UNIVERSIDAD POLITÉCNICA DE MADRID

ESCUELA TÉCNICA SUPERIOR DE
INGENIEROS DE CAMINOS, CANALES Y PUERTOS

Crystal Plasticity Simulation of the
Thermo-mechanical Behavior in
Polycrystalline Metals

TESIS DOCTORAL

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Directores: Prof. Javier Segurado

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*The journey ahead for seeking truth is long and tough, but I will search high
and low till the end of my life.*

— Qu, Yuan (*Famous ancient chinese poet.*)

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Abstract

Metals and alloys play an important role in our society. Hence, understanding and further predicting their behavior, and in particular under machining processes, is of great scientific and industrial interest. Such an understanding will prove instrumental for the optimization of machining conditions, which will further lead to a reduction of cost and an increase of productivity. Under thermo-mechanical processes including the machining process, polycrystalline metals usually undergo large deformations, high strain rates and high temperatures. The response of metals in these processes is very complex since their mechanical behavior is often strongly coupled with thermal phenomena. Accurate simulations of such processes require a fully coupled modeling framework that can accurately describe both the mechanical and the thermal behavior of the material, as well as their interaction. Such a complex multi-physics nonlinear framework could be established with the commonly used finite element method (FEM). In FEM, the simulation accuracy is largely dependent on the constitutive model employed. Conventional constitutive models are usually phenomenological and lack the description of the plasticity anisotropy and microstructure heterogeneity that polycrystalline metals exhibit, limiting their simulation accuracy. To address this issue, in this research an elasto-visco-thermo-plastic constitutive model based on crystal plasticity theory is developed for single crystals, which could connect the macroscopic plastic deformation behavior with the dislocation glide along slip systems and crystal reorientation.

Actual engineering metals and alloys are usually polycrystalline materials, made of numerous single crystals. Each macroscopic material point may represent a huge amount of grains, up to millions. For this reason it is difficult to precisely capture the detailed shapes and orientations of all the grains in a macroscopic point, and even more difficult to reproduce this microstructure in a finite element simulation due to the prohibitively computational cost. To link the macroscopic response of a material point and the underlying microstructure, homogenization approaches need to be constructed. In this research, the computational homogenization approach, which represents a macroscopic material point with a representative element volume (RVE) of the microstructure and obtains the macroscopic response and microscopic field distribution solving a boundary value problem on the RVE, is employed to study the response of polycrystalline metals during deformation. The modeling approach accounts for thermal strains, heat generation and conduction at the microscale, and the effect that this microscopic temperature field has on the crystal response through a temperature dependent crystal plasticity model.

Machining is one of the most commonly used manufacturing operations. Due to its crucial importance in modern industry, an in-depth understanding of the mechanisms and an accurate predictive simulation framework that could link the machining parameters with output variables could optimize the machining conditions and finally lead to notable enhancement of product quality, improvement of manufacturing productivity and reduction of economical cost. A machining process is a complicated nonlinear multiphysics problem as it usually involves contact, large deformations, fracture, as well as heat generation and conduction. Such a complex problem is usually resolved with the finite element method. In this study, the orthogonal cutting process of low carbon steel C45, a typical ferrite-pearlite steel, under various machining conditions is simulated. As the accuracy of a finite element analysis is mainly dependent on the constitutive relation employed, to better describe the material behavior of ferrite-pearlite steel subjected to large strain, high strain rate and high temperature and account for its plastic anisotropy and microstructure heterogeneity features, a microstructure informed elasto-visco-thermo-plastic constitute model based on the crystal plasticity model is proposed and integrated into ABAQUS/Explicit as a user defined subroutine VUMAT. A pure Lagrangian method with element deletion technique is adopted. The numerical results show acceptable agreement with experimental data and it could also capture the heterogeneous distribution of stress in the contact face due to the use of microstructure based constitutive model, which could not be observed with other conventionally used models, such as Jonhson-Cook's.

Resumen

Los metales y sus aleaciones juegan un papel importante en nuestra sociedad por lo que la comprensión y la predicción de su comportamiento, y en particular en los procesos de mecanizado, es de interés tanto científico como industrial. El resultado en este último caso debe conducir a la optimización del proceso, y en última instancia a una reducción de costes y aumento de productividad.

En los procesos termo-mecánicos que tienen lugar durante el mecanizado de metales, estos experimentan grandes deformaciones, altas velocidades de deformación y temperaturas. La respuesta de los metales en estas condiciones es muy compleja y se complica aún más debido al fuerte acoplamiento entre los fenómenos mecánicos y térmicos. Para simular con precisión dicha respuesta es necesario un entorno de simulación multi-campo que represente fielmente la respuesta mecánica, la térmica y también su interacción. Tal entorno se puede construir empleando el método de los elementos finitos (MEF).

Cuando se emplea el MEF, la precisión depende en gran medida del modelo constitutivo empleado. De hecho, los modelos constitutivos habitualmente empleados para modelar la respuesta de metales son, a menudo, fenomenológicos, ignorando la anisotropía propia de la plasticidad y la heterogeneidad debida a la microestructura de los policristales. Estas simplificaciones limitan, a priori, la precisión de las simulaciones que los emplean. Para subsanar estas limitaciones, en esta tesis se desarrolla un modelo termo-elasto-visco-plástico basado en plasticidad cristalina de metales. Con este modelo, formulado para monocristales, se podrá relacionar la deformación macroscópica con los procesos microscópicos de deslizamiento de dislocaciones y de reorientación cristalográfica.

Los metales y aleaciones que se usan habitualmente en ingeniería son materiales policristalinos, formados por numerosos cristales. Cada punto macroscópico puede representar un gran número de granos cristalinos, del orden de un millón. Es difícil representar la compleja geometría de estos granos y sus orientación, incluso para un único punto macroscópico, así que su modelado preciso mediante el MEF es imposible. Para relacionar la respuesta macroscópica de un punto material y su comportamiento microestructural han de emplearse técnicas de homogeneización. En este trabajo se desarrollan modelos homogeneizados computacionalmente. En ellos, cada punto material macroscópico se simula con un elemento de volumen representativo (RVE) de la microestructura. En este elemento, que incluye un gran número de granos cristalinos, se resuelve un problema de valores de contorno y se obtiene tanto la respuesta global como la de los campos microscópicos. El modelo empleado tiene en cuenta los fenómenos mecánicos y también las deformaciones de origen térmico, el calor generado por la plasti-

dad, la conducción en la micro-escala y los efectos que la temperatura tiene sobre las propiedades plásticas de los cristales.

El mecanizado es una de las técnicas de fabricación más comunes. Debido a su importancia crucial en la industria moderna, es interesante conocer con profundidad los mecanismos de deformación que ocurren en las piezas que son mecanizadas y, para ello, construir un entorno de simulación predictivo, capaz de relacionar parámetros materiales con propiedades finales. Si esto se lograra, se podría emplear para optimizar las condiciones del mecanizado, mejorar la calidad de las piezas fabricadas de esta manera y, en última instancia, lograr reducción de costes. Sin embargo, el proceso de mecanizado es extremadamente complejo, y desde el punto de vista de simulación involucra el modelado del contacto, de grandes deformaciones, de fractura, plasticidad y de calor generado por deformación plástica. Usando las técnicas desarrolladas en la primera parte de la tesis doctoral y el MEF se estudiará en la parte final el corte ortogonal de un acero ferrítico-perlítico C45 con bajo contenido de carbono. Para describir este acero se desarrollará un modelo constitutivo específico que tendrá en cuenta las heterogeneidades microestructurales del mismo, y se integrará en una subrutina VUMAT de Abaqus/Explicit. Empleando una discretización puramente Lagrangiana con eliminación de elementos e integración explícita se simulará el proceso de corte. Los resultados numéricos obtenidos muestran una concordancia aceptable con medidas experimentales del proceso y además proporcionan información microestructural (de tensiones, deformación plástica, etc.) que no pueden analizarse con modelos fenomenológicos habituales (por ejemplo, el modelo de Johnson-Cook).

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CHAPTER 1

Introduction and Objectives

1.1 Motivation

Metals and their alloys have been playing a crucial role in the formation and development of technology since the Bronze age, dating back to about five thousand years, when humans started to use metals to fabricate tools. Since then, metallic materials have been behind almost any technological development, from the basis of agriculture tools as sickles, passing through their fundamental role in the industrial revolution, to their central role in the aerospace industry. In the present, even with the progressive introduction of composites or high performance polymers, metallic alloys still play the most prominent role as structural materials due to their good performance and relative low cost. Moreover, there are no alternatives to replace metals when a combination of high strength, high working temperature and ductility is required as for example in engine blocks, turbines, nuclear applications, etc. Some applications of metals and alloys are illustrated in Fig. 1.1.

Fig. 1.1: Some applications of metals and alloys.

Due to the importance of metals and alloys in our society, it is of great scientific and industrial interest to understand and further predict the behavior of metallic material. In particular, understanding the behavior under extreme conditions (high strain rates, high temperature, large applied deformations) is specially helpful for the manufacturing industry since these are the typical conditions achieved during the solid-state processing of metallic parts by either rolling, drawing, machining, etc.

The introduction of a new metallic alloy in any technological application or the validation of its performance under the particular working condition (temperature, strain rate, level of stresses, etc) have been classically accounted by experimental testing. These tests range from lab test of the uniaxial material response to the very complex crash tests need to assess the safety of new designed automobiles or drop test in electronics industry to evaluate the durability of electronic appliances. Since the mechanical response depends on these conditions and also on the alloy microstructure (precipitation, presence of second phases, grain shape, size and orientation distribution, surface conditions, etc), the number of test needed and their associated cost implies the use of largely conservative assumptions during design and slows down the introduction of new alloys for a particular application. This limitations are maximized in the case of the behavior under extreme conditions where testing becomes more difficult and expensive.

To overcome these difficulties, reduce the production cost and improve the use or processing with a given alloy, it is fundamental the development of mathematical models able to predict the alloy response under any particular working condition and including the effect of the microstructure. Analytical models have the benefit of being simple and easy to be evaluated, allowing the parametric study of the model inputs. However, analytical approaches usually imply strong simplifications of the actual physics behind the problem and many times are not useful to provide accurate and quantitative predictions. An alternative approach is the development of complex physically based models of the mechanical behavior which requires numerical simulations to be evaluated. The objective of these computational approaches is to provide accurate predictions of the material response accounting for the physical mechanisms occurring at different length scales, from the atomistic scale to the macroscale, and including the effect of the microstructure on those predictions. The computational cost of this strategy becomes prohibitive in many cases and this fact has limited its application away from academic examples. Recent advances in simulation techniques, increase of computational power, and the development of new multiscale modeling strategies are rapidly overcoming this limitation. This new paradigm to quantitatively

predict the metal response for a given combination microstructure and working conditions is allowing the virtual testing of materials for any new condition or microstructure as well as its performance during a particular processing route, strongly reducing the number of tests needed and therefore reducing the time and cost of the introduction of a material in a particular application.

Focusing on the behavior of a metallic material under a thermo-mechanical processing route, it is common that they undergo large plastic deformation under a wide range of strain rates and at high temperature. The response of metals in these processes is very complex since their mechanical behavior is often strongly coupled with thermal phenomena. In one direction, the temperature influences the mechanical response. For example, the thermal variations may produce affect the mechanical behavior as the result of thermal expansion and/or contraction. Also temperature changes may notably affect the mechanical response as many mechanical material properties, such as the elastic modulus, are temperature dependent and their non-linear regime (yield and post-yielding behavior) is strongly temperature dependent. As an illustration of the temperature dependent elastic response and its modeling, the stiffness constants of single crystalline aluminum are temperature dependent [1], and this dependency can be approximated with a polynomial expression as function of the absolute temperature θ (in K) as follows ([1]):

$$\begin{aligned} c_{11} &= 123.323 - 7.8788 \times 10^{-3}\theta - 1.1342 \times 10^{-4}\theta^2 + 6.7008 \times 10^{-8}\theta^3, \\ c_{12} &= 70.6512 + 3.9992 \times 10^{-3}\theta - 7.5498 \times 10^{-5}\theta^2 + 4.4105 \times 10^{-8}\theta^3, \\ c_{44} &= 31.2071 - 8.3274 \times 10^{-3}\theta - 1.2136 \times 10^{-5}\theta^2 + 7.0477 \times 10^{-8}\theta^3. \end{aligned} \quad (1.1)$$

Away from the elastic response, temperature changes may even more significantly modify the metal response. As an example, the flow stress usually decreases with temperature (thermal softening), and the strain-rate dependency of the metal is strongly coupled with temperature. Moreover, temperature changes may even cause microstructural changes as solid state transformations (nucleation or transformation of the present phases) or grain structure changes as coarsening or recrystallization. These microstructural transformations can remarkably change the overall material response. On the contrary direction, the mechanical deformation itself can influence the temperature of the material through the heat generation caused by plastic work dissipation. Thus, accurate simulations of thermo-mechanical processes require a fully coupled modeling framework that can describe with precision both the mechanical and the thermal behavior of the material, as well as their interaction. In addition, the simulation of these processes imply the use of accurate constitutive equations that accounts for the

material response under mechanical and thermal fields and depending on the microstructure.

The fully coupled modeling framework for thermomechanical processes will be based on the balance equations of linear momentum and thermal energy that govern the mechanical and the thermal fields, respectively. A thermo-mechanical process can then be mathematically described by a coupled set of second order partial differential equations with given boundary and initial conditions. Such an initial-boundary value problem could be resolved by a variety of numerical approaches such as the finite difference method, the boundary element method, the finite element method and meshfree methods. Among these numerical methods, the finite element method (FEM) has been extensively studied and widely used in both academia and industry due to its capability of dealing with complicated boundary conditions. In finite element method, the weak form formulations for the balance equations of linear momentum and thermal energy are spatially discretized into a nonlinear system of algebraic equations and further solved for the nodal displacements and temperatures with iterative method in an implicit scheme or separately with the central difference method for the mechanical field and the forward difference method for the thermal field in an explicit scheme. All these procedures are standard in computational continuum mechanics and have been implemented in generalist commercial finite element code such as ABAQUS[2].

Contrary to the general thermomechanical framework, constitutive equations accounting for the material response under mechanical and thermal fields are much less developed and, with the exception of simple phenomenological approaches such as Jonson-Cook [3], and not included in general commercial codes. Moreover, it is very hard to find in the scientific literature any material models/computational strategy that account for the influence of the microstructure in the material thermo-mechanical response of a polycrystalline metallic alloy. The reason for the small number of studies proposing microstructure dependent models for the thermo-mechanical behavior of polycrystals is the complexity of the processes involved. It is well known that during plastic deformation polycrystalline metals exhibit a notable anisotropic response at the macro-scale, driven by the orientation dependent behavior of the single crystalline grains forming the polycrystal. The plastic accommodation of finite strains leads to the re-orientation of the grains (texture evolution) that also anisotropically influences the response. To further complicate the process, the heterogeneous plastic deformation at the grain level could lead to a heterogeneous distribution of temperature field, which strongly influences the crystal response.

As a summary of the above arguments, the accurate simulation of thermo-

mechanical processing routes in polycrystalline metals require the development of elasto-visco-thermo-plastic constitutive models able to model the microstructure dependent mechanical response and its coupling with temperature.

1.2 Thermo-mechanical material modeling

The vast majority of the constitutive models for the thermo-mechanical response of metals for engineering applications are phenomenological, lacking the description of material behavior at the microscopic level. Among them, the most widely used constitutive model for metallic materials in industrial field is the Johnson-Cook's model [3]. This model assumes that the flow stress σ_y of the alloy is determined by the plastic strain rate ($\dot{\epsilon}_p$) and temperature (θ) as well as by the material history, given by the accumulated plastic strain $\bar{\epsilon}_p$. The expression of this relation gives

$$\sigma_y = (A + B\bar{\epsilon}_p^n) \left[1 + C \ln \left(\frac{\dot{\epsilon}_p}{\dot{\epsilon}_0} \right) \right] \left[1 - \left(\frac{\theta - \theta_{ref}}{\theta_m - \theta_{ref}} \right)^m \right] \quad (1.2)$$

where A , B , C , n , m are material parameters measured at the reference temperature θ_{ref} , $\dot{\epsilon}_0$ is the reference strain rate and θ_m is the melting temperature. These material parameters can be generally determined by performing a series of split Hopkinson pressure bar (SHPB) tests under various temperatures and strain rates. This phenomenological model could favorably predict responses of metallic materials under low and moderate temperatures while for elevated temperature it may yield notable prediction inaccuracies compared to experimental observations, which may be caused by its uncoupled nature of strain rate hardening effect and thermal softening effect [4].

Another constitutive model is the dislocation mechanics based Zerilli-Armstrong model [5]. In the model the effects of strain rate and temperature are determined based on the theory of thermal activation processess. Contrary to Johnson-Cook's model [3], Zerilli-Armstrong model has a (weak) microscopical basis since its response depends on the lattice of the material under study. For bcc crystals, the Zerilli-Armstrong model is expressed as

$$\sigma_y = C_0 + C_1 \exp(-C_3\theta + C_4\theta \ln \dot{\epsilon}) + C_5 \bar{\epsilon}^n \quad (1.3)$$

while for fcc crystals it is given by

$$\sigma_y = C_0 + C_2 \bar{\epsilon}^{\frac{1}{2}} \exp(-C_3\theta + C_4\theta \ln \dot{\epsilon}) \quad (1.4)$$

where $C_0 \sim C_5$ are model parameters determined from dislocation dynamics analysis. The Zerilli-Armstrong model could give more accurate predictions at higher temperature compared to the Johnson-Cook model, but it is more complicated and still lacks the description of the plastic anisotropy and microstructure evolution required for accurate predictions of responses of polycrystalline metals as mentioned above.

The incorporation of the plastic anisotropy in the mechanical response can be introduced using anisotropic phenomenological models([6, 7, 8, 9]) However, the resulting models are very complex and they usually include a large number of parameters to account for the anisotropic yielding and its evolution during the plastic deformation. Moreover, a large number of tests are required to obtain those parameters, being some of them considerably complex since they imply different triaxialities or strain path changes.

1.3 Crystal plasticity based mechanical models

An alternative to phenomenological anisotropic plasticity is the use of approaches based on the single crystal plastic behavior, given by the crystal plasticity (CP) model [10, 11, 12, 13]. These models imply the individual representation of each grain and, therefore, can only be applied to the response of small volumes containing a relative small number of grains. The use of this models for macroscopic simulations can be achieved directly in the case where the grain size is comparable to the macroscopic domain under study [14]. On other more general cases, CP should first be combined with some homogenization technique to average the behavior of a representative set of grains. This can be achieved with either simplified mean-field models [15, 16, 17] or using polycrystalline computational homogenization [18, 19]. The response obtained under homogenization will directly represent the response under simple homogeneous macroscopic states. For general heterogeneous simulations, multiscale models are need which couple homogenization approaches at the microscale with FE models at the macroscale. This has been done using mean-field homogenization at the microscale [20, 21] or using more expensive FE^2 [22, 23] or FE-FFT[24, 25] models.

The crystal plasticity (CP) model was developed in [10, 11, 12, 13] based on the model envisioned by Taylor in the 30s. Since then, the model has been widely used in finite element frameworks as a constitutive equation for single crystalline metals, being this type of models known as CPFEM approaches. The crystal plasticity model considers the single crystalline plastic response by taking into account the plastic slip caused by moving dislocations through the slip planes characteristic of its lattice. Due to the verified predictive capacity, CPFEM has been exten-

sively applied for the direct modeling and simulating of some problems or phenomena at the microscale such as the nanoindentation testing [26, 27, 28], micro-pillar testing [29, 30] and microscale cutting [31, 32]. In addition, when adopting homogenization approaches as will be introduced in the next section, the model has been employed for predicting the mechanical responses of polycrystalline metals at the macroscale under monotonic loading [33, 34, 35, 36, 37, 38, 39], cyclic loading [40, 41, 42] and fatigue response [43, 44, 45, 46, 47] or simulating forming processes such as rolling [48, 49, 50, 51].

It must be noted however, that the models based on CP are usually pure mechanical models and with the exception of a few recent works, they neglect the effect of temperature on the mechanical response or/and the heat generation due to plastic deformation. As the first objective of this research, as will be described in Chapter 2, we will develop a finite element framework for predictions of thermomechanical behavior of polycrystalline metals by incorporating a temperature dependent physically based crystal plasticity model as constitutive equation.

1.3.1 Polycrystalline Homogenization

Actual engineering metals and alloys are usually polycrystalline materials, formed by numerous single crystals. As mentioned before, for the macroscopic application of the CPFEM to polycrystalline metals, every material point should be associated with a collection of single crystals being each one characterized by its shape and orientation. The behavior of a macroscopic material point can be extracted by the collective responses of all the associated single crystals whereas the behavior for each single crystal is determined by the CP model.

Since the typical mesh size in finite element model in a macroscopic application can be around 1.0 mm and the typical grain size is about 10 μm , the number of grains per each macroscopic material point may comprise a huge amount of grains, up to million of grains. Even with high resolution experimental techniques, it is still difficult to precisely capture the detailed shapes and orientations of all the grains in a macroscopic point and even more difficult would be the use of this microstructure in a finite element simulation due to the prohibitively computational cost caused from the huge number of degrees of freedom. To link the macroscopic responses of a material point and the underlying microstructure (grain shape and orientation distributions), homogenization approaches are adopted. In essence, the main task of a polycrystalline homogenization approach is to construct a homogenized constitutive relation at the macroscale based on the collective behavior of a statistically representative sample of grains while the response of each grain is described with the CP model. Thus, a homogenization model implies first a

statistically representative simplified description of the microstructure and second an approach to relate the relevant quantities between the macroscopic scale and the microscopic scale. Commonly used homogenization approaches could be classified into two categories: mean-field homogenization approaches and full field homogenization approaches.

Mean-field homogenization approaches assume a uniform distribution of the microscopic fields in each of the grains consider to statistically represent the microstructure. Therefore, the complex shape of stress and strain fields at the microstructure are replaced by a discrete set of values characterizing the state of each grain. The objective of any mean-field homogenization approach is providing a macroscopic strain-stress tensorial relation by assuming some hypothesis about how these fields are distributed in the different grains depending on their particular shape and orientation. The simplest mean-field homogenization model is the Taylor model [52], which assumes that the deformation gradient in each grain is identical to the deformation gradient of the macroscopic material point. Interactions between neighboring grains are neglected. The macroscopic quantities of the material point is then extracted by simply averaging the corresponding quantities in all the associated grains. In thermo-mechanical cases under the Taylor model, it is assumed that heat generated from plastic dissipation only contributes to the local temperature rise in each grain while heat transfer between neighborin grains is neglected due to the absence of their interactions. Taylor approach provides a very simple method to predict the macroscopic response but if might be inaccurate, specially when predicting the macroscopic response under large strains, since the model does not capture adequately the grain reorientation (texture evolution). the most commonly used mean-field homogenization approach is the viscoplastic self-consistent (VPSC) model [15, 16, 17], in which the plastic strain of each grain is linked to the applied macroscopic strain based on its particular orientation. In order to obtain this localization (the relation between the microscopic fields with the macroscopic one based on the particular size and orientation), an Eshelby [53] based approach is used. Due to the accuracy and relative simplicity, the VPSC model can be used as a constitutive equation for a polycrystal in multiscale macroscopic simulations [20].

The full field homogenization approach, which is also known as computational homogenization, represents a macroscopic material point with a representative element volume (RVE) of the microstructure and obtains the macroscopic response and microscopic field distribution solving a boundary value problem on the RVE in which boundary conditions, usually periodic, are used to introduce the macroscopic state [18, 19]. The RVE consists in a material volume containing an explicit representation of a number of grains representative of the distribution

of shapes, sizes and orientations (ODF) found in the actual polycrystalline alloy. In this case, each grain is represented by a subset of microscopic material points in order to resolve the microfield distribution within the grain. Compared to mean-field approaches, computational homogenization is computationally more expensive but more accurate due to the very precise representation of microstructure details and to the resolution of the microfields. This precise microstructure reproduction allows to account for the effect of the grain orientation and also the surrounding atmosphere of each grain, neglected in mean-field approaches, and fundamental to get an accurate description of the deformation and texture evolution.

At the end of the previous section some examples were given on the applications of CPFEM under homogenization frameworks to the prediction of mechanical behavior of polycrystalline metals under various loading. Regarding the temperature effect, some studies can be found [54, 55, 56] which adopt the computational homogenization framework to extract the mechanical response of an RVE of the polycrystal as function of the temperature and a purely mechanical CP finite element framework. In these works, temperature appears in the crystal plasticity model as a parameter, through which the mechanical response of the crystal was affected. This parameter was set constant to consider isothermal simulations and heat generation from plastic dissipation, heat conduction and temperature field evolution were not considered. The incorporation of heating due to plastic dissipation was considered in [57, 58] using the Taylor model to extract the thermo-mechanical response of a polycrystal. In these works each grain contributed to the local temperature rise based on its plastic deformation. Since the Taylor approach considers individual grain orientations, the effect of the texture evolution in the thermo-mechanical response was accounted. On the other hand, the state of each grain was represented by a single value for each field variable and all the grains shared the same deformation gradient, limiting the accuracy of the models. Heat conduction at the microscale was not considered as neighboring grains do not interact with each other.

More recently, computational polycrystalline homogenization based on FEM has been used to simulate the thermo-mechanical response of a polycrystal considering a detailed representation of the microstructure and resolving the full microfields within the grains. Most of the studies use microscopic adiabatic conditions and therefore neglect thermal transport phenomena at the microscale, resulting in a very heterogeneous temperature distribution due to the differences in plastic dissipation in different points of the microstructure. In the last years, two fully coupled models for crystal plasticity have been presented that include heat diffusion at the microscale. In [59], a fully coupled thermodynamical framework

using the FEM with implicit integration scheme is developed. The model includes heat generation and thermal strains but the crystal plastic behavior was assumed to be independent of the temperature. An alternative thermo-mechanical coupled framework was proposed recently for FCC materials [60] including a more physical description of the plastic flow in the crystal plasticity model, but formulated using explicit time integration scheme. It must be noted, finally, that none of the works reviewed proposing coupled thermo-mechanical frameworks for polycrystals considers the use of periodic boundary conditions for both thermal and mechanical fields, limiting the accuracy of the schemes proposed due to the inaccuracies near the RVE surfaces.

As the second objective in this research, the thermo-mechanical coupled crystal plasticity finite element framework described in Chapter 2 will be applied, together with the computational homogenization, to study the response of polycrystalline metals during deformation (Chapter 3). The modeling approach will account for thermal strains, heat generation and conduction at the microscale, and the effect that this microscopic temperature field has on the crystal response through a temperature dependent crystal plasticity model.

1.4 Simulation of Machining Process

As mentioned in the motivation section, the micromechanical modeling the polycrystalline response under extreme conditions opens the door to simulate thermo-mechanical processes accounting for the effect of the microstructure. The accurate modeling of these processes will lead to their better understanding and optimization for the particular material studied, with the corresponding material and energy savings. Among the different industrial processes to produce final parts for engineering applications, machining, or metal cutting, is maybe one of the most important operations since the resulting products of many other processing routes as casting or rolling, will require a further adaptation to the actual shape of the part under production.

Machining can be defined as a set of manufacturing operations that transform raw metallic materials into final products with desired shapes by removal of material from the workpiece. It was estimated that in developed countries in the year 2000 the machining expenditures contributed to as high as 5% of the GDP [61] and this number may have increased since then. Due to the economic impact of machining, many efforts have been invested in achieving a comprehensive understanding of the process and in developing predictive simulation frameworks that link the machining parameters such as the cutting speed, feed rate and cutting depth, to the output variables including the cutting forces, temperature field and

chip morphology. These models could be the key for a notable enhancement of the manufacturing productivity, improvement of the product quality and reduction of the economic costs.

The machining process is an extremely complicated thermo-mechanically coupled process involving contact, very large non-linear deformations and fracture as well as heat generation and conduction. The material of the workpiece that is processed is subjected, in the region near the cutting edge, to high temperature, at high strain rates and suffering large deformations leading to fracture. This complex problem is classically solved using coupled multiphysics finite element method. Typically three different finite element approaches are used for simulating the machining process, namely the Lagrangian method, Arbitrary Lagrangian Eulerian (ALE) method and Coupled Eulerian Lagrangian (CEL) method, as will be introduced below.

Lagrangian method is probably the most commonly used finite element method to simulate the machining process. In this method, the workpiece and the cutting tool are straightforwardly modeled with the conventional Lagrangian mesh. The material points in the workpiece and the cutting tool always coincide with the nodes and integration points in the mesh during deformation process, enabling an easy and natural way for dealing with the boundary conditions and visualization of the motion of the material. However, machining processes usually involve large deformation and fracture. Pure Lagrangian method for simulations of such processes, as illustrated in Fig. 1.2(a) usually suffer from excessive element distortion, leading to the degradation of element aspect ratios, loss of simulation accuracy, reduction of the size of stable time increment or even the termination of the entire analysis. In order to address this problem, a failure criterion is usually defined to delete severe distorted elements before they cause computational difficulties. This element deletion technique allows to simulate the formation of chip and separation of chip from the workpiece. However, element removal technique is just a numerical approximation without a robust physical ground that violates the conservation of mass due to the removal of material and its use may introduce a pathological dependency of the simulation results on the finite element discretization. Although machining simulations using the Lagrangian approach with element removal constitute an interesting approach to simulate the problem in some circumstances, the results are dependent on some non-physical simulation parameters, as element removal criterion, so simulations need to be carefully adjusted and benchmarked with experimental results or other approaches.

ALE (Adaptative Lagrangian Eulerian) method uses an adaptive meshing technique to maintain a high quality mesh throughout the analysis by dynamically relocating nodal positions to reduce element distortions. In this method, the

domain where the workpiece interacts with the cutting tool is pre-defined as an adaptive meshing domain, where most distorted elements are located and thus new refined mesh needs to be generated. Conventional Lagrangian computations are performed in every time increment followed by the possible execution of two extra tasks in specified time increments at a given frequency: adaptive meshing and remapping. In the adaptive meshing process, a new mesh with good element aspect ratios is created by iteratively sweeping over the domain and re-locating the position of the nodes based on the mesh smoothing method applied, as illustrated in Fig. 1.2(b). In this process the mesh topology (elements and connectivity) is not changed. The new mesh is built simply by moving nodes in the old mesh to proper new position, without deleting or adding any node or element. The remapping process transfers solution dependent variables (SDVs) such as the stress, temperature, internal variables from the old mesh to the new one. These SDVs are conserved in an integral sense during the remapping process, which implies that their integrals over the domain in the new mesh equal to that in the old mesh. The mass, momentum and energy of the system are also conserved. Compared to the pure Lagrangian method with element deletion, the ALE method can usually give more accurate simulation results, since it does not require the use of any non-physical failure criterion. However, the computational cost of ALE method is usually very high due to the frequent and costly meshing and remapping operations, limiting its applications mainly to simulations of machining processes under two dimensional cases.

CEL (Coupled Eulerian Lagrangian) is the most recently developed numerical approach for simulating machining processes. In this method, the cutting tool is usually discretized with pure Lagrangian mesh and the workpiece is placed in a large Eulerian mesh. At the initial time, the workpiece occupies a partial region of the Eulerian mesh while the rest of the mesh is empty, i.e. does not have any material point associated. The CEL method involves the evolution of two phases in each time increment: a Lagrangian phase and an Eulerian phase. In the Lagrangian phase, nodes in the Eulerian region are assumed to be temporarily fixed within the material occupying the region. Their new positions are determined by a Lagrangian computation. Then in the Eulerian phase, these nodes are remapped to their original positions, thus it seems that the nodes in the Eulerian region are fixed in space and the mesh never moves, as illustrated in Fig. 1.2(c). Unlike in ALE method where every element is always occupied by a single material, in CEL method, an element could be empty or occupied by various materials. Every increment, each element will update the volume fraction of all associated materials within it. The sum of volume fractions for all materials in an element always equal to one. As the material flows independently in the

Eulerian mesh, it is not possible to determine the material boundary directly from the mesh but trace it by computation of the volume fraction in all the elements in the Eulerian mesh. The CEL method is generally computational costly compared to the pure Lagrangian method with element deletion but behaves better and does not require unphysical assumptions as shown in Fig. 1.2.

Fig. 1.2: Illustration on the (a). Pure Lagrangian approach, (b). ALE approach and (c). CEL approach

As we have argued previously, the constitutive relation is the key ingredient responsible for the accuracy of a finite element analysis. The most common constitutive model used for simulating the machining processes of polycrystalline metals is the Johnson-Cook model coupled with heat generation due to plastic dissipation. However, this phenomenological model will yield notable error at moderate

to high temperatures. Moreover, since it is phenomenological macroscopic approach, it does not account for the microstructure heterogeneity, preventing its use to study the effect of the heterogeneity of the material in the workpiece in the machining process. Since many metallic alloys subjected to machining present different phases with very different strength and stiffness (for example, ferritic-perlitic steels or Ti6Al4- alloys), their study cannot be accurately afforded using this simple constitutive model.

Therefore, as the third objective of this research, the thermo-mechanically coupled crystal plasticity finite element framework described in Chapter 2 will be used together with a crystal plasticity based constitutive equation to study the effect of the microstructure heterogeneity of the workpiece material during an orthogonal cutting process. The material under study will be a ferrite-pearlite steel. Due to the problems of using an heterogeneous material combined with CEL or ALE methods caused by the inappropriate remapping of internal variables at integration points, a simple Lagrangian method with element deletion will be adopted.

1.5 Objectives

As a brief summary of the above discussion, the main objectives for this research are listed below:

- 1). Development of a fully coupled finite element framework incorporating a temperature dependent and physically based crystal plasticity model as constitutive equation for the simulation of the response of polycrystalline metals during thermo-mechanical processes.
- 2). Application of the coupled finite element framework under implicit integration with computational homogenization to study the thermo-mechanical response of polycrystalline metals during uniaxial traction at different strain rates and temperatures.
- 3). Adaptation of the coupled finite element framework to investigate the machining process in polycrystalline alloys explicitly accounting for heterogeneous microstructure. In particular, a crystal plasticity model will be developed for ferrite-pearlite and the orthogonal cutting process will be analyzed using a Lagrangian approach with element deletion technique.

CHAPTER 2

Thermo-Mechanically Coupled Crystal Plasticity Finite Element Framework

This chapter serves as the theoretic framework of this dissertation. We present a finite element framework incorporating the crystal plasticity constitutive model for fully coupled analysis of the response of crystalline materials during thermo-mechanical processes. We start from a systematic and comprehensive discussion of the implementation of a general thermo-mechanical coupled finite element framework, followed by the introduction of the crystal plasticity model and the incorporation of this constitutive model into the general framework through user defined material subroutines. First the weak formulation for thermo-mechanically coupled problems is constructed based on the balance equation of linear momentum that governs the evolution of the mechanical field and the balance equation of thermal energy that determines the evolution of the thermal field, as well as the initial and boundary conditions. Then the weak form is spatially discretized into a coupled system of nonlinear equations of the nodal displacements and temperatures with the finite element method. This system of equations is continuous in the time domain and is further discretized into a series of time increments and solved for the nodal displacements and temperatures at the end of each time increment by using an implicit or an explicit time integration scheme. Finally, the crystal plasticity model is introduced and integrated into the general framework discussed previously through user defined material subroutines. The implementation of this constitutive model is described in detail followed by some simple numerical examples for validation of the entire framework.

2.1 Finite Element Method for Fully Coupled Thermal-Mechanical Analysis

2.1.1 Problem Statement

For fully coupled thermo-mechanical analyses of the response of a deformable body to be studied, both the mechanical field and the thermal field need to be solved simultaneously for any time of interest during the loading process. An accurate solution of the coupled fields first requires a precise mathematical description of the corresponding initial boundary value problem for the thermal mechanical process, which is established in this subsection based on the governing equations and the initial and boundary conditions of the thermal and mechanical fields as introduced below.

Mathematical Description of the Mechanical Field

Considering a deformable body and let $\mathbf{X}$ be the coordinates of a material point in the reference configuration which occupies a domain $\mathcal{B}_0$, bounded by the surface $\partial\mathcal{B}_0$ in three-dimensional space $\mathcal{R}^3$, and $\mathbf{x}(t)$ denote the corresponding coordinates at time t in the current configuration occupying a domain $\mathcal{B}$, bounded by the surface $\partial\mathcal{B}$. The reference configuration is usually chosen to be the initial undeformed configuration (at $t = 0$).

The motion of the body could be described by a one-to-one, continuously differentiable mapping

$$\varphi(\mathbf{X}, t) : \mathbf{X} \in \mathcal{B}_0 \mapsto \mathbf{x}(t) \in \mathcal{B}. \quad (2.1)$$

The deformation gradient tensor $\mathbf{F}$ could be derived from this mapping as

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}. \quad (2.2)$$

The displacement field $\mathbf{u}(\mathbf{X}, t) := \mathbf{x}(\mathbf{X}, t) - \mathbf{X}$ is governed by the balance equation of linear momentum, which is generally written as

$$\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{b} = \rho \ddot{\mathbf{u}} \quad (2.3)$$

where ρ is the mass density, $\boldsymbol{\sigma}$ is the Cauchy stress tensor, $\mathbf{b}$ is the body force per unit volume in the deformed configuration, $\nabla \cdot$ is the spatial divergence operator and $\ddot{\mathbf{u}}$ is the second time derivative of $\mathbf{u}$.

For thermo-mechanical coupled problems, it is generally assumed that the stress

tensor depends on the deformation gradient $\mathbf{F}$, its rate $\dot{\mathbf{F}}$, the local value of the temperature θ and, possibly, some internal variables denoted collectively as $\boldsymbol{\psi}$. That is,

$$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F}, \dot{\mathbf{F}}, \theta, \boldsymbol{\psi}). \quad (2.4)$$

The boundary of the current configuration $\partial\mathcal{B}$ can be split into two disjoint parts denoted by $\partial_u\mathcal{B}$ and $\partial_t\mathcal{B}$ as

$$\begin{aligned} \partial_u\mathcal{B} \cap \partial_t\mathcal{B} &= \emptyset, \\ \partial_u\mathcal{B} \cup \partial_t\mathcal{B} &= \partial\mathcal{B}, \end{aligned} \quad (2.5)$$

The displacement and tractions on the boundary are constrained as

$$\mathbf{u} = \bar{\mathbf{u}}, \text{ on } \partial_u\mathcal{B}, \quad (2.6a)$$

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \bar{\mathbf{t}}, \text{ on } \partial_t\mathcal{B}, \quad (2.6b)$$

where $\mathbf{n}$ is the outer normal to the boundary, $\bar{\mathbf{u}}$ and $\bar{\mathbf{t}}$ are known fields of displacement and surface tractions, respectively. Eq. (2.6a) is usually called the essential boundary condition or the Dirichlet boundary condition, and Eq. (2.6b) is called the natural boundary condition or the Neumann boundary condition.

Due to the presence of the inertial term in Eq. (2.3) which has the second derivative of the displacement with respect to time, to close the description of the mechanical field, two initial conditions need to be specified

$$\begin{aligned} \mathbf{u}(\mathbf{X}, 0) &= \bar{\mathbf{u}}_0(\mathbf{X}), \\ \mathbf{v}(\mathbf{X}, 0) &= \bar{\mathbf{v}}_0(\mathbf{X}), \end{aligned} \quad (2.7)$$

where $\mathbf{v} := \dot{\mathbf{u}}$ is the velocity of the material point.

The initial values for the internal variables in the constitutive equation Eq. (2.4) are assumed to be known, which is expressed as

$$\boldsymbol{\psi}(\mathbf{X}, 0) = \bar{\boldsymbol{\psi}}_0(\mathbf{X}). \quad (2.8)$$

The weak form of the momentum equation expressed in Eq. (2.3) could be constructed by multiplication with the test function $\delta\mathbf{v}$ and integration over the current configuration

$$\int_{\mathcal{B}} \delta\mathbf{v} (\nabla \cdot \boldsymbol{\sigma} + \rho\mathbf{b} - \rho\dot{\mathbf{v}}) dV = 0. \quad (2.9)$$

The test function $\delta\mathbf{v}$ could be chosen as the virtual velocity field, which is arbitrary but satisfies the essential boundary condition given in Eq. (2.6a) and

has sufficient continuity.

Applying integration by parts, using Gauss's theorem and taking into consideration the boundary conditions, we could obtain the virtual power equation from Eq. (2.9)

$$\int_{\mathcal{B}} \boldsymbol{\sigma} : \nabla \delta \mathbf{v} dV - \int_{\mathcal{B}} \delta \mathbf{v} \cdot \rho \mathbf{b} dV - \int_{\partial_t \mathcal{B}} \delta \mathbf{v} \cdot \bar{\mathbf{t}} dS + \int_{\mathcal{B}} \delta \mathbf{v} \cdot \rho \dot{\mathbf{v}} dV = 0. \quad (2.10)$$

Mathematical Description of the Thermal Field

Analogously, the temperature field $\theta(\mathbf{X}, t)$ of the body is governed by the balance equation of thermal energy. This equation reads

$$\rho c \dot{\theta} = \nabla \cdot \mathbf{q} + Q, \quad (2.11)$$

where ρ is the mass density as mentioned before in the momentum equation Eq. (2.3), c is the specific heat capacity, Q is the volumetric heat generation rate, $\mathbf{q}$ is the heat flux per unit surface.

For most solids the heat conduction is assumed to follow Fourier's law, which relates the heat flux with the temperature gradient as

$$\mathbf{q} = -\mathbf{k} \cdot \nabla \theta, \quad (2.12)$$

where $\mathbf{k}$ is the spatial thermal conductivity tensor.

Substituting Eq. (2.12) into Eq. (2.11) yields

$$\rho c \dot{\theta} + \nabla \cdot (\mathbf{k} \cdot \nabla \theta) - Q = 0. \quad (2.13)$$

For thermo-mechanical coupled problems, the heat supply Q is mainly contributed from the mechanical dissipation due to the power of the stress conjugated with the viscoplastic strains. The efficiency of the conversion of mechanical into thermal energy is not perfect because some energy may be stored in microstructural transformations at the dislocation level for metallic materials. However, considering this phenomena from a physical view point implies the introduction of constitutive hypotheses that are material dependent (see, e.g., the discrete dislocation model presented by Benzerga et. al. for copper [62]). For simplicity, the model proposed by Taylor and Quinney is usually used, which takes the conversion efficiency to be constant. The internal heat generation could then be customarily expressed as

$$Q = \chi W^p = \chi \boldsymbol{\sigma} \dot{\boldsymbol{\epsilon}}^p \quad (2.14)$$

where W^p is the plastic power, $\dot{\boldsymbol{\epsilon}}^p$ is the plastic strain rate, χ is the so-called

Taylor-Quinney parameter, usually selected in the range $0.85 \leq \chi \leq 1.0$.

For the thermal field, the boundary of the current configuration $\partial\mathcal{B}$, as has been similarly described in the mechanical field, could also be split into two parts denoted by $\partial_\theta\mathcal{B}$ and $\partial_h\mathcal{B}$

$$\begin{aligned}\partial_\theta\mathcal{B} \cap \partial_h\mathcal{B} &= \emptyset, \\ \partial_\theta\mathcal{B} \cup \partial_h\mathcal{B} &= \partial\mathcal{B}.\end{aligned}\tag{2.15}$$

In the boundary $\partial_\theta\mathcal{B}$, the prescribed temperature condition is defined, which is given by

$$\theta = \bar{\theta}, \text{ on } \partial_\theta\mathcal{B},\tag{2.16}$$

where $\bar{\theta}$ is the known temperature.

In the boundary $\partial_h\mathcal{B}$, the boundary conditions may be applied in three different forms, namely the specified heat flux condition, the convection condition and the radiation condition. The specified heat flux condition reads

$$\mathbf{q} \cdot \mathbf{n} = \bar{q}, \text{ on } \partial_h\mathcal{B},\tag{2.17}$$

where $\bar{q}$ is the prescribed surface heat flux. The convection condition is given by

$$\mathbf{q} \cdot \mathbf{n} = h(\theta - \theta_e), \text{ on } \partial_h\mathcal{B}\tag{2.18}$$

where h is the film coefficient and θ_e is the environment temperature. The radiation condition is given by

$$\mathbf{q} \cdot \mathbf{n} = A(\theta^4 - \theta_e^4), \text{ on } \partial_h\mathcal{B}\tag{2.19}$$

where A is the radiation constant. Eq. (2.16) is the essential boundary condition and Eq. (2.17) $\sim$ Eq. (2.19) are the natural boundary conditions. In what follows, for brevity and clarity of the formulations for the thermal field, we only consider the specified heat flux condition but ignore the convection and radiation conditions. It is rather straightforward to include these two boundary conditions in relevant formulations if one wants to take them into consideration.

Finally, the initial conditions need to be specified to complete the description of the thermal field due to the presence of the first derivative of temperature with respect to time in Eq. (2.13), which is given by

$$\theta(\mathbf{X}, 0) = \bar{\theta}_0(\mathbf{X}).\tag{2.20}$$

The weak form of the balance equation of energy Eq. (2.13) could be estab-

lished by multiplying it with the test function $\delta\theta$ and integrating over the current configuration

$$\int_{\mathcal{B}} \delta\theta \left(\rho c \dot{\theta} + \nabla \cdot (\mathbf{k} \cdot \nabla \theta) - Q \right) dV = 0. \quad (2.21)$$

The test function $\delta\theta$ is an arbitrary field satisfying the essential boundary conditions given in Eq. (2.16).

Using Gauss's theorem and the boundary conditions defined in Eq. (2.16) and Eq. (2.17), the weak form of the balance equation of energy Eq. (2.21) could be rewritten as

$$\int_{\mathcal{B}} \delta\theta \rho c \dot{\theta} dV + \int_{\mathcal{B}} \nabla \delta\theta \cdot (\mathbf{k} \cdot \nabla \theta) dV - \int_{\partial_h \mathcal{B}} \delta\theta \bar{q} dS - \int_{\mathcal{B}} \delta\theta Q dV = 0. \quad (2.22)$$

**Box 2.1 Weak Form Formulation for Fully
Coupled Thermal Mechanical Problems**

Find the velocity field $\mathbf{v} \in \mathcal{V}$ and the temperature field $\theta \in \mathcal{T}$ such that

$$\int_{\mathcal{B}} \boldsymbol{\sigma} : \nabla \delta \mathbf{v} dV - \int_{\mathcal{B}} \delta \mathbf{v} \cdot \rho \mathbf{b} dV - \int_{\partial_t \mathcal{B}} \delta \mathbf{v} \cdot \bar{\mathbf{t}} dS + \int_{\mathcal{B}} \delta \mathbf{v} \cdot \rho \dot{\mathbf{v}} dV = 0, \quad \forall \delta \mathbf{v} \in \mathcal{V}_0$$

$$\int_{\mathcal{B}} \delta\theta \rho c \dot{\theta} dV + \int_{\mathcal{B}} \nabla \delta\theta \cdot (\mathbf{k} \cdot \nabla \theta) dV - \int_{\partial_h \mathcal{B}} \delta\theta \bar{q} dS - \int_{\mathcal{B}} \delta\theta Q(\boldsymbol{\sigma}) dV = 0, \quad \forall \delta\theta \in \mathcal{T}_0$$

where

$$\mathcal{V} = \{\mathbf{v} \in C^0(\mathbf{X}), \mathbf{v} = \dot{\mathbf{u}} \text{ on } \partial_u \mathcal{B}\}, \quad \mathcal{V}_0 = \{\delta \mathbf{v} \in C^0(\mathbf{X}), \delta \mathbf{v} = 0 \text{ on } \partial_u \mathcal{B}\},$$

$$\mathcal{T} = \{\theta \in C^0(\mathbf{X}), \theta = \bar{\theta} \text{ on } \partial_\theta \mathcal{B}\}, \quad \mathcal{T}_0 = \{\delta\theta \in C^0(\mathbf{X}), \delta\theta = 0 \text{ on } \partial_\theta \mathcal{B}\}.$$

Coupling Effects between the Mechanical and the Thermal Fields

It is obviously seen that the mechanical field and the thermal field are closely coupled. Temperature changes will induce thermal strains, and changes in mechanical properties such as the elastic constants and other physical quantities in the constitutive equation as indicated in Eq. (2.4), which will affect the stress field and the deformation field. In turn, changes in the stress and strain fields will result in the changes of the internal heat generation Q as described in Eq. (2.14), and changes in the deformation field will lead to changes of the domain and boundary of the thermal problem. All these could affect the distribution and evolution of the temperature field.

2.1.2 Finite Element Discretization

The finite element method is a powerful and efficient numerical tool that is extensively used in engineering and mathematical physics for finding the approx-

imation solution to partial differential equations. In this section, the coupled set of integral equations derived in previous subsection is spatially discretized into a coupled system of nonlinear equations of the nodal temperatures and displacements with the finite element method for future use.

Discretization of the Mechanical Field

In the finite element method, the current configuration $\mathcal{B}$ is geometrically partitioned by a mesh consisting of a set of elements. Each element occupies a subdomain $\mathcal{B}_e$ and contains a given number of vertices named nodes. For any material point $\mathbf{X}$, its velocity $\mathbf{v}$ at time t could be approximated as the interpolation of velocities of all nodes in the mesh, which is expressed by

$$\mathbf{v}(\mathbf{X}, t) = \sum_{I=1}^{n_N} N_I(\mathbf{X}) \mathbf{v}_I(t) := N_I \mathbf{v}_I = \mathbf{N} \mathbf{V}, \quad (2.23)$$

where n_N is the total number of nodes in the mesh, $\mathbf{V}$ is the global nodal velocity vector defined as

$$\mathbf{V} := (v_{1x}, v_{1y}, v_{1z}, v_{2x}, \dots, v_{n_N x}, v_{n_N y}, v_{n_N z})^T. \quad (2.24)$$

with $\mathbf{v}_I$ denoting the velocity of node I and $\mathbf{N}$ is the interpolation matrix for the mechanical field given by

$$\mathbf{N} = \begin{bmatrix} N_1 & 0 & 0 & N_2 & 0 & 0 & \cdots & N_{n_N} & 0 & 0 \\ 0 & N_1 & 0 & 0 & N_2 & 0 & \cdots & 0 & N_{n_N} & 0 \\ 0 & 0 & N_1 & 0 & 0 & N_2 & \cdots & 0 & 0 & N_{n_N} \end{bmatrix}. \quad (2.25)$$

with N_I being the global shape function for node I .

Following the standard Galerkin method, the virtual velocity field could be approximated by the same shape functions as used for the approximation of the velocity field. That is

$$\delta \mathbf{v}(\mathbf{X}, t) = N_I \delta \mathbf{v}_I = \mathbf{N} \delta \mathbf{V}. \quad (2.26)$$

By substituting Eq. (2.26) into the virtual power equation Eq. (2.10) and using the arbitrariness of $\delta \mathbf{v}_I$, the discretized version of the virtual power equation could be formulated as

$$\int_{\mathcal{B}} \boldsymbol{\sigma} \cdot \nabla N_I dV - \int_{\mathcal{B}} N_I \rho \mathbf{b} dV - \int_{\partial_t \mathcal{B}} N_I \bar{\mathbf{t}} dS + \int_{\mathcal{B}} N_I \rho N_J \dot{\mathbf{v}}_J dV = 0. \quad (2.27)$$

By differentiating Eq. (2.23) with respect to the coordinates at the current

configuration, one could obtain the velocity gradient tensor $\mathbf{L}$ given by

$$\mathbf{L} := \nabla \mathbf{v} = \sum_{I=1}^{n_N} \mathbf{v}_I \otimes \nabla N_I, \quad (2.28)$$

and the rate of deformation tensor $\mathbf{D}$, which is defined as the symmetric part of the velocity gradient

$$\mathbf{D} := \frac{1}{2} (\mathbf{L} + \mathbf{L}^T). \quad (2.29)$$

Following the Voigt notation, the rate of deformation tensor can be written as a column matrix

$$\{\mathbf{D}\} := (D_{xx}, D_{yy}, D_{zz}, 2D_{xy}, 2D_{xz}, 2D_{yz})^T. \quad (2.30)$$

This vectorial rate of deformation $\{\mathbf{D}\}$ could be regarded to be the true strain rate $\dot{\boldsymbol{\epsilon}}$ commonly used in finite strain problems. That is

$$\dot{\boldsymbol{\epsilon}} := (\dot{\epsilon}_{xx}, \dot{\epsilon}_{yy}, \dot{\epsilon}_{zz}, 2\dot{\epsilon}_{xy}, 2\dot{\epsilon}_{xz}, 2\dot{\epsilon}_{yz})^T = \{\mathbf{D}\}. \quad (2.31)$$

Hereafter the curly bracket $\{\cdot\}$ enclosing a second order tensor, which is used to indicate the corresponding vectorial form of the tensor under the Voigt notation, is omitted in case no ambiguity is caused, for the sake of brevity.

By substituting Eq. (2.28) ~ Eq. (2.30) into Eq. (2.31), the strain rate could be related to the nodal velocity vector as

$$\dot{\boldsymbol{\epsilon}} = \mathbf{B}\mathbf{V}, \quad (2.32)$$

where

$$\mathbf{B} = (\mathbf{B}_1, \mathbf{B}_2, \dots, \mathbf{B}_{n_N}) \quad (2.33)$$

with the matrices $\mathbf{B}_I$ given by

$$\mathbf{B}_I = \begin{bmatrix} \frac{\partial N_I}{\partial x} & 0 & 0 \\ 0 & \frac{\partial N_I}{\partial y} & 0 \\ 0 & 0 & \frac{\partial N_I}{\partial z} \\ \frac{\partial N_I}{\partial y} & \frac{\partial N_I}{\partial x} & 0 \\ \frac{\partial N_I}{\partial z} & 0 & \frac{\partial N_I}{\partial x} \\ 0 & \frac{\partial N_I}{\partial z} & \frac{\partial N_I}{\partial y} \end{bmatrix}. \quad (2.34)$$

Substituting Eq. (2.33) and Eq. (2.34) into the discrete virtual power equation

Eq. (2.27), and using Voigt notation of the Cauchy stress tensor defined as

$$\{\boldsymbol{\sigma}\} := (\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{xz}, \sigma_{yz})^T, \quad (2.35)$$

one could obtain the discrete momentum equation in matrix form as

$$\mathbf{M}\ddot{\mathbf{U}} = \mathbf{f}^{\text{ext}} - \mathbf{f}^{\text{int}} \quad (2.36)$$

where $\mathbf{M}$ is the consistent mass matrix expressed as

$$\mathbf{M} = \int_{\mathcal{B}} \rho \mathbf{N}^T \mathbf{N} dV, \quad (2.37)$$

$\mathbf{f}^{\text{ext}}$ and $\mathbf{f}^{\text{int}}$ are the external and internal nodal force vectors, respectively, which are given by

$$\mathbf{f}^{\text{ext}} = \int_{\mathcal{B}} \rho \mathbf{N}^T \mathbf{b} dV + \int_{\partial_t \mathcal{B}} \mathbf{N}^T \bar{\mathbf{t}} dS, \quad (2.38a)$$

$$\mathbf{f}^{\text{int}} = \int_{\mathcal{B}} \mathbf{B}^T \boldsymbol{\sigma} dV. \quad (2.38b)$$

For quasi-static problems, the inertial term in the left hand of the discrete momentum equation Eq. (2.36) vanishes, which is reduced to the equilibrium equation as

$$\mathbf{f}^{\text{ext}} - \mathbf{f}^{\text{int}} = 0. \quad (2.39)$$

Fig. 2.1: Illustration of the connectivity of a node I and its associated elements.

The global shape functions N_I have nonzero values only in elements associated with the node I . Thus, the computations of the global consistent mass matrix $\mathbf{M}_{IJ}$, internal nodal force $\mathbf{f}_I^{\text{int}}$ and external nodal force $\mathbf{f}_I^{\text{ext}}$ for node I are in

practice performed by adding the corresponding contributions from the associated elements. As illustrated in Fig. 2.1, the node I is shared by eight elements denoted by $e_1 \sim e_8$. The global internal force of node I could then be computed as

$$\mathbf{f}_I^{\text{int}} = \int_{\mathcal{B}} \mathbf{B}_I^T \boldsymbol{\sigma} dV = \sum_{e=e_1}^{e_8} \int_{\mathcal{B}_e} \mathbf{B}_k^{eT} \boldsymbol{\sigma} dV, \quad (2.40)$$

where k is the local number of node I in element e , which is 5 in element e_3 in Fig. 2.1, $\mathbf{B}^e$ denotes the elemental interpolation matrix of element e , which is similar to the global interpolation matrix $\mathbf{B}$ but defined in the domain of element e as

$$\mathbf{B}^e = (\mathbf{B}_1^e, \mathbf{B}_2^e, \dots, \mathbf{B}_m^e) \quad (2.41)$$

with m denoting the number of nodes in element e , and

$$\mathbf{B}_k^e = \begin{bmatrix} \frac{\partial N_k^e}{\partial x} & 0 & 0 \\ 0 & \frac{\partial N_k^e}{\partial y} & 0 \\ 0 & 0 & \frac{\partial N_k^e}{\partial z} \\ \frac{\partial N_k^e}{\partial y} & \frac{\partial N_k^e}{\partial x} & 0 \\ \frac{\partial N_k^e}{\partial z} & 0 & \frac{\partial N_k^e}{\partial x} \\ 0 & \frac{\partial N_k^e}{\partial z} & \frac{\partial N_k^e}{\partial y} \end{bmatrix}. \quad (2.42)$$

with N_k^e being the element shape functions. The superscript e in $\mathbf{B}^e$ and N^e may be dropped off when no indices confusion is caused, for the sake of brevity.

In a finite element code, it is more practical to build the global internal force vector with a so-called assembly procedure, which loops through all the elements in the mesh, and for each element computes the elementary internal force vector and assemble it to the proper components of the global vector. The global consistent matrix and external force vector could be computed analogously.

The computation of such elementary quantities requires the integration over the element domain, which is usually very difficult to perform analytically. To achieve this, it is convenient to transform the integrals over the element domain at the current configuration to the integrals over the domain of a standard isoparametric element as illustrated in Fig. 2.2, and perform the integration numerically, which is expressed as

$$\int_{\mathcal{B}_e} \mathbf{f}(\mathbf{x}) dV_e = \int_{\mathcal{B}_s} \mathbf{f}(\mathbf{x}(\boldsymbol{\xi})) J_{\boldsymbol{\xi}} dV_s = \sum_l w_l J_{\boldsymbol{\xi}} \mathbf{f}(\mathbf{x}(\boldsymbol{\xi}_l)), \quad (2.43)$$

where $\mathbf{x}$ is the spatial coordinates of a material point in the element domain $\mathcal{B}_s$, $\boldsymbol{\xi}$ is the corresponding coordinates of $\mathbf{x}$ at the isoparametric element domain $\mathcal{B}_s$ or usually being called the natural coordinates, $J_{\boldsymbol{\xi}}$ is the Jacobian of the

transformation defined as the determinant of the transformation matrix $\mathbf{F}_\xi$ given by

$$\mathbf{F}_\xi = \begin{pmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} & \frac{\partial x}{\partial \zeta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} & \frac{\partial y}{\partial \zeta} \\ \frac{\partial z}{\partial \xi} & \frac{\partial z}{\partial \eta} & \frac{\partial z}{\partial \zeta} \end{pmatrix}, \quad (2.44)$$

f is a function defined in the element domain, w_l and ξ_l are, respectively, the weight and the location of an integration point l within the isoparametric element.

Fig. 2.2: Mapping from a 3D 8-node element to the isoparametric element.

Now we could evaluate the integrals over the element domain as described in Eq.(2.43) with the commonly used Gaussian quadrature scheme. An n -point Gaussian quadrature scheme could yield an exact result for a $2n - 1$ order polynomial. For the C3D8T element used in this work, there are two integration points in each axis in the 3D space, so there are eight integration points in total within the element. For these integration points the weights are equally taken as 1.0 and the locations are tabulated in Table 2.1. This $2 \times 2 \times 2$ - points Gaussian

Table 2.1: Integration Points in C3D8T Isoparametric Element

Intg. Pt.	Natural Coordinates	Intg. Pt.	Natural Coordinates
1	$\frac{1}{\sqrt{3}} (-1, -1, -1)$	5	$\frac{1}{\sqrt{3}} (-1, -1, +1)$
2	$\frac{1}{\sqrt{3}} (+1, -1, -1)$	6	$\frac{1}{\sqrt{3}} (+1, -1, +1)$
3	$\frac{1}{\sqrt{3}} (+1, +1, -1)$	7	$\frac{1}{\sqrt{3}} (+1, +1, +1)$
4	$\frac{1}{\sqrt{3}} (-1, +1, -1)$	8	$\frac{1}{\sqrt{3}} (-1, +1, +1)$

quadrature scheme could give exact results if the integrands of the integral terms computed at the element level are cubic or lower order polynomial functions of the natural coordinates.

Sometimes, the reduced integration elements may be used for computational efficiency. For example for the C3D8RT element, which is also a three dimen-

sional eight nodes structural-thermal coupled continuum element as the C3D8T element, there is only a single integration point located at the center of the element. The weight and natural coordinates of this integration point in are 8.0 and (0.0, 0.0, 0.0), respectively. Compared to the full integration element that has eight integration points, this reduced integration point could reduce the time cost for the computation of quantities in the element, including the Cauchy stress, the element internal force vector and the element stiffness matrix, by about 87.5%, which is a huge save of the computational time. Nevertheless, the reduced integration element usually means the reduced computational accuracy. Compromise should be made between the efficiency and the accuracy. In addition, the use of the reduced integration element may give rise to the spurious hourglass mode, which will result in large amount of unphysical element distortion. This hourglass mode could be suppressed by some hourglass control approaches. In this work, for implicit analysis which will be introduced in later sections, the full integration element C3D8T is adopted while for explicit the reduced integration element C3D8RT is used.

Using Eq. (2.32), the strain increment $\Delta\boldsymbol{\varepsilon}$ in the time interval could be related to the nodal displacement increment $\Delta\mathbf{U}$ by

$$\Delta\boldsymbol{\varepsilon} = \dot{\boldsymbol{\varepsilon}}\Delta t = \mathbf{B}\mathbf{V}\Delta t = \mathbf{B}^e\Delta\mathbf{U} = \mathbf{B}^e(\mathbf{U}_{n+1} - \mathbf{U}_n). \quad (2.45)$$

The stress increment in this time interval could then be evaluated from a rate form constitutive model by

$$\Delta\boldsymbol{\sigma} := \overset{\circ}{\boldsymbol{\sigma}}\Delta t = \Delta\hat{\boldsymbol{\sigma}}(\boldsymbol{\sigma}_n, \Delta\boldsymbol{\varepsilon}, \theta_n, \theta_{n+1}, \psi_n) \quad (2.46)$$

where $\overset{\circ}{\boldsymbol{\sigma}}$ represents an objective stress rate. Two types of objective stress rate measures are commonly used in finite element analysis, namely the Jaumann rate of Cauchy stress and the Green-Naghdi rate of Cauchy stress. The former is defined as

$$\overset{\nabla}{\boldsymbol{\sigma}} = \dot{\boldsymbol{\sigma}} + \boldsymbol{\sigma} \cdot \mathbf{w} - \mathbf{w} \cdot \boldsymbol{\sigma} \quad (2.47)$$

where $\mathbf{w}$ is the skew symmetric part of the velocity gradient

$$\mathbf{w} = \frac{1}{2}(\mathbf{L} - \mathbf{L}^T), \quad (2.48)$$

and the latter is given by

$$\overset{\Delta}{\boldsymbol{\sigma}} = \dot{\boldsymbol{\sigma}} + \boldsymbol{\sigma} \cdot \boldsymbol{\Omega} - \boldsymbol{\Omega} \cdot \boldsymbol{\sigma} \quad (2.49)$$

where

$$\mathbf{\Omega} = \dot{\mathbf{R}}\mathbf{R}^T, \quad (2.50)$$

with the rotation matrix $\mathbf{R}$ determined by the polar decomposition of the deformation gradient as

$$\mathbf{F} = \mathbf{V}\mathbf{R} = \mathbf{R}\mathbf{U}, \quad (2.51)$$

and $\mathbf{U}$ and $\mathbf{V}$ being symmetric stretch tensors. Both $\mathbf{w}$ and $\mathbf{\Omega}$ are in essence measures of the rigid rotation during this time interval.

With the the stress increment obtained above, the Cauchy stress at time t_{n+1} could then be updated in a corotational framework by

$$\boldsymbol{\sigma}_{n+1} = \mathbf{R}_{n+1}\mathbf{R}_n^T\boldsymbol{\sigma}_n\mathbf{R}_n\mathbf{R}_{n+1}^T + \Delta\boldsymbol{\sigma} \quad (2.52)$$

Sometimes, it is more convenient to describe the constitutive behavior of the material to be studied directly with the second Piola-Kirchhoff stress $\mathbf{S}$, which could be written as

$$\mathbf{S}_{n+1} = \hat{\mathbf{S}}\left(\mathbf{E}_{n+1}, \dot{\mathbf{E}}_{n+1}, \theta_n, \theta_{n+1}, \psi_n\right). \quad (2.53)$$

Here $\mathbf{E}$ is the Green strain, which is the conjugate strain measure of the second Piola-Kirchhoff stress and given by

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{I}) \quad (2.54)$$

with $\mathbf{I}$ being the second order identity tensor. The Cauchy stress is the push forward of the second Piola-Kirchhoff stress to the current configuration, which could be evaluated by

$$\boldsymbol{\sigma}_{n+1} = (\det\mathbf{F}_{n+1})^{-1} \mathbf{F}_{n+1}\mathbf{S}_{n+1}\mathbf{F}_{n+1}^T. \quad (2.55)$$

With the Cauchy stress evaluated here from Eq. (2.52) or Eq. (2.55), and the elementary interpolation matrix $\mathbf{B}^e$ obtained from Eq. (2.42) for each integration point, the element internal nodal force could be computed by Eq. (2.40).

Based on the above discussion, the procedures for computation of the global consistent mass matrix, the global external nodal force vector and the global external nodal force vector in the discrete momentum equation Eq. (2.36) are briefly summarized in Box 2.2

**Box 2.2 Procedures for Computation of Global Consistent
Mass Matrix, External and Internal Nodal Force Vectors**

Given the global nodal displacement and temperature vectors at time t_{n+1} ,

1. Initialization: $\mathbf{M} = 0$, $\mathbf{f}^{\text{ext}} = 0$, $\mathbf{f}^{\text{int}} = 0$.
2. Loop for each element e :
 - (1). Initialization: $\mathbf{M}_e = 0$, $\mathbf{f}_e^{\text{ext}} = 0$, $\mathbf{f}_e^{\text{int}} = 0$.
 - (2). For each integration point l in element e :
 - a). Compute $\mathbf{F}(\boldsymbol{\xi}_l)$, $\mathbf{N}(\boldsymbol{\xi}_l)$ and $\mathbf{B}(\boldsymbol{\xi}_l)$.
 - b). $\mathbf{M}_e += w_l \rho \mathbf{N}^T \mathbf{N}$,
 - c). $\mathbf{f}_e^{\text{ext}} += w_l \rho \mathbf{N}^T \mathbf{b}$, modify it following boundary conditions.
 - d). Update the stress $\boldsymbol{\sigma}$ from the constitutive model.
 - e). $\mathbf{f}_e^{\text{int}} += w_l \mathbf{B}^T \boldsymbol{\sigma}$.
 - (3). Assemble elementary matrix and vectors to the global counterparts.

Discretization of the Thermal Field

Similarly as discussed for the mechanical field, the temperature field $\theta(\mathbf{X}, t)$, its rate $\dot{\theta}(\mathbf{X}, t)$ and its variation $\delta\theta(\mathbf{X})$ could be approximated by the interpolations of corresponding nodal values, which reads

$$\begin{aligned}\theta(\mathbf{X}, t) &= N_I \theta_I = \tilde{\mathbf{N}} \boldsymbol{\Theta}, \\ \dot{\theta}(\mathbf{X}, t) &= N_I \dot{\theta}_I = \tilde{\mathbf{N}} \dot{\boldsymbol{\Theta}}, \\ \delta\theta(\mathbf{X}, t) &= N_I \delta\theta_I = \tilde{\mathbf{N}} \delta\boldsymbol{\Theta}.\end{aligned}\tag{2.56}$$

where

$$\tilde{\mathbf{N}} := (N_1, N_2, \dots, N_{n_N})\tag{2.57}$$

is the interpolation matrix for the thermal field and

$$\boldsymbol{\Theta} := (\theta_1, \theta_2, \dots, \theta_{n_N})^T\tag{2.58}$$

denotes the nodal temperature vector. Substituting Eq. (2.56) into the weak form of the thermal energy balance equation Eq. (2.22), and using the arbitrariness of the virtual nodal temperature $\delta\theta_I$, we could obtained the discretized version of the thermal energy balance equation

$$\int_{\mathcal{B}} \rho c N_I N_J \dot{\theta}_J dV + \int_{\mathcal{B}} \nabla N_I \cdot (\mathbf{k} \cdot \nabla N_J \theta_J) dV - \int_{\partial_h \mathcal{B}} N_I \bar{q} dS - \int_{\mathcal{B}} N_I Q dV = 0.\tag{2.59}$$

This set of equations could be rewritten in matrix form as

$$\mathbf{C}\dot{\boldsymbol{\Theta}} + \mathbf{K}^{\text{th}}\boldsymbol{\Theta} = \mathbf{f}^{\text{th}}, \quad (2.60)$$

where $\mathbf{C}$ and $\mathbf{K}^{\text{th}}$ are the temperature dependent heat capacity matrix and conductivity matrix, respectively, which read

$$\mathbf{C} = \int_{\mathcal{B}} \rho c \tilde{\mathbf{N}}^T \tilde{\mathbf{N}} dV, \quad (2.61a)$$

$$\mathbf{K}^{\text{th}} = \int_{\mathcal{B}} \nabla \tilde{\mathbf{N}}^T \cdot (\mathbf{k} \cdot \nabla \tilde{\mathbf{N}}) dV, \quad (2.61b)$$

and $\mathbf{f}^{\text{th}}$ is the nodal heat supply vector given by

$$\mathbf{f}^{\text{th}} = \int_{\mathcal{B}} \tilde{\mathbf{N}}^T Q dV + \int_{\partial_h \mathcal{B}} \tilde{\mathbf{N}}^T \bar{q} dS. \quad (2.62)$$

As discussed in the mechanical field, the procedures for computation of the global heat capacity matrix, the conductivity matrix and the heat supply vector can be described in Box 2.3.

Box 2.3 Procedures for Computation of Global Heat Capacity and Conductivity Matrices, and Heat Supply Vector

Given the global nodal displacement and temperature vectors at time t_{n+1} ,

1. Initialization: $\mathbf{C} = 0$, $\mathbf{K}^{\text{th}} = 0$, $\mathbf{f}^{\text{th}} = 0$.
2. Loop for each element e :
 - (1). Initialization: $\mathbf{C}_e = 0$, $\mathbf{K}_e^{\text{th}} = 0$, $\mathbf{f}_e^{\text{th}} = 0$.
 - (2). For each integration point l in element e :
 - a). Compute $\tilde{\mathbf{N}}(\boldsymbol{\xi}_l)$ and $\nabla \tilde{\mathbf{N}}(\boldsymbol{\xi}_l)$.
 - b). $\mathbf{C}_e += w_l \rho \tilde{\mathbf{N}}^T \tilde{\mathbf{N}}$,
 - c). $\mathbf{K}_e^{\text{th}} += w_l \nabla \tilde{\mathbf{N}}^T \cdot (\mathbf{k} \cdot \nabla \tilde{\mathbf{N}})$
 - d). $\mathbf{f}_e^{\text{th}} += w_l \tilde{\mathbf{N}}^T Q$.
 - (3). Assemble elementary matrix and vectors to the global counterparts.

As a brief summary, in this subsection, the weak form formulation for fully coupled analysis of thermal mechanical processes is spatially discretized with the finite element method into a coupled system of nonlinear equations of the nodal displacements and nodal temperatures, which is stated in Box 2.4:

**Box 2.4 Finite Element Formulation for
Thermo-Mechanical Coupled Problems**

Solve the system of nonlinear equations

$$\begin{aligned} \mathbf{M}\ddot{\mathbf{U}} &= \mathbf{f}^{\text{ext}} - \mathbf{f}^{\text{int}} \\ \mathbf{C}\dot{\Theta} + \mathbf{K}^{\text{th}}\Theta &= \mathbf{f}^{\text{th}} \end{aligned}$$

for the nodal displacement vector $\mathbf{U}$ and temperature vector Θ , where

$$\begin{aligned} \mathbf{M} &= \int_{\mathcal{B}} \rho \mathbf{N}^T \mathbf{N} dV, \quad \mathbf{f}^{\text{ext}} = \int_{\mathcal{B}} \rho \mathbf{N}^T \mathbf{b} dV + \int_{\partial_t \mathcal{B}} \mathbf{N}^T \bar{\mathbf{t}} dS, \\ \mathbf{f}^{\text{int}} &= \int_{\mathcal{B}} \mathbf{B}^T \boldsymbol{\sigma}(\Theta) dV, \quad \mathbf{C} = \int_{\mathcal{B}} \rho c \tilde{\mathbf{N}}^T \tilde{\mathbf{N}} dV, \\ \mathbf{K}^{\text{th}} &= \int_{\mathcal{B}} \nabla \tilde{\mathbf{N}}^T \cdot (\mathbf{k} \cdot \nabla \tilde{\mathbf{N}}) dV, \quad \mathbf{f}^{\text{th}} = \int_{\mathcal{B}} \tilde{\mathbf{N}}^T Q(\boldsymbol{\sigma}) dV + \int_{\partial_h \mathcal{B}} \tilde{\mathbf{N}}^T \bar{q} dS. \end{aligned}$$

Numerical evaluations of these global matrices and vectors as function of $\mathbf{U}$ and Θ are described in Box 2.2 and Box 2.3.

It is shown that this nonlinear system of equations explicitly contains the time derivatives of the nodal displacements and temperatures. In addition, according to the constitutive equation described in Eq. (2.4), the stress is in general dependent on the strain rate as well as the history of the internal variables. Thus the system of equations described in Box 2.4 is actually a nonlinear set of ordinary differential equations in time and should be first discretized in the time domain before it could be finally solved numerically for the nodal displacements and temperatures at a give time. This time discretization and solution procedures will be discussed in detail in the following section.

2.1.3 Solution Procedures

In this section, the spatially discretized system of nonlinear differential equations given in Box 2.4 will be further discretized in the time domain to solve the nodal displacements and temperatures and to compute other solution dependent variables at a given time. Both implicit and explicit time integration schemes are introduced in detail.

The time domain for the loading process $[0, t_{\text{end}}]$ could be split into a series of time intervals as

$$[0, t_{\text{end}}] = [t_0, t_1] \cup (t_1, t_2] \cup \cdots \cup (t_{n_T-1}, t_{n_T}], \quad t_0 = 0, t_{n_T} = t_{\text{end}}. \quad (2.63)$$

Each interval is called a time increment defined as

$$(t_n, t_{n+1}], \quad 0 \leq n < n_T. \quad (2.64)$$

Δt_{n+1} is also used to represent the time increment size as

$$\Delta t_{n+1} = t_{n+1} - t_n, \quad 0 \leq n < n_T, \quad (2.65)$$

in this thesis depending on the context.

At the initial time $t = 0$, the nodal values of the displacements and temperatures as well as the values of internal variables for each integration point are obtained from the initial conditions given in Eq. (2.7), Eq. (2.20) and Eq. (2.8). For a typical time increment Δt_{n+1} we assume that at the beginning of the increment $t = t_n$ the solution to the system of nonlinear algebraic equations given in Box 2.4 is known, which means that all necessary information at $t = t_n$ including the nodal displacements, temperatures, and all other solution dependent variables including the stress, deformation gradient and internal variables at each integration point have been already solved or evaluated. If the values for these quantities at the end of the increment $t = t_{n+1}$ could be obtained based on their known values at time $t = t_n$ following a specific procedure, we could then march in the time domain by repeating the procedure from one increment to the next until the solution at every discrete time $t = t_k$ ($1 \leq k \leq n_T$) is incrementally determined. This procedure of advancing the solution of the system of equations, described in Box 2.4 from the beginning of an increment $t = t_n$ to the end of the increment $t = t_{n+1}$, is usually called the time integration procedure, which is briefly summarized in Box 2.5 for the sake of clarity.

**Box 2.5 Time Integration Procedure for
Thermal-Mechanical Coupled Problems**

1. At $t = 0$, apply the initial conditions Eq. (2.7), Eq. (2.20) and Eq. (2.8)

$$\mathbf{U}_0(\mathbf{X}_I) = \bar{\mathbf{u}}_0(\mathbf{X}_I), \quad \Theta_0(\mathbf{X}_I) = \bar{\theta}_0(\mathbf{X}_I), \quad \forall \text{ node } I,$$

$$\boldsymbol{\psi}_0(\mathbf{X}_l) = \bar{\boldsymbol{\psi}}_0(\mathbf{X}_l), \quad \forall \text{ integration point } l.$$

2. For time increment $(t_n, t_{n+1}]$ ($0 \leq n < n_T$), given

$$\mathbf{U}_n(\mathbf{X}_I), \Theta_n(\mathbf{X}_I), \forall I \quad \text{and} \quad \boldsymbol{\psi}_n(\mathbf{X}_l), \forall l,$$

determine

$$\mathbf{U}_{n+1}(\mathbf{X}_I), \Theta_{n+1}(\mathbf{X}_I), \forall I \quad \text{and} \quad \boldsymbol{\psi}_{n+1}(\mathbf{X}_l), \forall l,$$

by solving the system of equations in Box 2.4 at time $t = t_{n+1}$.

Typically there are two types of time integration algorithm, namely implicit time integration scheme and explicit time integration schemes. Both schemes have their own advantages in specific application scenarios and will be introduced in detail here.

Implicit Time Integration Schemes

For fully coupled thermal-mechanical analysis with the implicit time integration scheme, the inertial effect is usually neglected [2], i.e. the mechanical process is assumed to be quasi-static, which could be described with the discrete equilibrium equation given by Eq. (2.39). Taking such assumption and using the backward-Euler scheme for the temperature rate, the nonlinear system of equations described in Box 2.4 could be formulated at a typical time increment Δt_{n+1} as

$$\mathbf{R}^u(\mathbf{U}, \Theta) = \mathbf{f}^{\text{int}}(\mathbf{U}, \Theta) - \mathbf{f}^{\text{ext}} = 0, \quad (2.66a)$$

$$\mathbf{R}^\theta(\mathbf{U}, \Theta) = \mathbf{C} \frac{\Theta - \Theta_n}{\Delta t} + \mathbf{K}^{\text{th}} \Theta - \mathbf{f}^{\text{th}}(\mathbf{U}, \Theta) = 0. \quad (2.66b)$$

Here the subscript $n + 1$, which is used to represent the values of quantities at time t_{n+1} , is dropped off for brevity. That is

$$\mathbf{U} := \mathbf{U}_{n+1}, \quad \Theta := \Theta_{n+1}, \quad \psi := \psi_{n+1}, \quad \Delta t := \Delta t_{n+1}. \quad (2.67)$$

At the beginning of this increment $t = t_n$, as stated in Box 2.5 all necessary information including the nodal displacements, nodal temperatures and the internal variables for all integration points is known. Let $\mathbf{Y} := (\mathbf{U}, \Theta)^T$ denote the vector of unknowns of Eq.(2.66), which could be rewritten in compact residual form as

$$\mathbf{R}(\mathbf{Y}) := \begin{pmatrix} \mathbf{R}^u(\mathbf{Y}) \\ \mathbf{R}^\theta(\mathbf{Y}) \end{pmatrix} = 0 \quad (2.68)$$

The total number of unknowns, the degree of freedom in the model, is $4n_N$. This nonlinear system of algebraic equations could be solved by using the well known Newton-Raphson iterative solution scheme as introduced below.

Let $\mathbf{Y}_k$ be the approximation of $\mathbf{Y}$ at the k -th iteration. The residual vector of Eq. (2.68) at the next iteration could be derived by expanding the Taylor series in the neighborhood of $\mathbf{Y}_k$ as

$$\mathbf{R}(\mathbf{Y}_{k+1}) = \mathbf{R}(\mathbf{Y}_k - \Delta \mathbf{Y}_k) = \mathbf{R}(\mathbf{Y}_k) - \frac{\partial \mathbf{R}(\mathbf{Y}_k)}{\partial \mathbf{Y}_k} \Delta \mathbf{Y}_k + \mathcal{O}(\Delta \mathbf{Y}_k^2) \quad (2.69)$$

By neglecting the second and higher order terms in Eq. (2.69) and setting the residual vector to zero, the following iterative relation could be derived:

$$\mathbf{K} \Delta \mathbf{Y}_k = \mathbf{R}(\mathbf{Y}_k), \quad (2.70a)$$

$$\mathbf{Y}_{k+1} = \mathbf{Y}_k - \Delta \mathbf{Y}_k, \quad (2.70b)$$

where $\mathbf{K}$ is the global tangent stiffness matrix obtained by differentiating the residual vector with respect to the vector of unknowns as

$$\mathbf{K} = \frac{\partial \mathbf{R}(\mathbf{Y}_k)}{\partial \mathbf{Y}_k}. \quad (2.71)$$

The initial values for the vector of unknowns and the internal variables during the iterative process could be taken as the corresponding known values at time t_n . That is

$$\mathbf{Y}_0 = (\mathbf{U}_n, \Theta_n), \quad \psi_0 = \psi_n. \quad (2.72)$$

This iterative procedure expressed in Eq.(2.70) could then be repeated until the norm of the residual vector gets smaller than a given tolerance, which is written as

$$\|\mathbf{R}(\mathbf{Y}_k)\| \leq \varepsilon_{tol}. \quad (2.73)$$

This Newton-Raphson iterative method will converge at a quadratic rate as long as the initial guess for the unknowns falls into the radius of convergence.

The key task for an iteration is to determine the correction to the vector of unknowns by solving the linear system of algebraic equations given by Eq. (2.70a), which first requires the computation of the global residual vector and the global tangent stiffness matrix as will be discussed in detail as below.

By rewriting the global stiffness matrix in partitioned form, the linear system of equations Eq. (2.70a) could be reformulated as

$$\begin{pmatrix} \mathbf{K}^{uu} & \mathbf{K}^{u\theta} \\ \mathbf{K}^{\theta u} & \mathbf{K}^{\theta\theta} \end{pmatrix} \begin{pmatrix} \Delta \mathbf{U}_k \\ \Delta \Theta_k \end{pmatrix} = \begin{pmatrix} \mathbf{R}^u(\mathbf{U}_k, \Theta_k) \\ \mathbf{R}^\theta(\mathbf{U}_k, \Theta_k) \end{pmatrix}. \quad (2.74)$$

Following the procedures described in Box 2.2 and Box 2.3, the residual vectors in the displacement field $\mathbf{R}^u$ and the temperature field $\mathbf{R}^\theta$ could be evaluated straightforwardly. The computation of the submatrices of the global tangent stiffness matrix is discussed as below.

The submatrix $\mathbf{K}^{uu}$ could be derived from Eq. (2.66a) and further be divided into the three parts as

$$\mathbf{K}^{uu} := \frac{\partial \mathbf{R}^u}{\partial \mathbf{U}} = \frac{\partial \mathbf{f}^{\text{int}}}{\partial \mathbf{U}} - \frac{\partial \mathbf{f}^{\text{ext}}}{\partial \mathbf{U}} = \mathbf{K}^{uu,\text{mat}} + \mathbf{K}^{uu,\text{geo}} + \mathbf{K}^{uu,\text{load}}, \quad (2.75)$$

where $\mathbf{K}^{uu,\text{mat}}$ is the material tangent stiffness matrix, which can be computed by using Eq. (2.52) and Eq. (2.45) as

$$\mathbf{K}^{uu,\text{mat}} = \int_B \mathbf{B}^T \frac{\partial \boldsymbol{\sigma}}{\partial \mathbf{U}} dV = \int_B \mathbf{B}^T \frac{\partial \Delta \boldsymbol{\sigma}}{\partial \Delta \boldsymbol{\varepsilon}} \frac{\partial \Delta \boldsymbol{\varepsilon}}{\partial \mathbf{U}} dV = \int_B \mathbf{B}^T \frac{\partial \Delta \boldsymbol{\sigma}}{\partial \Delta \boldsymbol{\varepsilon}} \mathbf{B} dV, \quad (2.76)$$

$\mathbf{K}^{uu,\text{geo}}$ is the geometric tangent stiffness matrix, which is given here without proven as

$$\mathbf{K}^{uu,\text{geo}} = \int_{\mathcal{B}} \frac{\partial \mathbf{N}}{\partial X} \boldsymbol{\sigma} \frac{\partial \mathbf{N}}{\partial X} dV, \quad (2.77)$$

and $\mathbf{K}^{uu,\text{load}}$ is the contribution from the external load that is dependent on the deformation field. In case that this part of the stiffness matrix is absent, $\mathbf{K}^{uu}$ would be symmetric.

The submatrix $\mathbf{K}^{u\theta}$ could be computed by introducing the interpolation form for the temperature field given in Eq. (2.56) to Eq. (2.66a)

$$\mathbf{K}^{u\theta} := \frac{\partial \mathbf{R}^u}{\partial \Theta} = \int_{\mathcal{B}} \mathbf{B}^T \frac{\partial \Delta \boldsymbol{\sigma}}{\partial \Delta \theta} \frac{\partial \Delta \theta}{\partial \Theta} dV = \int_{\mathcal{B}} \mathbf{B}^T \frac{\partial \Delta \boldsymbol{\sigma}}{\partial \Delta \theta} \tilde{\mathbf{N}} dV. \quad (2.78)$$

The submatrix $\mathbf{K}^{\theta u}$ could be derived from Eq. (2.66b) by using Eq. (2.45) as

$$\mathbf{K}^{\theta u} := \frac{\partial \mathbf{R}^\theta}{\partial \mathbf{U}} = - \int_{\mathcal{B}} \tilde{\mathbf{N}}^T \frac{\partial Q}{\partial \mathbf{U}} dV = - \int_{\mathcal{B}} \tilde{\mathbf{N}}^T \frac{\partial \Delta Q}{\partial \Delta \boldsymbol{\varepsilon}} \mathbf{B} dV. \quad (2.79)$$

Finally, the submatrix $\mathbf{K}^{\theta\theta}$ could be derived from Eq. (2.66b) directly as

$$\begin{aligned} \mathbf{K}^{\theta\theta} := \frac{\partial \mathbf{R}^\theta}{\partial \Theta} = & \int_{\mathcal{B}} \left[\frac{\rho c}{\Delta t} \tilde{\mathbf{N}}^T \tilde{\mathbf{N}} + \nabla \tilde{\mathbf{N}}^T \cdot \left(\mathbf{k} \cdot \nabla \tilde{\mathbf{N}} \right) + \frac{\partial \Delta Q}{\partial \Delta \theta} \tilde{\mathbf{N}}^T \tilde{\mathbf{N}} \right] dV \\ & + \int_{\mathcal{B}} \left[\frac{\theta_k - \theta_n}{\Delta t} \frac{\partial \rho c}{\partial \theta} \tilde{\mathbf{N}}^T \tilde{\mathbf{N}} + \nabla \tilde{\mathbf{N}}^T \cdot \left(\frac{\partial \mathbf{k}}{\partial \theta} \cdot \nabla \theta_k \tilde{\mathbf{N}} \right) \right] dV. \end{aligned} \quad (2.80)$$

The second integral in $\mathbf{K}^{\theta\theta}$ is the contribution from the change of the material thermal properties including the heat capacity and thermal conductivity. It is usually neglected as the derivatives of thermal properties with respect to temperature are relatively small. In this case, the submatrix $\mathbf{K}^{\theta\theta}$ becomes symmetric.

It could be observed that although the diagonal submatrices $\mathbf{K}^{uu}$ and $\mathbf{K}^{\theta\theta}$ may be symmetric under some assumptions, the full global stiffness matrix $\mathbf{K}$ is still asymmetric as the off-diagonal submatrices $\mathbf{K}^{u\theta}$ and $\mathbf{K}^{\theta u}$ are not symmetric and $\mathbf{K}^{u\theta} \neq \mathbf{K}^{\theta u^T}$. However, it is shown from the component form of the submatrices expressed above that, due to the nodal support property of the global shape functions, the global stiffness matrix is sparse as its component $\mathbf{K}_{IJ}$ only has nonzero value when node I and node J are associated with the same element. Thus an asymmetric sparse matrix storage format could be used for the global stiffness matrix.

With the obtained residual vector and the global stiffness matrix discussed above, the estimated vector of unknowns at the next iteration could be updated with the correction vector $\Delta \mathbf{Y}_k$ determined by solving the linear system of equations with a sparse linear solver, as described in Eq. (2.70). This iterative process

is repeated until the converged solution to the nodal displacement vector and nodal temperature vector at the end of the time increment are determined. As a brief summary, the main procedures for performing thermo-mechanically coupled analysis with implicit finite element method are illustrated in Fig. 2.3.

**Box 2.6 Staggered Solution Scheme for Implicit Finite
Element Analysis of Thermal-Mechanical Coupled Problems**

1. Initialization: $k = 0$, $\mathbf{U}_k = \mathbf{U}_n$, $\Theta_k = \Theta_n$, $\psi_k = \psi_n$.
2. Solution to mechanical field:
 - a). Compute $\mathbf{K}^{uu}(\mathbf{U}_k, \Theta_k)$ and $\mathbf{R}^u(\mathbf{U}_k, \Theta_k)$,
 - b). Update Q_{k+1} and ψ_{k+1} from constitutive model.
 - c). Solve Eq.(2.82a) for $\Delta \mathbf{U}_k$,
 - d). Update displacement field: $\mathbf{U}_{k+1} = \mathbf{U}_k - \Delta \mathbf{U}_k$.
3. Solution to thermal field:
 - a). Compute $\mathbf{K}^{\theta\theta}(\mathbf{U}_{k+1}, Q_{k+1}, \Theta_k)$ and $\mathbf{R}^\theta(\mathbf{U}_{k+1}, Q_{k+1}, \Theta_k)$,
 - b). Solve Eq.(2.82b) for $\Delta \Theta_k$,
 - c). Update $\Theta_{k+1} = \Theta_k - \Delta \Theta_k$,
 - d). Check convergence for thermal and mechanical field.

In the previous discussion, we have discussed the implementation of the fully coupled thermomechanical problem. The displacement field and the temperature field are updated simultaneously in each iteration. However, as discussed previously, the global stiffness matrix is unsymmetric, which requires the use of unsymmetric matrix storage. Solving such linear system of equations also needs a more costly solution scheme compared to the one with symmetric stiffness matrix. This full implementation of the global stiffness matrix is more suitable for problems where the coupling effects between the mechanical field and the thermal field are strong. In cases that the coupling effects are weak, the linear system of equations given in Eq. (2.74) could be approximated as

$$\begin{pmatrix} \mathbf{K}^{uu} & \mathbf{0} \\ \mathbf{0} & \mathbf{K}^{\theta\theta} \end{pmatrix} \begin{pmatrix} \Delta \mathbf{U}_k \\ \Delta \Theta_k \end{pmatrix} = \begin{pmatrix} \mathbf{R}^u(\mathbf{U}_k, \Theta_k) \\ \mathbf{R}^\theta(\mathbf{U}_k, \Theta_k) \end{pmatrix}, \quad (2.81)$$

which in essence divides the original fully coupled system of equations into two

Fig. 2.3: Flowchart for fully coupled thermal-mechanical analysis with implicit finite element method

separated sets of equations as

$$\mathbf{K}^{uu} \Delta \mathbf{U}_k = \mathbf{R}^u, \quad (2.82a)$$

$$\mathbf{K}^{\theta\theta} \Delta \Theta_k = \mathbf{R}^\theta. \quad (2.82b)$$

The mechanical field and the thermal field at each iteration could now be updated in a staggered way as described in Box 2.6.

In this staggered solution scheme, if the load contribution to the stiffness matrix $\mathbf{K}^{uu}$ and the contribution to $\mathbf{K}^{\theta\theta}$ caused by thermal property changes is negligible, both the mechanical problem and the thermal problem have symmetric stiffness matrix and fewer unknowns, which can yield a reduction in storage and computational costs compared to the concurrent scheme where the two fields are solved simultaneously. Nevertheless, although the computational cost in each iteration is reduced, the staggered scheme usually needs more iterations before reaching convergence for both the mechanical and the thermal fields.

As long as the converged solution is obtained, the solution accuracy is not affected whether the staggered scheme or the concurrent scheme is chosen, since it is only determined by the given tolerance.

Explicit Time Integration Scheme

For fully coupled thermal-mechanical analysis with an explicit time integration scheme, the mechanical field and the thermal field are updated in a staggered fashion at each time increment. First for the mechanical field, the inertial effect now needs to be taken into consideration but the consistent mass matrix is usually replaced by the lumped mass matrix for the sake of computational efficiency. The elemental lumped mass matrix could be obtained by distributing the total mass of the element equally to each associated node as

$$\mathbf{M}_e^{\text{lump}} = \frac{1}{m} \int_{B_e} \rho dV_e \text{diag} \{ \mathbf{I}_1, \mathbf{I}_2, \dots, \mathbf{I}_m \} \quad (2.83)$$

where m is the number of nodes in the element and $\mathbf{I}_1 \sim \mathbf{I}_m$ are 3×3 identity matrices. By the assembly procedure of the elemental lumped mass matrix, the global lumped mass matrix could be formulated. As the nodal mass does not change in time, this global lumped mass matrix only needs to be computed once at the beginning of the analysis. It is diagonal and can be trivially inverted. The displacement field could then be updated by using the central difference integration scheme as follows.

At the beginning of time increment $n + 1$, the external and internal nodal force

vectors are first computed following the procedures described in Box 2.2. The nodal acceleration vector could then be computed from the discretized balance equation of linear momentum given in Eq. (2.36) as

$$\ddot{\mathbf{U}}_n = \mathbf{M}^{-1} (\mathbf{f}_n^{\text{ext}} - \mathbf{f}_n^{\text{int}}). \quad (2.84)$$

The nodal velocity vector at the middle of the increment could be obtained by

$$\dot{\mathbf{U}}_{n+\frac{1}{2}} = \dot{\mathbf{U}}_{n-\frac{1}{2}} + \frac{1}{2} (\Delta t_{n+1} + \Delta t_n) \ddot{\mathbf{U}}_n, \quad (2.85)$$

Finally, the nodal displacement vector at the end of the increment could be determined by

$$\mathbf{U}_{n+1} = \mathbf{U}_n + \dot{\mathbf{U}}_{n+\frac{1}{2}} \Delta t_{n+1}. \quad (2.86)$$

Actually the above equations Eq. (2.84) $\sim$ Eq. (2.86) are decoupled and is in practice solved node by node without the formulation and storage of the global mass matrix, the external and internal force vectors.

After the integration of the mechanical field, the new configuration of the body $\mathcal{B}$ are determined and the volumetric internal heat generation rate Q is evaluated. With the obtained information from the mechanical field, the thermal field could then be updated by using the explicit forward difference integration scheme as follows.

First, the consistent heat capacity matrix is replaced by the diagonal lumped heat capacity matrix as is done to the mass matrix in the mechanical field. Due to the temperature dependency, this matrix may need to be updated at the beginning of each increment. The procedures for computation of this heat capacity matrix, the thermal conductivity matrix $\mathbf{K}^{\text{th}}$ and the heat supply vector $\mathbf{f}^{\text{th}}$ are described in Box 2.3. The nodal temperature rate vector could then be computed from the discretized balance equation of thermal energy given in Eq. (2.60) as

$$\dot{\Theta}_n = \mathbf{C}^{-1} (\mathbf{f}_n^{\text{th}} - \mathbf{f}^{\text{int}}(\Theta_n)). \quad (2.87)$$

Finally, the nodal temperature vector at the end of the increment could be evaluated as

$$\Theta_{n+1} = \Theta_n + \dot{\Theta}_n \Delta t_{n+1}. \quad (2.88)$$

As discussed above, for each time increment, the mechanical field and the thermal field are updated explicitly by using the central difference integration scheme and the forward difference scheme, respectively. In contrast to the implicit time integration scheme as discussed in detail previously, this explicit time integration scheme does not require the expensive Newton-Raphson iteration process, which

means that neither the formation of the global tangent stiffness matrix nor the solution to the linear system of equations are required. However, both the central difference integration scheme and the forward difference scheme are conditionally stable. For every time increment, the increment size Δt , which is usually called the stable time increment, should be smaller than a critical value. It could be proved that for the central difference operator and the forward difference operator, the stability limit is determined by

$$\Delta t \leq \min(\Delta t_m, \Delta t_t) := \min\left(\frac{2}{\omega_{\max}}, \frac{2}{\lambda_{\max}}\right), \quad (2.89)$$

where Δt_m and Δt_t are the stability limit determined by the mechanical and thermal fields, respectively, $\omega_{\max}$ is the highest frequency in the system of equations for the mechanical response and $\lambda_{\max}$ is the largest eigenvalue in the system of equations for the thermal response. To avoid solving eigenvalue problems, in practice the stability limit for the mechanical field is usually chosen such that the time increment is too small for the dilatational wave to travel through any element in the mesh, which is written as

$$\Delta t_m \approx \frac{L_{\min}}{c_d} \quad (2.90)$$

where $L_{\min}$ is the smallest characteristic length of the elements and c_d is the dilatational wave speed given by

$$c_d = \sqrt{\frac{\bar{\lambda} + 2\bar{\mu}}{\rho}} \quad (2.91)$$

with $\bar{\lambda}$ and $\bar{\mu}$ being the effective Lamé's constants, and the stability limit for the thermal field is usually estimated by

$$\Delta t_t \approx \frac{\rho c L_{\min}^2}{2k} \quad (2.92)$$

where k is the thermal conductivity.

In most cases the stability limit is governed by the mechanical field unless huge amount of mass scaling is used. Mass scaling is a practical technique for improving the computational efficiency of explicit finite element analysis. The actual stable time increment calculated from Eqs. (2.90) and (2.92) is typically very small, which means a large number of time increments are required for the whole analysis. For some particular problems, the density could be treated as a parameter. By intentionally increasing the density, which is usually called mass scaling, the stable time increment could be increased accordingly as given

by Eq. (2.90) and Eq. (2.91). The computational costs could then be reduced significantly while causing little effect on the solution accuracy of the problems. Two typical problems the mass scaling technique may apply to are the quasi-static analysis or transit response simulations of a model consisting a few very small elements that dominate the stability limit. For quasi-static analysis, the inertial effect is weak and the fixed mass scaling approach is usually performed, which applies an appropriate and fixed mass scaling factor uniformly to the entire model. For example, a mass scaling factor of 100 may be applied to each element in the model, leading to an increase of the stable time increment by a factor of 10 and thus a reduction of the total computational time by about 90%. For the transit analysis, the inertial effect plays a crucial role in the response of the material. In this case the variable mass scaling approach may be used, which only scales the mass of a few elements with very small characteristic length that govern the stability limit. This could increase the stable time increment notably but yield a negligible effect on the overall response of the entire model. In practice, the effect of the mass scaling on the solution accuracy could be indicated by the ratio of the kinetic energy to the total strain energy in the model. It is believed that the increases of the mass and consequent inertial forces do not alter the solution significantly when the ratio remains under 5% throughout the analysis.

For the sake of clarity, the main procedures for performing thermo-mechanically coupled analysis with explicit finite element method are illustrated in Fig. 2.4.

Comparison between Implicit and Explicit Time Integration Schemes

In this subsection, both the implicit and explicit time integration schemes have been introduced in detail for updating the thermal and the mechanical fields in the model for each time increment. Comparisons between these two schemes are summarized as below.

First, the implicit time integration scheme determines the nodal temperatures and displacements at the end of each increment by solving a nonlinear system of algebraic equations with the Newton-Raphson iterative method. Typically tens of iterations may be required in each increment before the converged solutions are obtained for both the temperature field and the displacement field. In each iteration, a linear system of equations with a total number of $4n_N$ unknowns is solved with a sparse linear solver to determine the correction to the nodal temperatures and displacements. Prior to the solution of this linear system of equations, the left hand section and the right hand section, which are the global tangent stiffness matrix and the global residual vector, respectively, need to be formulated. The two fields could also be updated in each increment in a staggered way by solving one linear system of equations with a total number of $3n_N$ unknowns for

Fig. 2.4: Flowchart for fully coupled thermal-mechanical analysis with explicit finite element method

the mechanical field and another linear system of equations with n_N unknowns for the thermal field sequentially. In contrast, the implicit time integration scheme updates the mechanical field and the thermal field in a staggered fashion. For each increment, first the temperature field is frozen and the nodal displacements and other relevant quantities including the volumetric internal heat generation contributed from the mechanical dissipation are updated explicitly by using the central difference integration scheme. Then with the updated mechanical field, the temperature field can be updated straightforwardly with the forward difference integration scheme. No iteration is needed in each increment and therefore no need for formulation of the global tangent stiffness matrix and solution of the linear system of equations compared to the implicit scheme.

Second, for the implicit time integration scheme, the constitutive model needs to evaluate the Cauchy stress σ , the volumetric internal heat generation Q , the internal variables ψ as well as the derivatives of the increments of σ and Q with respect to the strain increment and the temperature increment. While for the explicit scheme, as the global tangent stiffness matrix is not needed, the constitutive model only has to compute σ , Q , and ψ , which is much more simple for implementation.

Third, the implicit time integration scheme unconditional stable for linear problems and large time increments may be used in the simulation, while the explicit scheme is conditionally stable. To get a stable and reliable solution, the chosen time increments should not exceed the stability limit determined by the mesh size and material properties. Typically the time increment used in implicit scheme could be larger than in explicit scheme by three to five orders of magnitude. However, as the Newton-Raphson iterations performed in one increment in the implicit analysis are much more expensive than the central difference scheme and the forward difference scheme applied in the explicit analysis, the explicit integration scheme may be more computational efficient than the implicit scheme, especially in cases where there is a huge number of degrees of freedom in the model or the mass scaling technique is adopted.

Fourth, for some quasi-static problems with high nonlinearity, in particular for processes where contact between different parts of the model is involved, for the implicit time integration scheme it may be difficult to achieve convergence in an increment with the Newton-Raphson iterative method. In these cases, the explicit time integration scheme might be preferred as it does not have convergence difficulties. And for some transient problems where the detailed history of the evolution of the mechanical and the thermal fields during the loading process is of interest, for instance the impact process or the machining process, the explicit time integration scheme may also be the first choice as it uses small time in-

crement and could give high resolution solution of the coupled fields in the time domain. Aside from these cases the implicit scheme might be adopted. As will be seen later, in chapter 3, the *implicit* finite element method is applied to study the plastic deformation behavior of polycrystalline metallic materials with the computational homogenization approach and in chapter 4, the *explicit* finite element method is adopted to study the thermal mechanical responses of ferrite-pearlite steels during machining processes.

2.1.4 Concluding Remarks

In section 2.1, we have introduced systematically and comprehensively a general finite element framework for fully coupled thermal mechanical analysis. First we started from the construction of the weak form formulation for fully coupled thermal mechanical problems in the form of coupled integral equations, based on the balance equations of linear energy and thermal energy that govern the evolution of the involved mechanical and thermal fields as well as the initial and boundary conditions as described in Box 2.1. Then, with the finite element method, we spatially discretized the weak form formulation derived before into a coupled system of nonlinear equations of the nodal displacements and temperatures as shown in Box 2.4. As each equation in this coupled system is actually an ordinary differential equation of time, we split the total time duration of the analysis into a series of time increments and temporally discretized the nonlinear system of ordinary differential equations accordingly, which were finally solved for the nodal displacements and temperatures at each increment by using the implicit or explicit time integration scheme, as summarized in Fig. 2.3 and Fig. 2.4, respectively.

It should be pointed out that all the procedures mentioned in the flowcharts for the implicit and explicit finite element analysis and as shown in Fig. 2.3 and Fig. 2.4 are standard. These fundamental procedures in finite element analysis have been implemented in most mature finite element codes such as the commercial FE codes ABAQUS, ANSYS and the research-centered FE codes Iris. For example, in Abaqus/standard there is a built-in element type C3D8R that is responsible for the computation of the element residual force and the element tangent stiffness matrix, and the assembly of these elemental quantities into the global counterparts. The Newton-Raphson iterative approach has been implemented to solve the discrete nonlinear set of balance equations for the thermal and the mechanical fields in each time increment, and linear sparse solvers have been implemented to solve the linear system of equations for the correction to the unknowns in each iteration. In Abaqus/explicit, the central difference inte-

grator and the forward difference integrator are developed for integration of the displacement field and the temperature field, respectively. All these built-in element types, nonlinear and linear solvers and integrators in ABAQUS could be commonly found in other FE codes. All these well developed FE codes should have similar performance in computational accuracy and efficiency for the same numerical example. Nevertheless, it should be emphasized that the key ingredient for the accuracy of a thermo-mechanically coupled finite element analysis is the accuracy of the Cauchy stress as well as other related quantities evaluated from the constitutive relation. Different material may have very different constitutive behavior in a thermal-mechanical process. Although most FE code may provide a material model library with tens of commonly used constitutive models, it is still not enough for these built-in constitutive models to accurately describe the constitutive behavior of all materials due to the diversity. Luckily, many finite element codes are well designed so that users could readily define their own constitutive relation. For instance, in ABAQUS user defined constitutive model could be integrated into ABAQUS/standard for an implicit analysis through the user subroutine UMAT, and ABAQUS/explicit for an explicit analysis through the user subroutine VUMAT. And in Iris, the material constitutive models are integrated as an open source library named Muesli. It is written in C++ and could be easily extended due to its well-designed code structure. Users could easily define one new constitutive model by deriving, in the terminology of object oriented programming, a pair of sub-classes from the appropriate base class and overloading a handful of essential virtual functions to update the relevant energies, Cauchy stress and material tangent stiffness matrix.

Regarding metallic materials we are interested in, in the material model library of these FE codes several constitutive models such as the Johnson-Cook's [3] and Zerilli-Armstrong [5] may be found. However, these constitutive models are phenomenological and could not capture the anisotropic plasticity behavior of metallic material during deformation. As the macroscopic behavior of materials is largely determined by the underlying microstructure, in order to get the most reliable possible model for metallic materials, in this work a microstructure based crystal plasticity model is employed in which the macroscopic plastic flow is connected to the crystallographic slip at the grain level. A general finite element framework for fully coupled thermal mechanical analysis of metallic materials will be developed by integrating the crystal plasticity constitutive model into ABAQUS/standard and ABAQUS/explicit through user defined subroutines UMAT and VUMAT, which will be applied to study the plastic deformation behavior of polycrystalline metals and the responses of ferrite-pearlite steels during machining processes as will shown in later chapters. In the next section, the

introduction, implementation and validation of the crystal plasticity model will be presented.

2.2 Crystal Plasticity Constitutive Model for Single Crystal

2.2.1 Crystal Plasticity Model

For finite strain inelastic mechanics of single crystal plasticity the deformation gradient $\mathbf{F}$ is assumed to be multiplicatively decomposed into its elastic and plastic parts as $\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$ [63]. The elastic and plastic deformation gradients define two different *local* deformed configurations: one *intermediate* configuration described by $\mathbf{F}^p$, and the final deformed configuration locally determined by $\mathbf{F}^e \mathbf{F}^p$. For a thermo-mechanical problem, as illustrated in Fig. 2.5, a third configuration is introduced accounting for thermal deformations [64]. The resulting decomposition reads

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p \mathbf{F}^\theta, \quad \det \mathbf{F}^e > 0, \quad \det \mathbf{F}^p = 1, \quad \det \mathbf{F}^\theta > 0. \quad (2.93)$$

where $\mathbf{F}^\theta$ now represents the thermal part of the deformation gradient. The elastic deformation gradient embodies the elastic distortions of the lattice, and the rigid body motions; the plastic part, $\mathbf{F}^p$, describes the irreversible deformations of the lattice, associated with plastic shearing along crystallographic planes; finally, the thermal contribution $\mathbf{F}^\theta$ includes the lattice distortion due solely to thermal effects. The local configuration defined by $\mathbf{F}^p \mathbf{F}^\theta$ is hereafter called the intermediate configuration, and can be regarded as being obtained by a pure elastic unloading from the current configuration.

The constitutive model relates the three parts of the deformation gradient with the stress and temperature, or their evolution. In particular, the evolution of the thermal deformation gradient of any metal can be expressed respect its lattice symmetry axis as

$$\dot{\mathbf{F}}^\theta \mathbf{F}^{\theta-1} = \dot{\theta} \boldsymbol{\beta}, \quad (2.94)$$

where $\boldsymbol{\beta}$ is a diagonal tensor of anisotropic thermal expansion coefficients

$$\boldsymbol{\beta} = \text{diag}(\beta_1, \beta_2, \beta_3). \quad (2.95)$$

Assuming that the plastic deformation takes place purely through dislocation glide, the evolution of the plastic deformation gradient could be expressed as a

Fig. 2.5: Illustration on decomposition of deform gradient into the thermal, plastic and elastic parts.

combination of the slip rate $\dot{\gamma}^\alpha$ in every slip system α as in

$$\mathbf{L}^p := \dot{\mathbf{F}}^p \mathbf{F}^{p-1} = \sum_{\alpha} \dot{\gamma}^\alpha \mathbf{S}_0^\alpha, \quad (2.96)$$

where $\mathbf{L}^p$ is the plastic velocity gradient and, for every slip system α , $\mathbf{S}_0^\alpha = \mathbf{s}_0^\alpha \otimes \mathbf{m}_0^\alpha$ is the Schmidt tensor, $\mathbf{s}_0^\alpha$ and $\mathbf{m}_0^\alpha$ are unit vectors along the slip direction and normal to the slip plane, respectively. For FCC crystals crystallographic slip occurs along the $\langle 1\ 1\ 0 \rangle$ direction in $\{1\ 1\ 1\}$ planes and for BCC crystals slip occurs in three different slip sets: $\langle 1\ 1\ 1 \rangle \{1\ 1\ 0\}$, $\langle 1\ 1\ 1 \rangle \{1\ 1\ 2\}$ and $\langle 1\ 1\ 1 \rangle \{1\ 2\ 3\}$. Usually the slip systems in the $\langle 1\ 1\ 1 \rangle \{1\ 1\ 2\}$ set are neglected for simplicity. Here for the sake of completeness the slip systems for FCC and BCC crystals are listed in Table 2.2 and Table 2.3, respectively.

Table 2.2: Slip Systems for FCC Crystals

α	$\mathbf{s}_0$	$\mathbf{m}_0$	α	$\mathbf{s}_0$	$\mathbf{m}_0$
1	$\frac{1}{\sqrt{2}} (0\ \bar{1}\ 1)$	$\frac{1}{\sqrt{3}} (1\ 1\ 1)$	7	$\frac{1}{\sqrt{2}} (1\ \bar{1}\ 0)$	$\frac{1}{\sqrt{3}} (1\ 1\ \bar{1})$
2	$\frac{1}{\sqrt{2}} (1\ \bar{1}\ 0)$	$\frac{1}{\sqrt{3}} (1\ 1\ 1)$	8	$\frac{1}{\sqrt{2}} (0\ 1\ 1)$	$\frac{1}{\sqrt{3}} (1\ 1\ \bar{1})$
3	$\frac{1}{\sqrt{2}} (1\ 0\ \bar{1})$	$\frac{1}{\sqrt{3}} (1\ 1\ 1)$	9	$\frac{1}{\sqrt{2}} (1\ 0\ 1)$	$\frac{1}{\sqrt{3}} (1\ 1\ \bar{1})$
4	$\frac{1}{\sqrt{2}} (1\ 1\ 0)$	$\frac{1}{\sqrt{3}} (1\ \bar{1}\ 1)$	10	$\frac{1}{\sqrt{2}} (1\ 1\ 0)$	$\frac{1}{\sqrt{3}} (\bar{1}\ 1\ 1)$
5	$\frac{1}{\sqrt{2}} (0\ 1\ 1)$	$\frac{1}{\sqrt{3}} (1\ \bar{1}\ 1)$	11	$\frac{1}{\sqrt{2}} (0\ \bar{1}\ 1)$	$\frac{1}{\sqrt{3}} (\bar{1}\ 1\ 1)$
6	$\frac{1}{\sqrt{2}} (1\ 0\ \bar{1})$	$\frac{1}{\sqrt{3}} (1\ \bar{1}\ 1)$	12	$\frac{1}{\sqrt{2}} (1\ 0\ 1)$	$\frac{1}{\sqrt{3}} (\bar{1}\ 1\ 1)$

Table 2.3: Slip Systems for BCC Crystals

α	$\mathbf{s}_0$	$\mathbf{m}_0$	α	$\mathbf{s}_0$	$\mathbf{m}_0$
1	$\frac{1}{\sqrt{3}}(11\bar{1})$	$\frac{1}{\sqrt{2}}(011)$	13	$\frac{1}{\sqrt{3}}(1\bar{1}1)$	$\frac{1}{\sqrt{6}}(21\bar{1})$
2	$\frac{1}{\sqrt{3}}(11\bar{1})$	$\frac{1}{\sqrt{2}}(101)$	14	$\frac{1}{\sqrt{3}}(11\bar{1})$	$\frac{1}{\sqrt{6}}(112)$
3	$\frac{1}{\sqrt{3}}(11\bar{1})$	$\frac{1}{\sqrt{2}}(1\bar{1}0)$	15	$\frac{1}{\sqrt{3}}(1\bar{1}1)$	$\frac{1}{\sqrt{6}}(\bar{1}12)$
4	$\frac{1}{\sqrt{3}}(\bar{1}11)$	$\frac{1}{\sqrt{2}}(01\bar{1})$	16	$\frac{1}{\sqrt{3}}(\bar{1}11)$	$\frac{1}{\sqrt{6}}(1\bar{1}2)$
5	$\frac{1}{\sqrt{3}}(\bar{1}11)$	$\frac{1}{\sqrt{2}}(101)$	17	$\frac{1}{\sqrt{3}}(111)$	$\frac{1}{\sqrt{6}}(1\bar{2}1)$
6	$\frac{1}{\sqrt{3}}(\bar{1}11)$	$\frac{1}{\sqrt{2}}(110)$	18	$\frac{1}{\sqrt{3}}(1\bar{1}1)$	$\frac{1}{\sqrt{6}}(121)$
7	$\frac{1}{\sqrt{3}}(1\bar{1}1)$	$\frac{1}{\sqrt{2}}(011)$	19	$\frac{1}{\sqrt{3}}(11\bar{1})$	$\frac{1}{\sqrt{6}}(\bar{1}21)$
8	$\frac{1}{\sqrt{3}}(1\bar{1}1)$	$\frac{1}{\sqrt{2}}(10\bar{1})$	20	$\frac{1}{\sqrt{3}}(111)$	$\frac{1}{\sqrt{6}}(1\bar{2}1)$
9	$\frac{1}{\sqrt{3}}(1\bar{1}1)$	$\frac{1}{\sqrt{2}}(110)$	21	$\frac{1}{\sqrt{3}}(\bar{1}11)$	$\frac{1}{\sqrt{6}}(12\bar{1})$
10	$\frac{1}{\sqrt{3}}(111)$	$\frac{1}{\sqrt{2}}(1\bar{1}0)$	22	$\frac{1}{\sqrt{3}}(\bar{1}11)$	$\frac{1}{\sqrt{6}}(211)$
11	$\frac{1}{\sqrt{3}}(111)$	$\frac{1}{\sqrt{2}}(10\bar{1})$	23	$\frac{1}{\sqrt{3}}(111)$	$\frac{1}{\sqrt{6}}(\bar{2}11)$
12	$\frac{1}{\sqrt{3}}(111)$	$\frac{1}{\sqrt{2}}(01\bar{1})$	24	$\frac{1}{\sqrt{3}}(11\bar{1})$	$\frac{1}{\sqrt{6}}(2\bar{1}1)$

In the intermediate configuration, the elastic Green-Lagrange strain $\mathbf{E}^e$, which is the work conjugate to the second Piola-Kirchhoff tensor $\mathbf{S}^*$, is defined as

$$\mathbf{E}^e = \frac{1}{2} (\mathbf{F}^{eT} \mathbf{F}^e - \mathbf{I}), \quad (2.97)$$

where $\mathbf{I}$ is the second order identity tensor. $\mathbf{E}^e$ and $\mathbf{S}^*$ are assumed to be connected with an elastic constitutive relation given by

$$\mathbf{S}^* = \mathcal{L} : \mathbf{E}^e, \quad (2.98)$$

where $\mathcal{L}$ is the fourth-order elasticity tensor.

The Cauchy stress is the push forward of the stress $\mathbf{S}^*$ to the current configuration, that is

$$\boldsymbol{\sigma} = (\det \mathbf{F}^e)^{-1} \mathbf{F}^e \mathbf{S}^* \mathbf{F}^{eT}. \quad (2.99)$$

To close the mechanical constitutive law, the evolution of the plastic slip γ^α must be specified for every slip plane. In a viscoplastic model for strain rate sensitive materials as metals, the slip rate is expressed with the flow model

$$\dot{\gamma}^\alpha = \hat{\gamma}^\alpha (\tau^\alpha, s^\alpha, \theta), \quad (2.100)$$

where τ^α is the resolved shear stress in slip system α , defined as

$$\tau^\alpha = \det \mathbf{F}^\theta \left(\mathbf{F}^{\theta T} \mathbf{S}^* \mathbf{F}^{\theta -T} \right) \cdot \mathbf{S}_0^\alpha, \quad (2.101)$$

and s^α is the slip resistance [64]. In this equation and below, the dot product refers to the full contraction of vectors or tensors over all their indices. The

quantity s^α evolves following the hardening model

$$\dot{s}^\alpha = \sum_{\beta} h^{\alpha\beta} |\dot{\gamma}^\beta|, \quad (2.102)$$

where

$$h^{\alpha\beta} = h^\alpha q^{\alpha\beta} \quad (2.103)$$

represents the hardening modulus, h^α stands for the self hardening modulus and $q^{\alpha\beta}$ denotes the latent hardening coefficients. $q^{\alpha\beta}$ is usually taken to be 1.4 if the slip systems α and β are non-coplanar and 1.0 if they are co-planar.

Power Law Type Flow Model

Several flow and hardening models have been proposed in the literature and are introduced here for the sake of completeness of our framework. Two flow models, one a phenomenological power law type model and the other a physically based model, are commonly used. The power law type flow model was first proposed by [65] and is given by

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{s^\alpha} \right|^m \text{sign}(\tau^\alpha) \quad (2.104)$$

where $\dot{\gamma}_0$ is the reference shearing rate, the exponent m is the strain rate sensitivity. This flow model is very simple, easy to implement in the user subroutine due to the simplicity of the formulation and easy for calibrating the model parameters as only two model parameters are involved. What is more, this flow model is computational very efficient compared to the physically based flow model that will be introduced later. However, this flow model also has some disadvantages. First it is phenomenological without clear physical meaning behind the formulation, which limits its reliability for description of flow mechanisms from the microscopic scale and hence the accuracy of the numerical analysis. Second, this flow model does not take into consideration the temperature effect, which is important in the fully coupled thermal mechanical problems we are studying. In order to get more accurate numerical results, the physically based flow model is usually adopted, which is discussed below.

Physically Based Flow Model

Assume that the slip resistance s^α could be decomposed as

$$s^\alpha = s_{at}^\alpha + s_t^\alpha, \quad (2.105)$$

where s_t and s_{at} denote the thermal and athermal parts due to thermally activated obstacles and athermal obstacles, respectively [57]. The resolved shear stress at a slip system α needs to overcome the athermal part of the slip resistance before slip starts. Beyond that value of the resolved shear stress, the thermal energy required to overcome the obstacle depends on the effective resolved shear stress τ_{eff}^α , defined as

$$\tau_{eff}^\alpha = |\tau^\alpha| - s_{at}^\alpha. \quad (2.106)$$

According to the flow model proposed by Frost and Ashby[65], the slip rate in a slip system α controlled by some thermal activation process can be obtained from the Orowan equation

$$\dot{\gamma}^\alpha = \rho_m^\alpha b^\alpha \bar{L} \bar{\nu}^\alpha(\tau_{eff}^\alpha, \theta). \quad (2.107)$$

where ρ_m^α denotes the mobile dislocation density, b^α is the Burgers vector of that system and $\bar{L}$ is a characteristic length of the distance between obstacles. $\bar{\nu}^\alpha$ is the average frequency of jumping events across the obstacles. It depends on both the effective resolved stress and the current temperature and is obtained by using the theory of thermally activated processes. If all the constants in the previous equation are grouped, a single parameter independent of the temperature $\dot{\gamma}_0^\alpha$, the reference slip rate, can be defined as

$$\dot{\gamma}_0^\alpha \approx \rho_m^\alpha b^\alpha \bar{L} \nu_0, \quad (2.108)$$

where ν_0 is the Debye frequency. Using this value, the shear rate can finally be expressed as

$$\dot{\gamma}^\alpha = \begin{cases} 0, & \tau_{eff}^\alpha \leq 0, \\ \dot{\gamma}_0^\alpha \exp\left(-\frac{\Delta G^\alpha}{k_B \theta}\right) \text{sign}(\tau^\alpha), & 0 < \tau_{eff}^\alpha \leq s_t^\alpha, \end{cases} \quad (2.109)$$

where k_B is Boltzmann's constant and ΔG^α is the activation enthalpy. The latter can be obtained with the expression

$$\Delta G^\alpha = \Delta F^\alpha \left[1 - \left(\frac{|\tau_{eff}^\alpha|}{s_t^\alpha} \right)^p \right]^q, \quad (2.110)$$

with ΔF^α being the activation energy at 0 K, p and q denoting model parameters with values $0 < p < 1$ and $1 < q < 2$.

The flow model based on thermal activation is valid for any alloy in which dislocation glide is controlled by thermal activation. In BCC crystals, the lattice friction is the main energy barrier and it is usually assumed that the thermal

part of the slip resistance s_t^α is constant [57]. For FCC crystals, the short range dislocation-dislocation interactions are the main thermal process and it was investigated experimentally [66] that both the thermal and athermal parts of the slip resistance evolve with the deformation but their ratio s_t^α/s_{at}^α could be regarded as a constant over a broad range of strains.

The self hardening modulus h^α in Eq. (2.103) for describing the evolution of the slip resistance is given by the hardening models. The most commonly used hardening models are all phenomenological and briefly introduced below.

Assaro-Needleman Hardening Model

This hardening model was presented by Assaro and Needleman [67]. The self-hardening modulus in different slip systems are considered to be identical as:

$$h = h_0 \text{sech}^2 \left(\frac{h_0 \Gamma}{s_s - s_0} \right) \quad (2.111)$$

where h_0 is the initial hardening modulus, s_0 and s_s are the initial and the saturation value of the slip system resistance, Γ is the accumulated shear strain on all the active slip systems.

Voce-Tome Hardening Model

This hardening model was first proposed by Voce [68] and later modified by Tome. It is also assumed that the self-hardening modulus in all slip systems are identical as:

$$h = h_0 + \left(h_0 - h_s + \frac{h_0 h_s}{s_s} \right) \exp(-h_0 \Gamma / s_s) \quad (2.112)$$

where h_0 and h_s are initial and saturation hardening modulus, respectively, s_s is the saturation value of the slip system resistance and Γ is the accumulated shear strain.

Voce-Kock Hardening Model

This hardening model was presented by Kock [69] by making some modification to the Voce-type hardening model. In this model the self-hardening moduli at slip system α is expressed as

$$h^\alpha = h_0 \frac{s_s - s^\alpha}{s_s - s_0} \quad (2.113)$$

where h_0 is the initial hardening modulus, s_0 is the initial value of slip system resistance and s_s is the saturated value of slip system which evolves with the sum

of shearing rate at all slip systems as:

$$s_s = h_{s0} \left(\frac{\sum_{\beta} |\dot{\gamma}_{\beta}|}{\dot{\gamma}_{s0}} \right)^{k_b \theta / A} \quad (2.114)$$

where K_b is the Boltzmann constant, h_{s0} , $\dot{\gamma}_{s0}$ and A are model parameters.

Brown Hardening Model

This hardening model was proposed by Brown[70]. In this model the self-hardening modulus at slip system α is give by

$$h^{\alpha} = h_0^{\alpha} (1 - s^{\alpha}/s_s^{\alpha})^{r_1} \text{sign} (1 - s^{\alpha}/s_s^{\alpha}). \quad (2.115)$$

where h_0^{α} is the initial hardening moduli, r_1 is a model parameter and s_s^{α} is the saturation value of s^{α} .

Finally, to close the description of this crystal plasticity constitutive model, the volumetric heat generation contributed from plastic work dissipation defined in Eq. (2.14) can be evaluated by

$$Q = \chi \sum_{\alpha} \tau_{\alpha} \dot{\gamma}_{\alpha}. \quad (2.116)$$

2.2.2 Numerical Schemes

In this subsection, we will discuss the numerical schemes for implementing the crystal plasticity constitutive model discussed in the previous subsection in ABAQUS/standard through the user subroutine UMAT for an implicit finite element analysis, and in ABAQUS/explicit through the user subroutine VUMAT for an explicit analysis.

Numerical Schemes in Implicit Analysis

As discussed before in section 2.1.3, in an implicit finite element analysis, the nodal displacements $\mathbf{U}_n$, nodal temperatures Θ_n and the internal variables $\boldsymbol{\psi}_n$ at the beginning of a typical time increment n are known. And for each iteration in this increment in the Newton-Raphson iterative process, the best estimation of the nodal temperature Θ_{n+1} and displacements $\mathbf{U}_{n+1}$ at the end of the increment are also known. The corresponding values of these quantities at the integration points could obtained easily. The value of the deformation gradient at the beginning of the increment $\mathbf{F}_n$ and the estimated value at the end of the increment $\mathbf{F}_{n+1}$ at each integration point could be computed from the estimated nodal displacements.

Now the key task for the user defined material subroutine UMAT may be stated as follows: Given $\mathbf{F}_n$, $\mathbf{F}_{n+1}$, θ_n , θ_{n+1} and $\boldsymbol{\psi}_n$, update the Cauchy stress $\boldsymbol{\sigma}$, the internal volumetric heat generation contributed from plastic dissipation Q , their derivatives with respect to strain increments and temperature increments $\Delta\sigma/\Delta\varepsilon$, $\Delta Q/\Delta\varepsilon$, $\Delta\sigma/\Delta\theta$, $\Delta Q/\Delta\theta$, as well as the internal variables $\boldsymbol{\psi}$, at each iteration.

Update of Cauchy Stress

During each iteration, the thermal deformation gradient can be calculated directly from Eq. (2.94) as

$$\mathbf{F}_{n+1}^\theta = \exp(\Delta\theta\boldsymbol{\beta}) \mathbf{F}_n^\theta \approx (\mathbf{I} + \Delta\theta\boldsymbol{\beta}) \mathbf{F}_n^\theta, \quad (2.117)$$

with $\Delta\theta = \theta_{n+1} - \theta_n$. Next, using Eq. (2.93), the plastic deformation gradient can be evaluated with the expression

$$\mathbf{F}_{n+1}^p = \exp\left(\Delta t \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{S}_0^{\alpha}\right) \mathbf{F}_n^p \approx \left(\mathbf{I} + \Delta t \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{S}_0^{\alpha}\right) \mathbf{F}_n^p. \quad (2.118)$$

Replacing Eqs. (2.117) and (2.118) in Eq. (2.93), the elastic deformation gradient can be also obtained as

$$\mathbf{F}_{n+1}^e = \mathbf{F}_{n+1} \mathbf{F}_{n+1}^{\theta}{}^{-1} \mathbf{F}_n^{p-1} \left(\mathbf{I} - \Delta t \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{S}_0^{\alpha} \right). \quad (2.119)$$

This expression can be rewritten as

$$\mathbf{F}_{n+1}^e - \mathbf{F}_{n+1} \mathbf{F}_{n+1}^{\theta}{}^{-1} \mathbf{F}_n^{p-1} \left(\mathbf{I} - \Delta t \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{S}_0^{\alpha} \right) = 0. \quad (2.120)$$

Using a backward-Euler scheme, the increment of the accumulated shear strain is given by

$$\Delta\gamma^{\alpha} = \dot{\gamma}^{\alpha} \Delta t. \quad (2.121)$$

Combining Eqs. (2.120) and (2.121), a set of nonlinear equations is formed, and the elastic deformation gradient $\mathbf{F}_{n+1}^e$ and the increment of the accumulated shear strain $\Delta\gamma^{\alpha}$ can be solved simultaneously, at the level of the quadrature point, with Newton-Raphson's iterative method as detailed below.

For simplicity, the subindex $n + 1$ is omitted, which implies that $\mathbf{F}^e := \mathbf{F}_{n+1}^e$, $\Delta\gamma^{\alpha} := \Delta\gamma_{n+1}^{\alpha}$, $\dot{\gamma}^{\alpha} := \dot{\gamma}_{n+1}^{\alpha}$, $\tau^{\alpha} := \tau_{n+1}^{\alpha}$, $s^{\alpha} = s_{n+1}^{\alpha}$ and $\theta := \theta_{n+1}$.

Let $\mathbf{X} := (\text{vec}(\mathbf{F}^e), \Delta\boldsymbol{\gamma})^T$ be the vector of unknowns of the nonlinear equations, where

$$\text{vec}(\mathbf{A}_{mn}) = (A_{11}, A_{12}, \dots, A_{1n}, \dots, A_{mn})^T \quad (2.122)$$

is the function that converts the matrix $\mathbf{A}$ to a vector by stacking the rows of the matrix on top of one another sequentially. Let n_s be the number of slip systems, the dimension of the unknown vector $\mathbf{X}$ will be $9+n_s$, which is 21 for FCC crystals and 33 for BCC crystals.

The residual vector $\mathbf{R}(\mathbf{X}) := (\mathbf{R}_{\mathbf{F}^e}, \mathbf{R}_{\Delta\gamma})^T$ is given by

$$\begin{aligned}\mathbf{R}_{\mathbf{F}^e} &= \text{vec} \left(\mathbf{F}^e - \mathbf{F}_{aux} \left(\mathbf{I} - \Delta t \sum_{\alpha} \dot{\gamma}^{\alpha} (\tau^{\alpha}, s^{\alpha}, \theta) \cdot \mathbf{S}_0^{\alpha} \right) \right) \\ \mathbf{R}_{\Delta\gamma} &= \Delta\gamma^{\alpha} - \dot{\gamma}^{\alpha} \Delta t\end{aligned}\tag{2.123}$$

where

$$\mathbf{F}_{aux} := \mathbf{F}_{n+1} \mathbf{F}_{n+1}^{\theta}{}^{-1} \mathbf{F}_n^{p-1}\tag{2.124}$$

The non-linear system of equations consist then in finding $\mathbf{X}$ such that

$$\begin{aligned}\mathbf{R}_{\mathbf{F}^e}(\mathbf{X}) &= \mathbf{0} \\ \mathbf{R}_{\Delta\gamma}(\mathbf{X}) &= \mathbf{0}.\end{aligned}\tag{2.125}$$

The linearization of the equation 2.125 around the last iteration of $\mathbf{X}_k$ leads to the Newton-Raphson iterative procedure where the new iteration of the solution $\mathbf{X}^{k+1}$ is given by

$$\mathbf{X}_{k+1} = \mathbf{X}_k - \delta\mathbf{X}.\tag{2.126}$$

The vector $\delta\mathbf{X}$ is the solution of a linear system of equations

$$\mathbf{J}\delta\mathbf{X} = \mathbf{R}(\mathbf{X}_k)$$

in which $\mathbf{J}$ is the jacobian matrix, that can be written in block form as

$$\mathbf{J} = \frac{\partial \mathbf{R}}{\partial \mathbf{X}} = \begin{bmatrix} \mathbf{J}^{11} & \mathbf{J}^{12} \\ \mathbf{J}^{21} & \mathbf{J}^{22} \end{bmatrix}\tag{2.127}$$

where

$$\begin{aligned}\mathbf{J}_{IJ}^{11} &= \frac{\partial (\mathbf{R}_{\mathbf{F}^e})_I}{\partial (\text{vec}(\mathbf{F}^e))_J} = \delta_{IJ} + \Delta t \sum_{\alpha} \text{vec}(\mathbf{F}_{aux} \mathbf{S}_0^{\alpha})_I \frac{\partial \dot{\gamma}_{\alpha}}{\partial \text{vec}(\mathbf{F}^e)_J}, \quad I, J = 1, \dots, 9 \\ \mathbf{J}_{IJ}^{12} &= \frac{\partial (\mathbf{R}_{\mathbf{F}^e})_I}{\partial \Delta\gamma^J} = \Delta t \sum_{\alpha} \text{vec}(\mathbf{F}_{aux} \mathbf{S}_0^{\alpha})_I \frac{\partial \dot{\gamma}_{\alpha}}{\partial \Delta\gamma^J}, \quad I = 1, \dots, 9; J = 1, \dots, n_s \\ \mathbf{J}_{IJ}^{21} &= \frac{\partial (\mathbf{R}_{\Delta\gamma})_I}{\partial (\text{vec}(\mathbf{F}^e))_J} = -\Delta t \frac{\partial \dot{\gamma}^I}{\partial \text{vec}(\mathbf{F}^e)_J}, \quad I = 1, \dots, n_s; J = 1, \dots, 9 \\ \mathbf{J}_{IJ}^{22} &= \frac{\partial (\mathbf{R}_{\Delta\gamma})_I}{\partial (\text{vec}(\mathbf{F}^e))_J} = \delta_{IJ} - \frac{\partial \dot{\gamma}^I}{\partial \Delta\gamma^J}, \quad I, J = 1, \dots, n_s\end{aligned}\tag{2.128}$$

Some auxiliary quantities used in Eq. (2.128) are given by

$$\begin{aligned}\frac{\partial \dot{\gamma}^\alpha}{\partial \mathbf{F}^e} &= \frac{\partial \dot{\gamma}^\alpha}{\partial \tau^\alpha} \frac{\partial \tau^\alpha}{\partial \mathbf{F}^e} = \frac{\partial \dot{\gamma}^\alpha}{\partial \tau^\alpha} \left(\frac{\partial \mathbf{S}^*}{\partial \mathbf{F}^e} : \mathbf{S}_0^\alpha \right) \\ \frac{\partial \mathbf{S}^*}{\partial \mathbf{F}^e} &= \frac{\partial (\mathcal{L} : \mathbf{E}^e)}{\partial \mathbf{F}^e} = \mathcal{L} : \frac{\partial \mathbf{E}^e}{\partial \mathbf{F}^e} = \frac{1}{2} \mathcal{L} : \frac{\partial (\mathbf{F}^{eT} \mathbf{F}^e)}{\partial \mathbf{F}^e} \\ \frac{\partial \dot{\gamma}^\alpha}{\partial \Delta \gamma^\beta} &= \frac{\partial \dot{\gamma}^\alpha}{\partial s^\alpha} \frac{\partial \dot{s}^\alpha}{\partial \dot{\gamma}^\beta} \text{sign}(\dot{\gamma}^\beta)\end{aligned}\quad (2.129)$$

The derivatives of the slip rate $\dot{\gamma}^\alpha$ with respect to the slip resistance s^α , and the slip resistance rate $\dot{s}^\alpha$ with respect to the slip rate $\dot{\gamma}^\beta$ could be evaluated from Eqs. (2.100) and (2.102), respectively.

The initial value of the vector of unknowns is taken as

$$\mathbf{X}_0 = (\text{vec}(\mathbf{F}_n^e), \mathbf{0})^T \quad (2.130)$$

and Eq. (2.126) is updated until the norm of the residual given by Eq. (2.123) is smaller than the given tolerance.

Once the elastic deformation gradient of the current increment is obtained, the Cauchy stress is updated with Eqs. (2.97) ~ (2.99). The internal volumetric heat generation Q is calculated with Eq. (2.116). The internal variables for our crystal plasticity model, the plastic deformation gradient $\mathbf{F}^p$, the plastic deformation gradient $\mathbf{L}^p$ and the slip resistance s^α , are automatically updated to the latest values obtained in the iteration. Now, we will discuss how to calculate the derivatives of stress increment and heat generation increment with respect to strain increment and temperature increment.

Calculation of the material Jacobian matrix

In order to formulate the element tangent stiffness matrix at each iteration, the following Jacobian matrices should be provided by the constitutive relation:

$$\begin{aligned}\mathbf{J}^{Me} &:= \frac{\partial \Delta \boldsymbol{\sigma}}{\partial \Delta \boldsymbol{\varepsilon}}, & \mathbf{J}^{he} &:= \frac{\partial \Delta Q}{\partial \Delta \boldsymbol{\varepsilon}}, \\ \mathbf{J}^{Mt} &:= \frac{\partial \Delta \boldsymbol{\sigma}}{\partial \Delta \theta}, & \mathbf{J}^{ht} &:= \frac{\partial \Delta Q}{\partial \Delta \theta}.\end{aligned}\quad (2.131)$$

Due to the complexity, it is usually very difficult to give analytical expressions of these matrices from the constitutive relation. Thus a numerical procedure is employed in this work to evaluate these matrices as described below.

According the previous discussion the procedures for computation of Cauchy stress and internal heat generation rate could be literally represented by the

following equations

$$\begin{aligned}\boldsymbol{\sigma}_{n+1} &= \hat{\boldsymbol{\sigma}}(\mathbf{F}_n, \mathbf{F}_{n+1}, \theta_n, \theta_{n+1}, \psi_n), \\ Q_{n+1} &= \hat{Q}(\mathbf{F}_n, \mathbf{F}_{n+1}, \theta_n, \theta_{n+1}, \psi_n).\end{aligned}\tag{2.132}$$

Employing Voigt notation, the stress and strain in Eq. (2.131) could be written as 6-dimensional vectors. That is

$$\begin{aligned}\boldsymbol{\sigma} &= (\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{12}, \sigma_{13}, \sigma_{23})^T \\ \boldsymbol{\varepsilon} &= (\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, \varepsilon_{12}, \varepsilon_{13}, \varepsilon_{23})^T.\end{aligned}\tag{2.133}$$

At the end of increment $n + 1$, the stress and the volumetric heat generation rate are known as $\boldsymbol{\sigma}_{n+1}$ and Q_{n+1} , respectively. Giving a small increment $\Delta\varepsilon$ to the i -th component of the strain vector in Eq. (2.133) and keeping the other components fixed, the corresponding increment to the strain tensor is given by

$$\Delta\mathbf{E}_i = \begin{cases} \Delta\varepsilon e_i \otimes e_i & \text{if } i = 1, 3 \\ \frac{1}{2}\Delta\varepsilon e_1 \otimes e_2 + \frac{1}{2}\Delta\varepsilon e_2 \otimes e_1 & \text{if } i = 4 \\ \frac{1}{2}\Delta\varepsilon e_1 \otimes e_3 + \frac{1}{2}\Delta\varepsilon e_3 \otimes e_1 & \text{if } i = 5 \\ \frac{1}{2}\Delta\varepsilon e_2 \otimes e_3 + \frac{1}{2}\Delta\varepsilon e_3 \otimes e_2 & \text{if } i = 6 \end{cases}\tag{2.134}$$

and the total deformation gradient at this new configuration is calculated as

$$\mathbf{F}_i^{new} = (\mathbf{I} + \Delta\mathbf{E}_i) \mathbf{F}_{n+1}.\tag{2.135}$$

The value of the Cauchy stress and the volumetric heat generation rate at this new configuration, $\boldsymbol{\sigma}_i^{\Delta\varepsilon}$ and $Q_i^{\Delta\varepsilon}$, are obtained from Eq. (2.132) by following the procedure for computation of Cauchy stress and heat generation rate discussed in detail previously as

$$\begin{aligned}\boldsymbol{\sigma}_i^{\Delta\varepsilon} &= \hat{\boldsymbol{\sigma}}(\mathbf{F}_n, \mathbf{F}_i^{new}, \theta_n, \theta_{n+1}, \psi_n), \\ Q_i^{\Delta\varepsilon} &= \hat{Q}(\mathbf{F}_n, \mathbf{F}_i^{new}, \theta_n, \theta_{n+1}, \psi_n).\end{aligned}\tag{2.136}$$

The i -th column of the matrix $\mathbf{J}^{Me}$ and the i -th component of $\mathbf{J}^{he}$ could then be computed using numerical differentiation as

$$\begin{aligned}\mathbf{J}_{:,i}^{Me} &= \frac{\partial \Delta\boldsymbol{\sigma}}{\partial \Delta\varepsilon_i} \Big|_{n+1} = \frac{\boldsymbol{\sigma}_i^{\Delta\varepsilon} - \boldsymbol{\sigma}_{n+1}}{\Delta\varepsilon_i} \\ J_i^{he} &= \frac{\partial \Delta Q}{\partial \Delta\varepsilon_i} \Big|_{n+1} = \frac{Q_i^{\Delta\varepsilon} - Q_{n+1}}{\Delta\varepsilon_i}\end{aligned}\tag{2.137}$$

Similarly, giving a small increment $\Delta\theta$ to the temperature at the end of the increment and keeping others quantities fixed, the corresponding stress and in-

ternal heat generation rate could be calculated from Eq. (2.132) by following the procedure for computation of Cauchy stress and heat generation rate discussed in detail previously as

$$\begin{aligned}\boldsymbol{\sigma}^{\Delta\theta} &= \hat{\boldsymbol{\sigma}}(\mathbf{F}_n, \mathbf{F}_{n+1}, \theta_n, \theta_{n+1} + \Delta\theta, \boldsymbol{\psi}_n), \\ Q^{\Delta\theta} &= \hat{Q}(\mathbf{F}_n, \mathbf{F}_{n+1}, \theta_n, \theta_{n+1} + \Delta\theta, \boldsymbol{\psi}_n).\end{aligned}\tag{2.138}$$

The i -th column of the matrix $\mathbf{J}^{Mt}$ and the i -th component of $\mathbf{J}^{ht}$ could then be computed using numerical differentiation as

$$\begin{aligned}\mathbf{J}^{Mt} &= \frac{\partial \Delta \boldsymbol{\sigma}}{\partial \Delta \theta} \Big|_{n+1} = \frac{\boldsymbol{\sigma}^{\Delta\theta} - \boldsymbol{\sigma}_{n+1}}{\Delta\theta} \\ J^{ht} &= \frac{\partial \Delta Q}{\partial \Delta \theta} \Big|_{n+1} = \frac{Q^{\Delta\theta} - Q_{n+1}}{\Delta\theta}\end{aligned}\tag{2.139}$$

Numerical Schemes in Explicit Analysis

Similarly to what discussed for the implicit analysis, in an explicit finite element analysis, the key task for the user defined material subroutine VUMAT could be stated as follows: Given $\mathbf{F}_n$, $\mathbf{F}_{n+1}$, θ_n , θ_{n+1} and $\boldsymbol{\psi}_n$, update the Cauchy stress $\boldsymbol{\sigma}_{n+1}$, the internal volumetric heat generation contributed from plastic dissipation Q_{n+1} , as well as the internal variables $\boldsymbol{\psi}_{n+1}$ at the end of each time increment. Compared to the UMAT used in the implicit analysis, in VUMAT there is no need to calculate the material Jacobian matrices. In the UMAT we developed for the crystal plasticity model, the elastic deformation gradient $\mathbf{F}_{n+1}^e$ at the end of the increment $n + 1$ was obtained by solving a nonlinear system of equations with the Newton-Raphson iterative method, while in this VUMAT designed to be used in an explicit finite analysis with a huge number of time increments, it is very computational costly to use the iterative method to determine $\mathbf{F}_{n+1}^e$ in each increment. Here it is computed in an explicit manner.

The thermal deformation gradient at the end of the increment $\mathbf{F}_{n+1}^\theta$ could be directly from Eq.(2.117). Using the forward Euler scheme, the plastic deformation gradient at the end of the increment could be approximated from Eq. (2.96) as

$$\mathbf{F}_{n+1}^p = \mathbf{F}_n^p + \mathbf{F}_n^p \mathbf{L}_n^p \Delta t\tag{2.140}$$

The elastic deformation gradient could then be explicitly determined from Eq. (2.93) by

$$\mathbf{F}_{n+1}^e = \mathbf{F}_{n+1} (\mathbf{F}_{n+1}^p \mathbf{F}_{n+1}^\theta)^{-1}\tag{2.141}$$

The Cauchy stress then could be evaluated from Eqs. (2.97) $\sim$ (2.99). From the definition given in Eq.(2.101), the resolved shear stress τ_{n+1}^α could be determined

and the slip rate can be evaluated from Eq. (2.100) by

$$\dot{\gamma}_{n+1}^{\alpha} = \hat{\gamma}^{\alpha}(\tau_{n+1}^{\alpha}, s_n^{\alpha}, \theta_{n+1}). \quad (2.142)$$

The slip resistance now is updated from Eq. (2.102) by

$$s_{n+1}^{\alpha} = s_n^{\alpha} + \sum_{\beta} h^{\alpha\beta} |\dot{\gamma}^{\beta}| \Delta t, \quad (2.143)$$

and the plastic velocity gradient $\mathbf{L}^p$ could be updated using Eq. (2.96). $\mathbf{F}^p$, $\mathbf{L}^p$ and s^{α} are stored as the internal variables for further use in the next increment. Finally, the internal volumetric heat generation Q_{n+1} is calculated with Eq. (2.116).

2.2.3 Validation

In this subsection, several simple numerical examples are presented to validate the thermal-mechanically coupled crystal plasticity finite element framework we have developed.

For the first numerical example, let's consider a single crystal with only two slip systems as shown in Table 2.4: Numerical simulations for uniaxial tension of

Table 2.4: Slip Systems for a Simple Single Crystal

α	$\mathbf{s}_0$	$\mathbf{m}_0$	α	$\mathbf{s}_0$	$\mathbf{m}_0$
1	$\frac{1}{\sqrt{2}}(0\ 1\ 1)$	$\frac{1}{\sqrt{2}}(0\ 1\ \bar{1})$	2	$\frac{1}{\sqrt{2}}(0\ 1\ \bar{1})$	$\frac{1}{\sqrt{2}}(0\ 1\ 1)$

the crystal in the (0, 1, 0) direction under a constant true strain rate of $1.0\ s^{-1}$ at an initial temperature of 300 K were carried out in the following different cases.

a) (Case 1). The elastic modulus of the crystal is temperature independent and the thermal expansion is not considered.

b) (Case 2). The elastic modulus (in GPa) of the crystal is a linear function of temperature given by:

$$\begin{aligned} c_{11} &= 110.0 - 0.20\theta \\ c_{12} &= 60.0 - 0.10\theta \\ c_{14} &= 22.0 - 0.04\theta \end{aligned} \quad (2.144)$$

but the thermal expansion is not considered.

c). (Case 3). The elastic modulus of the crystal is temperature independent but the thermal expansion is now taken into consideration. The thermal expansion coefficient is taken to be $10^{-3}K^{-1}$.

The power law type flow model and the Brown type hardening law as introduced in section 2.2.1 are used in the simulations. The other model parameters and material properties are arbitrarily chosen as listed in Table 2.5.

Table 2.5: Material Properties of a Simple Single Crystal

Model Parameter	Value
$\dot{\gamma}_0$	1.0 s^{-1}
m	0.02
r_1	2.0
s_0	200 MPa
s_s	210 MPa
h_0	100 MPa
ρ	$1.0\text{E}+03 \text{ Kg/m}^3$
c	$1.0\text{E}+03 \text{ J/(Kg} \cdot \text{K)}$
χ	0.9

For case 1, some analytic results could be obtained. The resolved shear stresses in the two slip systems are identical and as the deformation proceeds it first increases from 0.0 to the initial slip resistance 200 MPa and then equals to the slip resistance, which slowly increases to reach the saturated value of 210 MPa. The plastic shearing rate increases from 0.0 to 1.0 according to the flow model. The temperature increase rate can be approximated from Eq. (2.13) and Eq. (2.116) by:

$$\dot{\theta} = \frac{Q}{\rho c} = \frac{\chi \sum_{\alpha} \dot{\gamma}^{\alpha} \tau^{\alpha}}{\rho c} \approx \frac{0.9 \times 2 \times 1.0 \times 200 \times 10^6}{1.0 \times 10^3 \times 1.0 \times 10^3} = 360 \text{ K/s} \quad (2.145)$$

The numerical results are shown in Fig. 2.6. It can be seen that for case 1 the numerical results are in good agreement with the analytic solutions. For case 2 with a temperature dependent elastic properties, as the traction proceeds, the temperature increases and the elastic modulus decreases accordingly. Compared to case 1, the resolved shear stress is a little smaller, thus the Cauchy stress in the tension direction, the plastic shearing rate and the temperature increase rate is smaller than those in case 1. For case 3 with thermal expansion but no temperature dependency of elastic modulus, due to the presence of thermal strain, the resolved shear stress is a bit smaller than the other two cases. Therefore the plastic shearing rate and the temperature increase rate also gets smaller. A softening in the Cauchy stress is also observed in this case.

This simple example shows that the framework we have developed could give reasonable numerical results, which to some extent validated the reliability of our framework.

For the second numerical example, let's consider a BCC single crystal. The elastic modulus (in GPa) of the crystal is taken to be linearly dependent on the

Fig. 2.6: Comparative numerical results on (a). temperature increase rate, (b). plastic shearing rate, (c). resolved shear stress, (d). uniaxial Cauchy stress for uniaxial tension of a single crystal under different cases.

absolute temperature θ given by:

$$\begin{aligned} c_{11} &= 268.2 - 0.24\theta \\ c_{12} &= 159.6 - 0.011\theta \\ c_{14} &= 87.1 - 0.015\theta \end{aligned} \tag{2.146}$$

The physically based flow model and the Brown hardening law as introduced in section 2.2.1 are used. The model parameters and necessary material properties are listed in Table 2.6.

A pair of comparative simulations, one using the explicit finite element method and the other one using the implicit method, are performed to study the responses of the crystal under uniaxial traction in the $(0, 0, 1)$ crystalline direction under a constant engineering strain rate of 1.0 s^{-1} at an initial temperature of 300 K. The C3D8R and C3D8RT element types are chosen for the implicit analysis and the explicit analysis, respectively. For the implicit analysis, the staggered solution technique as introduced in section 2.1.3 is adopted for solving the coupled fields. The numerical results on the uniaxial stress and the temperature during

Table 2.6: Material Properties of a BCC single crystal

Model Parameter	Value
ΔF^α	$2.77 \cdot 10^{-19} \text{ J}$
$\dot{\gamma}_0$	$1.732 \cdot 10^7 \text{ s}^{-1}$
h_0	181 MPa
s_s	121 MPa
r_1	1.10
p	0.28
q	1.40
$s_{at,0}$	50.0 MPa
$s_{t,0}$	445 MPa
α	$6.3 \cdot 10^{-6}$
ρ	$1.669 \cdot 10^{-8}$
c	57.5
χ	0.9

traction are shown in Fig. 2.7. It is shown in Fig. 2.7 that the numerical results

Fig. 2.7: Comparisons on numerical results obtained from explicit and implicit schemes for (a). uniaxial stress-strain and (b). temperature-strain curves of a single BCC crystal under uniaxial traction.

obtained with the implicit method and the explicit method are in good accordance, especially for the temperature-strain curve. This accordance could also to some extent cross validate the thermo-mechanically coupled implicit and explicit crystal plasticity finite element framework we have developed.

The computational efficiency of the explicit method and implicit method is also compared as shown in Table 2.7. For the implicit analysis, the initial and maximum time increment are given as $10^{-4}s$ and $10^{-2}s$ while for the explicit analysis, the time increment is automatically determined by the stability limit calculated at each increment. Although this comparison is rather coarse as we did not make an absolute equivalent conditions for the two method, we could still get some conclusions from Table 2.7. It is shown that the time increment size in

Table 2.7: Comparison on computational efficiency for explicit and implicit analysis

	Implicit Analysis	Explicit Analysis
Total Increments	133	7.5 Million
Min Inc. Size	1.0E-4 s	1.2E-7 s
Max Inc. Size	1.0E-2 s	1.5E-7 s
Normalized Time Cost	1.0	28.4

the explicit analysis may be typically smaller by three to five orders of magnitude than that in the implicit analysis, thus the total increments for the former may accordingly be three to five orders of magnitude greater than that for the latter case. In this quasi-static problem, the total time cost for the explicit analysis is about 30 times longer than that for the implicit analysis, but in other cases the former one may be more efficient than the latter one, depending on the specific problem we are solving.

For explicit finite element analysis, the mass scaling technique may be applied to improve the computational efficiency. Here, a series of explicit analysis with mass scaling factors of 1.0, 10^3 and 10^5 are performed to study the effect of the mass scaling technique on the accuracy and efficiency of explicit analysis. The numerical results for the uniaxial stress-strain curve and the temperature-strain curve are plotted in Fig. 2.8. As shown in Fig. 2.8, for this quasi-static

Fig. 2.8: Comparisons on numerical results obtained with various mass scaling factors for (a). uniaxial stress-strain and (b). temperature-strain curves of a single BCC crystal under uniaxial traction.

problem the numerical simulation performed with a mass scaling factor of as high as 10^5 yields little accuracy loss compared to the one conducted without the use of mass scaling technique while achieve huge computational efficiency gain as the total increments greatly drops from about 7.5 million to 20 thousand, corresponding to a sharp decrease of the total computational time by 99.8%. In

order to improve the computational efficiency, the mass scaling technique may be adopted in explicit analysis performed in later chapters.

CHAPTER 3

Application to Polycrystal Homogenization

In the previous chapter, a thermo-mechanically coupled finite element framework was developed that incorporates the crystal plasticity constitutive model for single crystals and which could be directly applied to study the thermal-mechanical responses of crystalline materials at the grain scale. However, from a practical viewpoint, it is necessary to obtain the response at the macroscale as function of the microstructure, and this response should be based on the behavior at the grain scale. This scale bridging will help to better model thermomechanical process and improve the efficiency and reduce the costs in engineering applications.

An engineering alloy is in general a polycrystalline aggregate of grains with sizes usually ranging $10 - 200\mu\text{m}$. The polycrystalline alloy microstructure is then characterized by the grain size, shape and orientation distributions. As the grain scale is usually several orders of magnitude smaller than the macroscale, determining the macroscopic behavior explicitly modelling all the grains contained in the component under study is not possible due to high computational cost.

The scale gap between the microscopic and the macroscopic responses can be strongly simplified considering scale separation in the problem. Under this approach, macroscopic fields gradients can be considered negligible at the microscopic level, and the material point behavior can then be studied as the collective response of a set grains representing the microstructure subjected to homogeneous stress/strain states. Homogenization theories are used then to obtain the macroscopic or effective response of the polycrystal from the behavior of the grains, given by the crystal plasticity model, and the microstructure, characterized by the grain size, shape and orientation distributions.

In this chapter, we will first present the main aspects of the Taylor homogenization approach and the framework of finite element based computational homogenization. Then, the crystal plasticity finite element framework developed in the previous chapter will be combined with computational homogenization to

study the thermo-mechanical behavior of polycrystalline Tantalum in uniaxial traction process under various initial temperatures and strain rates. To validate the model, simulations will be compared with experiments and with the results provided by a simpler Taylor homogenization model.

3.1 Polycrystalline Homogenization

The main task for a homogenization approach in a thermo-mechanical problem is to establish a homogenized constitutive relation between the macroscopic deformation gradient $\bar{\mathbf{F}}$, temperature $\bar{\theta}$ and the stress $\bar{\boldsymbol{\sigma}}$ for a material point $\mathbf{x}$ in the current configuration $\mathcal{B}$, from the statistical average of the corresponding deformation gradient field $\mathbf{F}$, temperature field θ and stress field $\boldsymbol{\sigma}$ in the underlying microstructure of $\mathbf{x}$. Thus, a homogenization model consists of the following two aspects: first, how to establish a microstructure to represent the material point $\mathbf{x}$ in a statistical sense and second, how to link the relevant quantities between the macroscopic scale and the microscopic scale.

3.1.1 Taylor model

Typically there are two types of homogenization approaches, namely the mean-field homogenization approach and the full field homogenization approach. Mean-field homogenization approaches assume a uniform distribution of the microscopic fields in each of the grains. In this work, the Taylor model [52], will be considered. In this model, a macroscopic material point is represented by a polycrystal consisting of a collection of grains and each grain is considered to be an independent single crystal with prescribed initial volume and orientation, while the shape of each grain and interactions between neighboring grains are neglected. The model assumes that the local deformation gradient in each grain is constant and identical to the deformation gradient $\bar{\mathbf{F}}$ of the macroscopic material point, independently on the grain orientation respect the loading axes.

The macroscopic response of the material point is extracted simply by averaging the responses of all the associated grains as illustrated in Fig. 3.1, where k labels a grain and ϕ_k denotes the initial orientation of grain k .

In the adaptation of the Taylor model to the thermo-mechanical case, it is assumed that there is no heat transfer between neighboring grains and the temperature evolution of each grain evolves as function of the local plastic work assuming an adiabatic condition. These conditions emulate very fast heating where the time associated to heat transfer from grain to grain is much larger than the time of the process under study. Under these approaches, the micro-

Fig. 3.1: Illustration of Taylor homogenization model.

and macro- fields are related as

$$\begin{aligned}\bar{\mathbf{F}} &= \mathbf{F}^{(k)} \\ \bar{\boldsymbol{\sigma}} &= \frac{1}{N_c} \sum_{k=1}^{N_c} \boldsymbol{\sigma}^{(k)} \\ \bar{\theta} &= \frac{1}{N_c} \sum_{k=1}^{N_c} \theta^{(k)}\end{aligned}\tag{3.1}$$

where N_c is the total number of grains/orientations in the representative polycrystal.

More complex mean-field models allow that each grain deforms independently based on its actual orientation. The viscoplastic self-consistent model (VPSC) is the most common approach within mean-field approaches [15, 16, 17] and due to its accuracy and relative simplicity can be used as constitutive equation of a polycrystal in macroscopic simulations [20]. However, mean-field approaches are not accurate enough for some purposes and full field homogenization schemes are preferred.

3.2 Computational homogenization

The full field homogenization approach is also called the computational homogenization approach. For polycrystalline materials, the computational homogenization approach is based on the numerical resolution of the governing equations at the microscopic level in a representative volume element (RVE) of the polycrystalline microstructure [18, 19]. Finite elements ([71, 72]) or other simulation approaches as FFT based algorithms ([73, 74, 75]) are used to solve the boundary value problem

As illustrated in Fig. 3.2, the RVE typically contains hundreds of grains, each

one with an assigned initial orientation and represented by a subset of microscale material points which define its shape. The collection of grains in the RVE is synthetically generated to be representative of the orientation distribution function (ODF) and the distribution of the grain sizes experimentally measured.

The macroscopic fields are obtained as the volume average of the microscopic fields obtained by the numerical resolution of a boundary value problem in the RVE. Compared to mean-field approaches, the computational homogenization approach is usually computationally more expensive but it accounts for a more detailed description of the microstructure and its evolution and the full resolution of the fields at the microscale result in a more accurate prediction of the macroscopic behavior of the material. For these reasons, this is the approach adopted in this chapter to study the response of polycrystalline Tantalum under uniaxial traction.

Fig. 3.2: Illustration of computational homogenization model.

The computational homogenization framework used here is based on solving numerically the weak form of the balance equation of linear momentum and the balance equation of thermal energy as given in Box 2.1 in the previous chapter, with periodic boundary conditions using the finite element method. The stress tensor and the temperature of a macroscopic material point are calculated, respectively, with the averages:

$$\begin{aligned}\bar{\mathbf{F}} &= \frac{1}{V} \int \mathbf{F} dV = \frac{\sum_{l=1}^{N_i} \mathbf{F}^{(l)} V^{(l)}}{\sum_{l=1}^{N_i} V^{(l)}}, \\ \bar{\boldsymbol{\sigma}} &= \frac{1}{V} \int \boldsymbol{\sigma} dV = \frac{\sum_{k=1}^{N_i} \boldsymbol{\sigma}^{(k)} V^{(k)}}{\sum_{k=1}^{N_i} V^{(k)}}, \\ \bar{\theta} &= \frac{1}{V} \int \theta dV = \frac{\sum_{k=1}^{N_i} \theta^{(k)} V^{(k)}}{\sum_{k=1}^{N_i} V^{(k)}},\end{aligned}\tag{3.2}$$

where N_i is the total number of integration points within the RVE and $V^{(l)}$ is the volume associated to the l -th integration point, which is obtained from its weight within the associated element and the volume of that element.

3.2.1 Generation of the Representative Volume Elements

Under the computational homogenization approach, one of the key ingredients for an accurate prediction of the behavior of polycrystalline materials is the precise reproduction of the associated microstructure with the RVE. RVE should contain a statistical sample of the actual grain size, shape and orientation distribution. The number of grains in the RVE should be sufficiently large to be representative of the grain size distribution and the orientation density function (ODF), providing the same symmetry in the mechanical response as the macroscopic material (i.e. isotropic response for a polycrystal with random texture).

Grain shapes in a polycrystal are well represented by a Voronoi tessellation in which the seeds can be set to mimic a target grain size distribution [33], which can be experimentally measured using optical microscopy or EBSD data. The procedure followed consists first in generating randomly N_c seed points in the RVE and then use these seed points to generate a Voronoi tessellation (performed here using the open source code Voropp [76]) to divide the RVE into n_c subdomains with each one representing a grain. With the volumes of these polyhedra, the numerical grain size distribution is obtained, as well as the quadratic error between this distribution and the target distribution. In a second step, a Monte Carlo process is used to modify the locations of the seed points until the error gets smaller than a given tolerance as summarized in a flowchart in Fig. 3.3. An example of a periodic RVE generated following the procedure introduced above is shown in Fig. 3.4. The error evolution during the Monte-Carlo process and the comparison of the grain size distribution in the generated RVE with the experimental one are also represented in Fig. 3.5.

Once the geometry is generated, the orientation of each grain, represented by three Euler angles as $\phi = (\phi_1, \phi_2, \phi_3)$, is randomly selected such that the RVE texture well represents the experimental ODF, usually obtained by X-ray diffraction or electron backscatter diffraction (EBSD) data [77, 78, 79]. In the case of uniform/isotropic texture (no preferential directions in the crystal orientations), the initial crystalline orientations are randomly distributed in the orientation space SO3.

The Finite Element model is constructed from the geometry generated by the Voronoi procedure. Two type of FE discretization have been considered, adaptive meshes and voxelized models. The first approach (Fig. 3.2) is used to represent the microstructure during the machining process (chapter 4). In this case the generated optimal Voronoi tessellation is exported and an unstructured mesh is generated with Gmsh [80] using triangular/tetrahedral in the cases of 2D/3D.

Fig. 3.3: Flowchart for generating a RVE with grain size following experimental distribution.

Fig. 3.4: Demonstration on a periodic RVE generated following the experimental grain size distribution.

The second approach, voxelized models, is performed by the discretizing the RVE in a regular array of hexahedral elements and rastering the Voronoi tessellation generated. This type of discretization is used in this chapter to simulate the thermomechanical response of polycrystals under uniaxial tension. Usually each grain is represented by tens or hundreds of elements. An example of a voxel-based RVE with 400 randomly distributed grains discretized by 30^3 elements is shown in Fig. 3.6. It must be noted that for any of the two discretization approaches considered, mesh convergence tests usually need to be performed to check the effect of the mesh size and the number of grains on the numerical results.

3.2.2 Periodic Boundary Conditions

The microstructure of a polycrystalline material can be idealized as an infinite periodic arrangement of RVEs. Under this approach, periodic boundary conditions need to be imposed to enforce shape compatibility between adjacent deformed RVEs as periodic boundary conditions reproduce exactly the deformation of an infinite media constructed by a periodic arrangement of the RVE. Moreover, it has been observed that, among the different boundary conditions that fulfill the Hill-Mandel condition, periodic boundary conditions give solutions that converge faster than any other to the solution of an infinite RVE [81]. For a cubic

Fig. 3.5: (a). Error evolution and (b). comparison on grain size distribution between the generated RVE and the experimental data

RVE, let P_i^+ be an arbitrary node lying on a boundary surface S_i^+ , and P_i^- be its counterpart lying on surface S_i^- , where S_i^+ and S_i^- are a pair of surfaces perpendicular to the X_i axis. According to the requirement of periodicity and continuity of boundary conditions, the deformations of nodes P_i^+ and P_i^- are linked by the multiple point constraints given by [82],

$$\mathbf{u}(P_i^+) - \mathbf{u}(P_i^-) = (\bar{\mathbf{F}} - \mathbf{I})\mathbf{L}_i = \mathbf{u}(M_i) - \mathbf{u}(O) \quad (i = 1, 2, 3), \quad (3.3)$$

where $\bar{\mathbf{F}}$ is the deformation gradient of the corresponding macroscopic material point, $\mathbf{L}_i$ is a vector with the length of the cubic RVE along the X_i axis and O and M_i being its two associated vertices. The vertex O is called the reference point and its deformation $\mathbf{u}(O)$ is set to zero for convenience.

In the case of the thermal problem, the use of periodic boundary conditions on temperature in the RVE also provides the microscopic temperature distribution in an idealized medium formed as an infinite periodic arrangement of the RVE. In this case, the corresponding equations are

$$\theta(P_i^+) - \theta(P_i^-) = \nabla \bar{\theta} \cdot \mathbf{L}_i = \theta(M_i) - \theta(O) \quad (i = 1, 2, 3), \quad (3.4)$$

where $\nabla \bar{\theta}$ is the temperature gradient of the macroscopic material point and $\mathbf{L}_i, M_i, O$ are as before.

From the macroscopic view point, two cases of interest can be analyzed with the periodic RVE, namely, adiabatic and isothermal processes. In the case of an adiabatic process the average temperature gradient $\nabla \bar{\theta}$ is equal to zero. In this case, Eq. (3.4) is reduced to

$$\theta(P_i^+) - \theta(P_i^-) = 0 \quad (i = 1, 2, 3). \quad (3.5)$$

Fig. 3.6: Example of a cubic RVE generated with the voxel-based method.

In standard constitutive models at the macroscale, the adiabatic condition assumes that the plastic work contributes to the macroscopic temperature increase locally and that its effect on the mechanical response is instantaneous. On the contrary when two scales are considered, the heat generation at the micro-scale is not uniform due to the inhomogeneous distributions of the stress, plastic strain and temperature fields caused by the heterogeneity of the microstructure. In this case thermal conduction exists between grains at the microscopic level even under macroscopic adiabatic conditions and the mechanical effect of the temperature at the macro-scale might not be instantaneous. Such a detailed description of the distribution and evolution of the temperature field within the RVE is obtained in this work by solving the thermo-mechanically coupled problem under the periodic boundary conditions given in Eqs. (3.3) and (3.5). The additional complexity of the coupled problem leads to a better prediction of the material behavior during thermo-mechanical processes, as compared to the conventional approaches.

The second case of interest is a macroscopic isothermal process. In this case, to ensure that the temperature of the macroscopic material point does not change in time, the average temperature increase of the associated RVE should be kept equal to zero at all times. This could be implemented simply by setting equal to zero the Taylor-Quinney factor χ defined in Eq. (2.14).

3.3 Numerical Methods

Under Taylor's homogenization model, the macroscopic deformation is prescribed and it is assumed that its value is equal to the deformation gradient of each crystal. Hence, there is no need to solve any boundary value problem at the microscale. The problem is reduced to solve, for each time increment, the system of non-linear equations defined by the constitutive equations as discussed in section 2.1.3, and the Taylor approach given by Eq. (3.1).

To obtain the macroscopic stress and temperature as function of the current deformation gradient, the backward Euler method is used to integrate the equations in time. The time interval of interest is divided into subintervals of size Δt . Let $\bar{\mathbf{F}}_{n+1}$ be the prescribed macroscopic deformation gradient at time $t = t_{n+1}$ and $\boldsymbol{\sigma}^{(k)}$ the stress in the k -th grain of the polycrystal. The problem to solve consists in finding for each grain k its stress $\boldsymbol{\sigma}^{(k)}$, temperature, $\theta^{(k)}$ and the internal variables $\boldsymbol{\psi}^{(k)}$ that satisfy the constitutive equation (2.4) at time t_{n+1} , that is,

$$\boldsymbol{\sigma}^{(k)} = \hat{\boldsymbol{\sigma}}\left(\mathbf{F}^{(k)}, \dot{\mathbf{F}}^{(k)}, \theta^{(k)}, \boldsymbol{\psi}^{(k)}\right) = \hat{\boldsymbol{\sigma}}\left(\bar{\mathbf{F}}_{n+1}, \dot{\bar{\mathbf{F}}}_{n+1}, \theta^{(k)}, \boldsymbol{\psi}^{(k)}\right). \quad (3.6)$$

The numerical scheme for updating the local stress of each grain in Eq. (3.6) is discussed in detail in Section 2.2.2.

The temperature at each grain, $\theta^{(k)}$ in Eq. (3.6) is computed from the local temperature at time t_n and its increment from t_n to t_{n+1} , denoted as $\Delta\theta^{(k)}$, using the thermal balance equation and neglecting heat conduction between grains. The resulting temperature of each grain reads

$$\theta^{(k)} = \theta_n^{(k)} + \Delta\theta^{(k)} = \theta_n^{(k)} + Q^{(k)}(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)})\Delta t / (\rho c). \quad (3.7)$$

A fixed-point iteration algorithm is used to solve, for each grain, the system of non-linear equations (3.6) and (3.7). The values of $\theta^{(k)}$ and $\boldsymbol{\psi}^{(k)}$ are initialized at the beginning of the time step with the corresponding values at the previous time and are updated iteratively. This iterative procedure is repeated until the differences of the stress and temperature between two consecutive iterations are below the given tolerances.

Once the non-linear equations are solved, the macroscopic stress $\bar{\boldsymbol{\sigma}}$ and the temperature $\bar{\theta}$ at the material point are computed as the average of the values in

each grain as

$$\begin{aligned}\bar{\boldsymbol{\sigma}} &= \frac{1}{N_c} \sum_{k=1}^{N_c} \boldsymbol{\sigma}^{(k)} \\ \bar{\theta} &= \frac{1}{N_c} \sum_{k=1}^{N_c} \theta^{(k)}\end{aligned}\tag{3.8}$$

For the computational homogenization approach, the stress field and the temperature field within the RVE are obtained from the thermo-mechanically coupled crystal plasticity finite element framework proposed in the previous chapter, and the deformation gradient $\bar{\mathbf{F}}$, the Cauchy stress $\bar{\boldsymbol{\sigma}}$ and the temperature $\bar{\theta}$ at the macroscopic material point are calculated by the volumetric averages of the corresponding quantities in the RVE as given in Eq. (3.2).

3.4 Numerical Analysis on Uniaxial Traction of Polycrystalline Tantalum

The computational homogenization framework combined with the implicit version of the thermo-mechanically coupled crystal plasticity finite element framework proposed in the previous chapter is applied to study the thermo-mechanical responses of a polycrystalline alloy under uniaxial traction. In this chapter, pure BCC tantalum is selected as a benchmark to validate the model since a full thermo-mechanical experimental campaign is available on the literature [83], which was also modelled using a Taylor model in [57].

The results obtained with this numerical framework will be compared at the end of this section with the response obtained using the Taylor homogenization approach.

A RVE with 400 randomly oriented grains is defined and discretized in hexahedral finite elements, as illustrated in Fig. 3.7. To determine the size of the models a mesh sensitivity study was done. In particular, simulations considering the macroscopic adiabatic condition were conducted using meshes containing 20^3 , 25^3 and 30^3 elements to check the effects of mesh. The comparative results on the macroscopic uniaxial stress and temperature in a tension process are shown in Fig. 3.8. It is observed that the difference of both the macroscopic temperature-strain curves and the stress-strain curves between the model with 20^3 mesh and 30^3 mesh are below 1%. In addition, the distributions of the Von Mises stress and the temperature within the RVE models with 20^3 mesh and 30^3 mesh are also compared as shown in Fig. 3.9. It could be observed that the mechanical and thermal fields at the microscopic scale were also very similar. These results

Fig. 3.7: Representative volume element of BCC Ta containing 400 randomly-oriented crystals discretized with 8000 cubic finite elements.

suggest that the mesh containing 20^3 elements is accurate enough, and this size is then used for the following part of this thesis. Moreover, to check the effect of the total number of grains in the RVE model on the numerical results, a pair of simulations were conducted, both using meshes containing 20^3 elements but one was divided with 400 grains and the other with 800 grains. The simulation results are plotted in Fig. 3.10. It is shown that the difference of the macroscopic temperature-strain curves and the stress-strain curves between the model with 400 grains and 800 grains are below 1% and 3%, respectively. This good agreement suggests that 400 is a number sufficiently large to provide statistically representative results and isotropic response, having also a better in-grain resolution.

The elastic moduli (in GPa) of this metallic material is approximated by a linear function of the temperature θ as follows [84]:

$$\begin{aligned} c_{11} &= 268.2 - 0.024 \theta, \\ c_{12} &= 159.6 - 0.011 \theta, \\ c_{44} &= 87.1 - 0.015 \theta. \end{aligned} \tag{3.9}$$

The density, the specific heat, the thermal conductivity and the thermal expansion

Fig. 3.8: Mesh convergence check on (a). uniaxial stress-strain and (b). Temperature elevation-strain curves with 20^3 , 25^3 and 30^3 elements within the RVE.

are taken to be $16.69 \times 10^3 \text{ Kg/m}^3$, $1.506 \times 10^8 \text{ J/(Kg} \cdot \text{K)}$, $57.5 \text{ W/(m} \cdot \text{K)}$ and $6.3 \times 10^{-6} \text{ K}^{-1}$, respectively.

Regarding the plastic response, in BCC metals three sets of slip systems are normally responsible of the plastic deformation, $\langle 111 \rangle \{110\}$, $\langle 111 \rangle \{112\}$ and $\langle 111 \rangle \{123\}$. In this work, only the first two slip sets are taken into consideration as proposed in [57] and the corresponding slip systems are listed in Table 2.3 in the previous chapter.

The experimental behavior of Tantalum was taken from [83], where an enhanced compression recovery split Hopkinson bar technique was used to obtain the plastic flow in wide range of strains, strain rates, and temperatures during uniaxial compression. In particular, the model parameters defining both flow and hardening models were adjusted to fit the stress-strain response of the polycrystalline RVE with the experimental result for uniaxial traction under isothermal condition in [83].

This fitting procedure used in the study started using as an initial guess the set of parameters for the flow and hardening model in [57], who model these experiments using a Taylor approach and a similar crystal plasticity model. It must be noted that the resulting parameters using computational homogenization are different to the ones obtained in [57] because Taylor model gives an upper bound for the stress predictions. The resulting set of parameters obtained are listed in Table 3.1.

To assess the validity of the fitting procedure, the parameters listed in Table 3.1 (fitted using isothermal experiments) are used in the numerical framework to predict the stress-strain response of the RVE under an adiabatic condition. The numerical results and corresponding experimental values obtained from [83] are plotted in Fig. 3.11. It is shown that the numerical predictions provided by the

Fig. 3.9: Mesh convergence check on distributions of (a). Von Mises stress with 20^3 elements, (b). Von Mises stress with 30^3 elements, (c). Temperature with 20^3 elements, and (d). Temperature with 30^3 elements within the RVE models.

current work are in good agreement with the experimental results, which validates the reliability of the framework proposed.

3.4.1 Effect of initial orientation

To study the effect of the initial orientation on the response of single crystal Ta, a single crystal RVE is created and discretized into $20 \times 20 \times 20$ regular finite elements, as in the first simulation. The solid is strained at three different crystalline directions $[1\ 0\ 0]$, $[1\ 1\ 0]$ and $[1\ 1\ 1]$. The uniaxial stress-strain curves and the temperature changes at these directions during traction processes under adiabatic condition are plotted in Fig. 3.12.

It is shown that the response of the single crystal is strongly dependent on the traction direction, being the strength obtained when loading in direction $[1\ 1\ 1]$ the highest of all the three cases. In the model, the same value of s_{at} and

Fig. 3.10: Mesh convergence check on (a). uniaxial stress-strain and (b). Temperature elevation-strain curves with RVE model containing 400 grains and 800 grains.

Table 3.1: Material Properties of BCC Ta

Model Parameter	Value
ΔF^α	$2.77 \cdot 10^{-19} \text{ J}$
$\dot{\gamma}_0$	$1.732 \cdot 10^7 \text{ s}^{-1}$
h_0	181 MPa
s_s	121 MPa
r_1	1.10
p	0.28
q	1.40
$s_{at,0}$	50.0 MPa
$s_{t,0}$	445 MPa

s_t are chosen for all the slip systems so the result obtained is simply due to the Schmidt factor of the systems. In particular, when loading in a $[1\ 1\ 1]$ direction the Schmidt factor of the best oriented planes is lower than in the other two loading directions and therefore, the material plastifies at a larger applied stress.

The effect of loading direction in the thermal response of the single crystal can be observed in Fig. 3.12. The temperature rises faster when loading in the $[111]$ direction and this is due to the higher strength in this direction. Heat generation is proportional to the plastic dissipation which rate depends on the sum of the product of resolved stress and shear rates on all the systems (Eq. (2.116)). Because the accumulated plastic shear is the same for all the three loading directions, the temperature increases faster when pulling in the $[111]$ direction due to its larger strength.

Fig. 3.11: Comparison of experimental and predicted stress-strain responses of BCC Ta during uniaxial traction.

3.4.2 Effect of initial temperature

To study the effect of the initial temperature on the thermo-mechanical behavior of polycrystalline Ta, the RVE is strained at three different initial temperatures: 298 K, 398 K, and 498 K with an engineering strain rate of 5000 s^{-1} . Two sets of simulations are performed, under isothermal conditions and under adiabatic conditions in order to quantify the effect of considering heat generation during the test. The numerical results of the mechanical response of both type of tests are plotted in Fig. 3.13(a). It can be observed that the effect of the initial temperature is a decrease in the material strength. In the isothermal case, all the three curves are proportional and hardening is not affected by the initial temperature. Under adiabatic conditions, the material plastifies at the same stress than as in the corresponding isothermal case but the stress-strain curve deviates with the strain showing less hardening. Moreover, in contrast with the isothermal case, the effective hardening rate increases when decreasing the initial temperature. The reason of this behavior can be found in the heat generation due to plastic dissipation. As it can be observed in Fig. 3.13(b) the temperature rise is higher for the lowest temperature due to the higher value of the strength (as it happened when analyzing the effect of loading direction). This temperature increase produces a softening of the material that is more evident for the lower initial temperature where the differences between isothermal and adiabatic cases are maximal. The resulting behavior is in agreement with the experimental observations showing a reduction of the strength for BCC Ta as a function of the initial temperature.

Fig. 3.12: (a). Uniaxial stress-strain and (b). Temperature change-strain curves of single crystalline BCC Ta during uniaxial traction at various crystallographic directions

Fig. 3.13: (a). Stress- (b). Temperature change-strain curves of BCC Ta during uniaxial traction at various initial temperatures

3.4.3 Effect of strain rate

To study the effect of the strain rate on the behavior of polycrystal Ta, the RVE is strained at three different engineering strain rates: $5 \cdot 10^{-3}$, 5, and $5 \cdot 10^3 \text{ s}^{-1}$, all of them at 298K and under adiabatic conditions. The stress-strain response of the polycrystal for the three strain rates considered are plotted in Fig. 3.14(a). In this figure the effect of the strain rate can be clearly observed, the strength of the polycrystal increases when increasing the strain rate applied. These results are in quantitative agreement with the experimental results in [83]. The hardening effect is due to the elasto-visco-plastic nature of the CP selected and shows that increasing the strain rate is equivalent to reducing the temperature. The large differences found in the initial yield indicate a high strain rate sensitivity of the model for the energy parameters chosen even at room temperature. The effect of the strain rate in the thermal response of the polycrystal can be observed

in Fig. 3.14(b) where the temperature increase is represented as a function of the applied strain for the three strain rates considered. The larger strain rates result in higher values of the effective strength and, as a consequence, the plastic dissipation increases and the temperature increases faster. It is interesting to note that the current framework is able to reproduce the analogous effect of decreasing the applied strain rate or increasing the initial temperature in both the mechanical response and in the temperature evolution.

Fig. 3.14: (a). Stress- (b). Temperature change-strain curves of BCC Ta during uniaxial traction tests at various engineering strain rates

3.4.4 Effects of considering heat conduction at the microscale

Conventional approaches of thermo-mechanical coupled crystal plasticity often neglect the heat transfer. To study the effect of heat transfer on the responses of BCC Ta, comparative simulations were carried out to study the responses of the RVE during uniaxial traction tests, under macroscopic adiabatic conditions. Two different cases are considered, one where heat conduction at the microscale is considered and a second one where heat transfer is disabled also at the microscopic level. The maximum, minimum, and average value of the microscopic temperature field obtained for the three strain rates considered are given in Table 3.2. When heat diffusion is considered, it can be observed that for the two smallest strain rates, namely 5s^{-1} and $5 \cdot 10^{-3}\text{s}^{-1}$, the temperature distribution on the microstructure is homogeneous. In contrast, when microscopic heat conduction is not allowed (microscopic adiabatic condition), temperature distributions are heterogeneous and the differences between the maximum and minimum local temperatures are 83 K and 63 K, respectively, for the two strain rates. In contrast, for the highest strain rate ($5 \cdot 10^3\text{s}^{-1}$) the full model with diffusion predicts an het-

	$\dot{\epsilon} = 5000 \text{ s}^{-1}$		$\dot{\epsilon} = 5 \text{ s}^{-1}$		$\dot{\epsilon} = 0.005 \text{ s}^{-1}$	
	No diff.	Full model	No diff.	Full model	No diff.	Full model
T_{min} (K)	304.2	316.3	302.3	333.2	300.9	324.5
T_{max} (K)	422.8	401.2	385.1	333.5	364.0	324.5
T_{ave} (K)	349.1	349.1	333.2	333.3	324.4	324.5

Table 3.2: Maximum, minimum, and average local temperatures considering heat diffusion (full model) or a microscopic adiabatic condition (no diffusion)

erogeneous temperature distribution. This is an important result of the model because it shows that a characteristic time scale is introduced. Then, when strain rates are low, temperature becomes homogeneous, while for fast deformations the material behaves almost as microscopic-adiabatic.

To further analyze this behavior, the temperature field distribution at the end of the tensile simulation for the case at a nominal strain rate of 5000 s^{-1} is plotted in Fig. 3.15(a) for the case in which thermal conduction is considered and (b) for the microscopic-adiabatic case. Both figures show an heterogeneous distribution of the temperature due to the non-homogeneous distribution of the plastic deformation within the RVE. In both cases, the temperature hot-spots are the points in which plastic dissipation is maximum and correspond to the regions in which plastic strain is localized, near grain boundary or triple points. The comparison between the two figures suggests that the heat transfer plays a smoothing role, as expected. Allowing heat transfer at the microscale diffuses the temperature near the hottest points of the microstructure and the temperature gradients in Fig. 3.15(a) are reduced in comparison to the case without transfer, as shown in Fig. 3.15(b). This redistribution is very incipient here (time is $5 \cdot 10^{-5} \text{ s}$) and temperature heterogeneities are still significant, but the heterogeneities disappear for larger times, as it happens at the end of the tests at 5 s^{-1} and $5 \cdot 10^{-3} \text{ s}^{-1}$ (Table 3.2).

3.4.5 Comparison with Taylor homogenization model

To illustrate the difference between the results obtained using the full-field computational homogenization approach proposed in this work and the Taylor model, the cases studied in the previous sections are now simulated using this last approximation. In particular, the model was used to simulate uniaxial tensile tests performed at nominal strain rates of 0.005 , 5.0 and 5000 s^{-1} , under both macroscopic adiabatic and isothermal conditions. The initial temperature was chosen to be 298 K in all cases.

The polycrystal was represented using 400 grains and the orientations of these grains were exactly the same as those in the RVE. The model parameters were

Fig. 3.15: Temperature distributions of BCC Ta during uniaxial traction tests at $\dot{\epsilon} = 5.0 \cdot 10^3 \text{ s}^{-1}$ under cases (a). with heat transfer and (b). without heat conduction

also the same as in previous simulations. The results under isothermal conditions are represented in Fig. 3.16. It can be observed that, for all the strain rates considered, the Taylor model produces a stiffer stress-strain response compared with the results obtained by the computational homogenization approach. The stiffer response of the Taylor model is well known and is due to the iso-strain assumption. This approach imposes that grains badly oriented for accommodating the plastic deformation deform identically to well oriented grains, artificially increasing their elastic strain level and therefore their contribution to the macroscopic stress. It must be noted that in the isothermal case the temperature does not play any role and the differences between (a), (b) and (c) are only due to the strain rate sensitivity of the crystal plasticity model.

The results obtained for macroscopic adiabatic conditions are represented in Fig. 3.17. It is shown that, similar to the isothermal case, under an adiabatic condition Taylor model still gives stiffer stress-strain response compared with the computational homogenization approach. However, the difference in strength between Taylor model and computational homogenization for this adiabatic condition is slightly smaller than the difference obtained under isothermal conditions. This small weakening of the Taylor model respect the computational homogenization approach may be due to higher heat generated from overestimated stress response, which further produces a higher temperature and in return softens the stress response.

More interesting is the comparison of the temperatures obtained using the two homogenization approaches at the end of the simulation as listed in Table 3.3. First, as pointed out in the previous section, it can be observed that allowing heat diffusion at the microscale influences the local temperature distribution. This re-

Fig. 3.16: Comparison of stress-strain curves obtained by computational homogenization approach and Taylor model of BCC Ta during uniaxial tensile tests at various engineering strain rates and isothermal conditions. (a). $\dot{\epsilon} = 5.0 \cdot 10^3 \text{ s}^{-1}$ (b). $\dot{\epsilon} = 5.0 \text{ s}^{-1}$ (c). $\dot{\epsilon} = 5.0 \cdot 10^{-3} \text{ s}^{-1}$

distribution of temperature has an effect on the local behavior and therefore on the actual macroscopic response. In contrast with this effect, it can be observed that in the Taylor approach temperature differences persist for every strain rate. This is due to the grain-adiabatic condition used in the Taylor model that does not allow heat redistribution within the grains, similarly to what happened when microscopic adiabatic condition was used in the computational model. In summary, the use of a Taylor approach results in a stiffer response and in a time-independent artificial temperature heterogeneity that might influence the mechanical results.

Table 3.3: Comparison of Temperature Distribution in Polycrystal Obtained by Taylor and Computational Homogenization

	$\dot{\epsilon} = 5000 \text{ s}^{-1}$		$\dot{\epsilon} = 5 \text{ s}^{-1}$		$\dot{\epsilon} = 0.005 \text{ s}^{-1}$	
	Taylor	Comp.	Taylor	Comp.	Taylor	Comp.
T_{min} (K)	340.7	316.3	327.4	333.2	319.8	324.5
T_{max} (K)	368.8	401.2	347.3	333.5	335.4	324.5
T_{ave} (K)	353.8	349.1	336.7	333.3	327.2	324.5

Fig. 3.17: Comparison of stress-strain curves obtained by computational homogenization approach and Taylor model of BCC Ta during uniaxial tensile tests at various engineering strain rates and adiabatic conditions. (a). $\dot{\epsilon} = 5.0 \cdot 10^3 \text{ s}^{-1}$ (c). $\dot{\epsilon} = 5.0 \text{ s}^{-1}$ (e). $\dot{\epsilon} = 5.0 \cdot 10^{-3} \text{ s}^{-1}$

CHAPTER 4

Application to Orthogonal Cutting of Ferrite-pearlite Steel

4.1 Motivation

Machining, or metal cutting, is one of the most commonly used manufacturing operations for producing industrial components with high-precision dimensions and smooth surfaces by the removal of unwanted material from a metallic workpiece. Due to its crucial importance in modern industry, many attempts have been made to gain an in-depth understanding of the mechanisms behind this process. Moreover, there is a big scientific and technological interest in developing predictive simulation frameworks which allows to link the machining parameters with output variables such as cutting and feed forces, temperature on the cutting zone, contact length and chip morphology. These frameworks will help to optimize the machining conditions leading to a notable enhancement of the product quality, an improvement of manufacturing productivity and the reduction of economical cost.

The typical simulation approach for the machining process is based on coupled thermo-mechanical implementations of the finite element method due to their capacity to account for contact, large deformations, fracture as well as heat generation and conduction. Three different approaches are usually followed for simulating the machining process, namely the Lagrangian method, Arbitrary Lagrangian Eulerian (ALE) method and Coupled Eulerian Lagrangian (CEL) method, as have been comparatively introduced in Chapter 1. The pure Lagrangian method requires an element deletion criterion to delete excessive distorted elements and enable the formation of chip but the results of the simulations might depend on the specific expressions and parameters of the chosen criterion. The ALE method is based on remeshing of elements with poor aspect ratio and in CEL method the material of the workpiece independently flows on the fixed Eulerian mesh avoiding distortion. However, ALE and CEL method are computationally more complex

and expensive and simulations are generally limited to 2D cases.

Under any of these three approaches, the improvement of the fidelity and predictive capacity of the simulations implies the use of realistic constitutive models specially suited for the raw material under study. In particular, the incorporation of the effect of the material micro-heterogeneity on the process is crucial for the improvement of the simulation accuracy. Only a few recent studies can be found in this direction. In [85] the microstructure of a ferrite-pearlite dual-phase steel was explicitly introduced in the simulations using differentiated properties for each phase and CEL approach. The model was able to account for the effect microstructure in the tool wear, but the material model considered for both phases was a phenomenological macroscopic approach and the possible effect of the anisotropy of the perlite was not considered. In [86], a similar approach was followed for austempered ductile iron, while in [87], a two-phase steel AISI 1045 was studied also considering the microstructure explicitly, but using simple Johnson-cook models for the two phases. The use of more physically based constitutive models is also taking interest in the simulation of machining. For example in [88] a physically based model was used to model the flow stress of a ferrite-perlite steel including strain hardening, thermal softening and strain rate hardening based on microstructure parameters and mechanisms. This study is a first important step in linking microscopic deformation mechanisms with the response during machining but due to the complex response, microstructure is not explicitly considered. To account for the possible influence of microstructural heterogeneities, recently the crystal plasticity theory has been applied to the simulation of cutting processes. For instance, In [89] a 2D cutting simulation in small deformation was carried out and in [90] the crystal plasticity theory was applied to study the cutting process of Ti alloys.

In this chapter, the crystal plasticity thermo-mechanical simulation framework proposed in previous chapters will be used to simulate the orthogonal cutting of a low carbon steel C45, a typical ferrite-pearlite steel under various machining conditions. A Lagrangian method will be employed and the alloy microstructure will be considered explicitly. Finally, as first time in this type of simulation, a physically based crystal plasticity approach will be used for the mechanical behavior of the two phases. The crystal plasticity model will account for the elastic and plastic anisotropy in the deformation of each phase considering large strains, high strain rates and the effect of temperature on their mechanical response. The thermo-mechanical model is introduced into ABAQUS/Explicit as a user defined subroutine VUMAT. Some of the simulation results will be compared with the experimental ones reported by Mikel et.al. [91].

4.2 Microstructure informed constitutive model for ferrite-pearlite steels

4.2.1 Microstructure of ferrite-pearlite steels

The microstructure of ferrite-pearlite steel is experimentally characterized as pearlite blocks surrounded by ferrite crystal grains. A pearlite block contains several lamella-structured pearlite colonies composed by cementite phase and ferrite phase and the mechanical behavior of a pearlite colony is dependent on the number of lamellas and the inter-lamella spacing. This hierarchical microstructure is shown in Fig. 4.1 [92].

Fig. 4.1: Microstructures of (a) ferrite-pearlite steel and (b) pearlite block

The typical length scale for the geometry model in a finite element simulation of machining process is about 1.0 mm and the element size is about 10 μm , which is comparable to the actual grain size of ferrite crystals or pearlite colonies. Thus in the model, the workpiece will be divided into a set of ferrite grains and pearlite blocks following the experimentally observed microstructure of ferrite-pearlite steel in a statistical sense. Ferrite grains will be considered as single crystals with a BCC lattice and their behavior will be accounted using a CP model. Pearlite colonies will be modeled using a homogenization approach in which the behavior of the full multilayered phase will be represented by a lamella of cementite and one lamella of ferrite, as illustrated in Fig. 4.2. The orientation of the BCC lattice of the ferrite grains will be randomly generated. The orientation of the pearlite block, considered as the normal to the ferrite/cementite lamellas, will also be set randomly, but the orientation of the ferrite within the pearlite colony is determined by the crystalline orientation relationship between ferrite phase and

cementite phase [92]

$$(0, 0, 1)_c // (2, 1, 1)_f, \quad [1, 0, 0]_c // (0, \bar{1}, 1)_f, \quad [0, 1, 0]_c // (\bar{1}, 1, 1)_f \quad (4.1)$$

Fig. 4.2: Illustration of microstructure of pearlite colony

Let V^c be the volume fraction of the cementite phase in the pearlite colony. According to the steel-carbon equilibrium diagram, the overall carbon content in the pearlite colony is estimated to be about wt. 0.76%, and from the chemical composition of the cementite (Fe_3C), the resulting carbon content in cementite phase is about wt. 6.69%. Thus a carbon equilibrium equation can be written as,

$$0.76 [(1.0 - V^c) \rho^f + V^c \rho^c] = 6.69 V^c \rho^c \quad (4.2)$$

where

$$\rho^f = 7.85 g/cm^3, \quad \rho^c = 7.68 g/cm^3 \quad (4.3)$$

are the densities of ferrite phase and cementite phase, respectively. By solving Eq. (4.2) and Eq. (4.3), the resulting volume fraction of the cementite phase in pearlite colony V^c is determined to be around 11.6%.

Once the microstructure of the steel and its approximation for the present simulations are described, constitutive equations for each of the materials or phases considered should be derived. As mentioned above, the hierarchical microstructure of ferrite-pearlite steel is composed by two phases, the pearlite colony and the ferrite grains being the former composed by two materials, ferrite and cementite. Therefore, the constitutive equations for the ferrite and the cementite will be presented together with the homogenization approach to obtain the response of the pearlite colony from the other two materials.

4.2.2 Constitutive Model for Single Crystalline Ferrite

The crystal plasticity constitutive model implemented in Chapter 2 is directly employed here to describe the constitutive relation of single crystalline ferrite and the ferrite phase in the pearlite colony. As the ferrite grain has a BCC structure, the slip systems listed in Table. 2.3 are also used here. The physically based flow rule and the Brown's hardening law are employed. Numerical scheme for update of Cauchy stress and volumetric heat generation could be found in detail in section 2.2.2.

4.2.3 Constitutive Model for Cementite

For simplicity, cementite phase is described with the Mises plasticity model with isotropic hardening. In elastic stage, the stress increment $\Delta\sigma$ is expressed in terms of strain increment $\Delta\epsilon$ as,

$$\Delta\sigma = 2\mu\Delta\epsilon + \lambda \text{tr}(\Delta\epsilon) \quad (4.4)$$

where λ and μ are Lamé constants and can be derived from the Young's modulus E^c and the shear modulus G^c by

$$\lambda = \frac{G^c(E^c - 2G^c)}{3G^c - E^c}, \quad \mu = G^c \quad (4.5)$$

The yield stress σ^y is expressed in terms of the effective plastic strain $\bar{\epsilon}^p$ as,

$$\sigma^y = \sigma_0 + E^p \bar{\epsilon}^p \quad (4.6)$$

where σ_0 is the initial yield stress and E^p is the hardening modulus.

The conventional elastic prediction and radial return scheme is employed for update of stress at each time increment $n+1$. First, an elastic response is assumed and a trial stress is predicted as,

$$\sigma^{pr} = \sigma_n + 2\mu\Delta\epsilon + \lambda \text{tr}(\Delta\epsilon) \quad (4.7)$$

The deviatoric trial stress is calculated as:

$$\mathbf{S}^{pr} = \sigma^{pr} \mathbf{I} - \text{tr}(\sigma^{pr}) \mathbf{I} \quad (4.8)$$

Then the yield function is given as,

$$f = \bar{\sigma} - \sigma_n^y \quad (4.9)$$

where

$$\bar{\sigma} = \frac{1}{2} \mathbf{S}^{pr} : \mathbf{S}^{pr} \quad (4.10)$$

is the Von. Mises stress.

If the yield function is less than zero, which indicates that the material point lies in the elastic regime, the plastic strain increment is zero and the predicted stress is accepted as the stress measure at the new time step as

$$\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}^{pr}. \quad (4.11)$$

Otherwise, the effective plastic strain increment is determined by

$$\Delta \bar{\varepsilon}^p = \frac{\bar{\sigma} - \sigma_n^y}{3\mu + E^p}, \quad (4.12)$$

and the yield stress is updated from the newly obtained effective plastic strain increment as,

$$\sigma_{n+1}^y = \sigma_n^y + E^p \Delta \bar{\varepsilon}^p. \quad (4.13)$$

The deviatoric stress can then be calculated by scaling the predicted one back to the yield surface as,

$$\mathbf{S}_{n+1} = \frac{\sigma_{n+1}}{\sigma_{n+1} + 3\mu \Delta \bar{\varepsilon}^p} \mathbf{S}^{pr} \quad (4.14)$$

Finally, The stress is calculated by

$$\boldsymbol{\sigma}_{n+1} = \mathbf{S}_{n+1} + \text{tr}(\boldsymbol{\sigma}^{pr}) \mathbf{I}. \quad (4.15)$$

The volumetric heat generation rate contributed from plastic dissipation can be calculated from Eq. (2.14) by,

$$Q^c = \chi \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p \quad (4.16)$$

where $\dot{\boldsymbol{\varepsilon}}^p$ is the plastic strain rate and is calculated during the above stress update procedure.

4.2.4 Constitutive Model for Pearlite Colonies

As previously mentioned, the behavior of a full pearlite colony will be accounted by homogenization. The pearlite is represented as a perfect layered structure, and

the macroscopic stress and strains of the colony will be obtained as the volume average of their counterparts in the ferrite and cementite phases. The distribution of the fields in each phase will be obtained exactly by solving the stress equilibrium and deformation compatibility of a two-layer structure with a perfect interface (iso-stress or iso-strain conditions depending on the field component), as described below.

Let $\boldsymbol{\sigma}^c$ and $\boldsymbol{\sigma}^f$ respectively be the stresses of the cementite phase and the ferrite phase in a material point of pearlite colony and $\boldsymbol{\sigma}$ be its overall stress, and $\boldsymbol{\varepsilon}^c$, $\boldsymbol{\varepsilon}^f$ and $\boldsymbol{\varepsilon}$ be the corresponding strain measures. The overall stress and strain increments of pearlite colony could be approximated as the volumetric average of the corresponding stress and strain increments of cementite phase and ferrite phase as

$$\Delta \boldsymbol{\sigma} = V^c \Delta \boldsymbol{\sigma}^c + (1 - V^c) \Delta \boldsymbol{\sigma}^f, \quad (4.17a)$$

$$\Delta \boldsymbol{\varepsilon} = V^c \Delta \boldsymbol{\varepsilon}^c + (1 - V^c) \Delta \boldsymbol{\varepsilon}^f. \quad (4.17b)$$

Under a cartesian coordinate systems $Ox_1x_2x_3$ defined in the corotational configuration as illustrated in Fig. 4.2, for thermo-viscoplastic constitutive models, assuming that the constitutive models for both cementite phase and ferrite phase could be generally written in an incremental form as

$$\Delta \boldsymbol{\sigma}^c = \mathbf{D}^c \Delta \boldsymbol{\varepsilon}^c + \Delta \boldsymbol{\sigma}^{ct}, \quad (4.18a)$$

$$\Delta \boldsymbol{\sigma}^f = \mathbf{D}^f \Delta \boldsymbol{\varepsilon}^f + \Delta \boldsymbol{\sigma}^{ft}, \quad (4.18b)$$

where $\mathbf{D}^c$ and $\mathbf{D}^f$ are the elastic plastic stiffness matrices of cementite phase and ferrite phase, respectively, $\Delta \boldsymbol{\sigma}^{ct}$ and $\Delta \boldsymbol{\sigma}^{ft}$ are thermal stress increments for the two phases. These four quantities are updated at every time increment by corresponding constitutive models of the two phases as will be discussed later.

Under this corotational coordinates system, where the interface of the two phases is parallel to the Ox_1x_2 plane, the tangential and normal components of stress and strain measures of pearlite colony could be written as

$$\mathbf{Y}_{\parallel} := (Y_{11}, Y_{22}, Y_{12})^T, \quad \mathbf{Y}_{\perp} := (Y_{33}, Y_{13}, Y_{23})^T \quad (4.19)$$

where $\mathbf{Y}$ can represent $\boldsymbol{\sigma}^c$, $\boldsymbol{\sigma}^{ct}$, $\boldsymbol{\sigma}^f$, $\boldsymbol{\sigma}^{ft}$, $\boldsymbol{\sigma}$, $\boldsymbol{\varepsilon}^c$, $\boldsymbol{\varepsilon}^f$ or $\boldsymbol{\varepsilon}$.

On the interface of the two phases, to avoid relative sliding, the strain components along the interface plane need to be compatible as,

$$d\boldsymbol{\varepsilon}_{\parallel}^c = d\boldsymbol{\varepsilon}_{\parallel}^f \quad (4.20)$$

And to avoid relative separation of the two phases, the stress components along the normal direction of the plane should satisfy,

$$d\sigma_{\perp}^c = d\sigma_{\perp}^f \quad (4.21)$$

For each material point, the overall strain increment $d\epsilon$ is known, while the overall stress increment $d\sigma$ as well as both the strain increment and stress increment of ferrite phases and the cementite phase are unknown, which leaves us $6 \times 5 = 30$ independent unknowns in total. Eqs. (4.17a)-Eqs. (4.21) provide a set of exactly 30 linear equations. Thus the overall stress increment of the pearlite colony could be obtained as below.

First, Eq. (4.18a) could be rearranged as,

$$\begin{Bmatrix} \Delta\sigma_{\parallel}^c \\ \Delta\sigma_{\perp}^c \end{Bmatrix} = \begin{bmatrix} A_1^c & A_2^c \\ A_3^c & A_4^c \end{bmatrix} \begin{Bmatrix} \Delta\epsilon_{\parallel}^c \\ \Delta\epsilon_{\perp}^c \end{Bmatrix} + \begin{Bmatrix} \Delta\sigma_{\parallel}^{ct} \\ \Delta\sigma_{\perp}^{ct} \end{Bmatrix} \quad (4.22)$$

where

$$\begin{aligned} A_1^c &= \begin{bmatrix} D_{1111}^c & D_{1122}^c & D_{1112}^c \\ D_{2211}^c & D_{2222}^c & D_{2212}^c \\ D_{1211}^c & D_{1222}^c & D_{1212}^c \end{bmatrix}, \\ A_2^c &= \begin{bmatrix} D_{1133}^c & D_{1123}^c & D_{1131}^c \\ D_{2233}^c & D_{2223}^c & D_{2231}^c \\ D_{1233}^c & D_{1223}^c & D_{1231}^c \end{bmatrix}, \\ A_3^c &= \begin{bmatrix} D_{3311}^c & D_{3322}^c & D_{3312}^c \\ D_{2311}^c & D_{2322}^c & D_{2312}^c \\ D_{3111}^c & D_{3122}^c & D_{3112}^c \end{bmatrix}, \\ A_4^c &= \begin{bmatrix} D_{3333}^c & D_{3323}^c & D_{3331}^c \\ D_{2333}^c & D_{2323}^c & D_{2331}^c \\ D_{3133}^c & D_{3123}^c & D_{3131}^c \end{bmatrix}. \end{aligned} \quad (4.23)$$

Remembering that

$$\Delta\sigma_{\perp}^c = \Delta\sigma_{\perp}, \quad \Delta\epsilon_{\parallel}^c = \Delta\epsilon_{\parallel}, \quad (4.24)$$

Eq. (4.22) could be rewritten as,

$$\begin{Bmatrix} \Delta\sigma_{\parallel}^c \\ \Delta\epsilon_{\perp}^c \end{Bmatrix} = \mathbf{B}^c \begin{Bmatrix} \Delta\sigma_{\perp} \\ \Delta\epsilon_{\parallel} \end{Bmatrix} + \mathbf{R}^c \quad (4.25)$$

where

$$\mathbf{B}^c = \begin{bmatrix} A_2^c (A_4^c)^{-1} & A_1^c - A_2^c (A_4^c)^{-1} A_3^c \\ (A_4^c)^{-1} & -(A_4^c)^{-1} A_3^c \end{bmatrix}, \quad \mathbf{R}^c = \begin{Bmatrix} \Delta\sigma_{\parallel}^{ct} - A_2^c (A_4^c)^{-1} \Delta\sigma_{\perp}^{ct} \\ -(A_4^c)^{-1} \Delta\sigma_{\perp}^{ct} \end{Bmatrix} \quad (4.26)$$

Similarly, for ferrite phase, four matrix blocks A^f equivalent to eqs. (4.23) can be defined from the tangent behavior. Using the same orientation considerations than in the case of cementite, we have

$$\begin{Bmatrix} \Delta \sigma_{\parallel}^f \\ \Delta \epsilon_{\perp}^f \end{Bmatrix} = \mathbf{B}^f \begin{Bmatrix} \Delta \sigma_{\perp} \\ \Delta \epsilon_{\parallel} \end{Bmatrix} + \mathbf{R}^f \quad (4.27)$$

where

$$\mathbf{B}^f = \begin{bmatrix} A_2^f (A_4^f)^{-1} & A_1^f - A_2^f (A_4^f)^{-1} A_3^f \\ (A_4^f)^{-1} & - (A_4^f)^{-1} A_3^f \end{bmatrix}, \mathbf{R}^f = \begin{Bmatrix} \Delta \sigma_{\parallel}^{ft} - A_2^f (A_4^f)^{-1} \Delta \sigma_{\perp}^{ft} \\ - (A_4^f)^{-1} \Delta \sigma_{\perp}^{ft} \end{Bmatrix} \quad (4.28)$$

Combining Eq. (4.25) and Eq. (4.27) and making use of Eq. (4.17a) and Eq. (4.17b), we have

$$\begin{Bmatrix} \Delta \sigma_{\parallel} \\ \Delta \epsilon_{\perp} \end{Bmatrix} = \mathbf{B} \begin{Bmatrix} \Delta \sigma_{\perp} \\ \Delta \epsilon_{\parallel} \end{Bmatrix} + \mathbf{R} \quad (4.29)$$

where

$$\begin{aligned} \mathbf{B} &= V^c \mathbf{B}^c + (1 - V^c) \mathbf{B}^f, \\ \mathbf{R} &= V^c \mathbf{R}^c + (1 - V^c) \mathbf{R}^f. \end{aligned} \quad (4.30)$$

which finally leads to the expression of the increment of the overall stress with the increment of the overall strain as,

$$\begin{Bmatrix} \Delta \sigma_{\parallel} \\ \Delta \sigma_{\perp} \end{Bmatrix} = \begin{bmatrix} B_2 - B_1 B_3^{-1} B_4 & B_1 B_3^{-1} \\ -B_3^{-1} B_4 & B_3^{-1} \end{bmatrix} \begin{Bmatrix} \Delta \epsilon_{\parallel} \\ \Delta \epsilon_{\perp} \end{Bmatrix} + \begin{bmatrix} \mathbf{I} & -B_1 B_3^{-1} \\ \mathbf{0} & B_3^{-1} \end{bmatrix} \mathbf{R}. \quad (4.31)$$

The overall heat generation rate, which will be contributed as a heat source to the temperature field, could be approximated as the volume average of the heat generation rate of the two phases as,

$$Q = V^c Q^c + (1 - V^c) Q^f. \quad (4.32)$$

For each phase the heat generation rate could be obtained by the corresponding constitutive model, as previously discussed.

4.2.5 Model Parameters Calibration

The elastic behavior for both the ferrite phase and the cementite phase are temperature dependent. However, a detailed characterization of this temperature dependency is not available for the two phases, so for simplicity the elastic

behavior is considered temperature independent. In the case of cementite the Young's Modulus and shear modulus are taken as [93]

$$E^c = 210GPa, \quad G^c = 80GPa. \quad (4.33)$$

For the single crystals of ferrite phase, the components of elastic modulus at room temperature are used as representative of all the temperature range, and are taken from the database [84]

$$C_{11}^f = 230GPa, \quad C_{12}^f = 130GPa, \quad C_{44}^f = 110GPa. \quad (4.34)$$

The plastic response of the cementite phase, as mentioned above, is represented with the Mises plasticity model with isotropic hardening. For simplicity, it is considered that this response is also temperature independent so the initial yield stress and the hardening modulus are taken constant with values $\sigma_0 = 2200MPa$ and $E_p = 600MPa$, which are estimated from the stress-strain curves in [94]. It is expected that these assumptions will not have a strong influence in the machining simulations, since the elastic response has a limited effect for the large strains reached. The thermal material properties are considered identical for the two phases and temperature dependent as [91]

Table 4.1: Thermal Material Properties for Ferrite-pearlite Steels

Material Properties	Value
$\rho \text{ (Kg} \cdot \text{m}^{-3}\text{)}$	7765(293K), 7685(473K), 7535(973K)
$K \text{ (W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}\text{)}$	32.2(293K), 34.3(473K), 20.7(973K)
$C_p \text{ (J} \cdot \text{Kg}^{-1} \cdot \text{K}^{-1}\text{)}$	395(293K), 545(473K), 800(973K)

Finally, the parameters of the CP model used for the ferrite phase are obtained using an inverse optimization procedure, following the procedure given in [35], to fit the numerical results obtained in the simulation of uniaxial compression tests of polycrystals with the actual experimental results [88]. For efficiency, the reference shear strain rate is taken to be $1.73 \cdot 10^6 \text{ s}^{-1}$, the exponent r_1 in the hardening law is taken to be 1.1. The rest of the model parameters are obtained from the curve fitting procedure. The final parameters obtained model are listed in Table 4.2. The validity of the parameters used for the mechanical simulation can be analyzed in Fig. 4.3 where the result of isothermal polycrystalline simulations at two different temperatures and a strain rate of 50 s^{-1} are compared with the corresponding experimental stress-strain curves. It can be observed that model reproduces well the experiments for both temperatures. Nevertheless, it should be remarked that since this set of parameters have been obtained with limited experimental data and neglecting the temperature dependency of elastic

Table 4.2: Material Properties of Ferrite-pearlite Steels

Model Parameter	Value
ΔF^α	$2.77 \cdot 10^{-19}$ J
$\dot{\gamma}_0$	$1.73 \cdot 10^6$ s $^{-1}$
h_0	200 MPa
s_s	120 MPa
r_1	1.10
p	0.20
q	1.40
$s_{at,0}$	60.0 MPa
$s_{t,0}$	380 MPa

constants, the temperatures and strain rates in which the model can be applied should near the testing data. In order to improve the model adjustment in future developments, experimental results of pure ferrite crystals would help to identify the parameter of its phase. From those results, the cementite properties could then be obtained using inverse fitting procedure with the ferrite-pearlite steel, from the set of tests here presented. The newly calibrated model parameters may hopefully fits experimental results better in a much wider range of strain rates and temperatures, as observed in metal cutting processes.

Fig. 4.3: Fitting of model parameters for ferrite-pearlite steels

4.3 Simulations on orthogonal turning of ferrite-pearlite steels

4.3.1 Orthogonal Turning Process

In this section, the orthogonal turning process of C45 will be simulated and compared with the experimental results given in [91]. In a turning process, the cutting tool is fixed and the workpiece, which is usually a cylindrical tube, rotates at a given angular velocity as depicted in Fig. 4.4(a), where V_c is the linear velocity of the outer radius of the workpiece. Since the typical length scale for the study of such cutting process is several millimeters, much more smaller than the radius of the workpiece, this process could be simply modeled as in Fig. 4.4(b) and Fig. 4.4(c), where f is called the feed, a_p is the cutting depth, t_c is the chip thickness, α , β and γ are the rake angle, clearance angle and shear angle, respectively. The surface in the tool that contacts with the chip is called the rake face and the other bottom face in the tool that contact with the workpiece is called the flank face. In an orthogonal turning experiment, the cutting force and feed force can be measured by a dynamometer; the temperature at the side face of the cutting tool can be obtained with an infrared (IR) camera, and based this measurement the temperature in the contact face could be estimated; the chip thickness and contact length can be measured with a microscope IR and a profilometer, respectively.

4.3.2 Setup of finite element model for orthogonal cutting simulation

A finite element model was established to simulate the orthogonal cutting of C45 as illustrated in Fig. 4.5. The length, width and depth of the workpiece in the model are taken as 1.2mm, 0.5mm, and 0.3mm, respectively. The microstructure of the workpiece is represented by about 3000 grains discretized into about 300,000 hexagonal elements with each grain being either a ferrite crystal or a pearlite block. The initial orientations of these grains are assumed to be random. The actual orientations and distributions of grains within the workpiece are slightly different for simulations with different feed due to the randomness of the grain generation process, but this is expected to have minor effect on the simulation results. The volume fraction of the ferrite single crystals in the model is taken to be 0.25 as in the specimen of the experiments [91]. The cutting tool is deformable with a radius of 40 μm of the cutting edge, and a rake and clearance angles of 5°

Fig. 4.4: (a). Illustration of an orthogonal turning process. (b). Oblique view and (c) Front view on a simplified model of turning process

and 6° , respectively. A Coulomb friction law is employed to describe the frictional behavior between the tool and the chip and the friction coefficient is taken to be 0.50. The bottom face of the workpiece is fixed.

Fig. 4.5: Finite element model for simulations of turning processes of C45. (a). Distributions of grains and blocks and (b). Distribution of phases (Blue for ferrite crystals and Red for pearlite blocks) in the workpiece.

The pure Lagrangian method is adopted to study the thermo-mechanical behavior of C45 during turning process. In this method, an element deletion criterion is needed to remove the excessively distorted elements and enable the formation and evolution of chips. For simplicity, the maximum effective plastic strain

criteria is employed. An element will be removed when its effective plastic strain reaches a critical value of 1.6. It should be pointed out that this parameters will affect the simulation results notably and was chosen after several times of trial. If it is too large, the analysis may be terminated due to the excessive distorted elements. While if it is too small, the workpiece may behaves too fragile and too much mass loss will be found, which leads to a reduction of the simulation accuracy.

4.4 Simulation Results and Discussion

A series of simulations were carried out with cutting speed of 100m/min and 200m/min and feed of 0.1mm and 0.2mm to study the thermo-mechanical behavior of C45 under orthogonal turning processes. The cutting length for all these simulations are taken to be 0.5mm. Thus, for cases with cutting speed of 200m/min, the cutting time simulated is one half of that for cutting speed of 100m/min. The time histories of cutting forces for these cases, which are obtained as the total contact forces on the rake face of the tool in the cutting direction, are plotted in Fig. 4.6. It is shown that the cutting forces first increase rapidly and

Fig. 4.6: Time histories on cutting forces during cutting process.

then oscillate around corresponding mean values after cutting time of about 0.1 ms, indicating that steady cutting states have been reached. The cutting force changes slightly as the cutting speed increases, but it rises almost proportionally as the feed rises, since the cutting area and the amount of material to be removed

in this case increases accordingly. The specific cutting force K_{sc} , which is defined as

$$K_{sc} = F_c / a_p f \quad (4.35)$$

where F_c is the average cutting force at steady state, a_p is the cutting depth and f is the feed, is compared to the experimental results given in [91] as shown in Fig. 4.7. It is shown that the model follows the same trends than the experiments

Fig. 4.7: Comparison on numerical and experimental results of specific cutting forces for cases (a). $V_c=100\text{m/min}$, $f=0.1\text{mm}$, (b). $V_c=100\text{m/min}$, $f=0.2\text{mm}$, (c). $V_c=200\text{m/min}$, $f=0.1\text{mm}$ and (d). $V_c=200\text{m/min}$, $f=0.2\text{mm}$

in terms of the dependency of K_{sc} with the cutting speed and the feed. Quantitatively, the difference between the numerical and experimental results are about 20% to 40%, which suggests that our proposed numerical framework is reasonable accurate, considering the complexity of the problem and the lack of fitting data for the material response.

The chip forms at a cutting length of 0.45 mm for the four cases are given in Fig. 4.8. It can be observed that the simulated chip forms are in good agreement with experimental observations [91]. In order to observe how the chip is separated from the workpiece and how the chip form evolves, the distribution of the effective plastic strain within the workpiece at various cutting length for the case with cutting speed of 200m/min and feed of 0.1mm are shown in Fig.4.9. It can be observed that the material in contact with the cutting edge is the one first fails due to the large shear deformations that has to accommodate. Moreover, the model clearly reproduces the typical shear band formed from the tool edge to

Fig. 4.8: Chip form at cutting length of 0.45 mm for (a). $V_c=100\text{m/min}$, $f=0.1\text{mm}$, (b). $V_c=100\text{m/min}$, $f=0.2\text{mm}$, (c). $V_c=200\text{m/min}$, $f=0.1\text{mm}$ and (d). $V_c=100\text{m/min}$, $f=0.2\text{mm}$.

Fig. 4.9: Distributions of effective plastic strain in the workpiece at cutting length of (a). 0.05mm, (b). 0.15mm, (c). 0.3 mm and (d). 0.45mm for cutting speed of 200m/min and feed of 0.1mm.

the workpiece surface. Near the contact face in the chip, due to the pressure transmitted by the cutting tool a high compression area was formed. In this area, the compressed material also moved upward due to the Poisson effect and formed a bump-up, resulting in an increasing contact length between the chip and the tool. The movement of the chip along the contact face was also effected by the frictional force between the surfaces of the chip and the tool. It can also be observed that the plastic strain at first was localized near the chip tip and then propagated in the chip.

The evolution of the Von. Mises stress is shown in Fig. 4.10. It can be seen that the stress distribution within the chip is more complex. The complex stress patterns are caused by the smooth stress concentration due to the contact with the tool and, on the other side, by the local changes of the tangent stiffness due to the heterogeneity of the microstructure. The evolution of the temperature field

Fig. 4.10: Distributions of Von. Mises stress in the workpiece at cutting length of (a). 0.05mm, (b). 0.15mm, (c). 0.3mm and (d). 0.45mm for cutting speed of 200m/min and feed of 0.1mm.

within the workpiece is shown in Fig. 4.11. It is observed that the distribution is similar to that of the effective plastic strain as shown in Fig. 4.9. The average temperature rise is about 500K.

Fig. 4.11: Distributions of temperature in the workpiece at cutting length of (a). 0.05mm, (b). 0.15mm, (c). 0.3mm and (d). 0.45mm for cutting speed of 200m/min and feed of 0.1mm.

As a brief summary, in this chapter, we successfully applied the thermo-mechanically coupled crystal plasticity framework into the study of the machining process of ferrite-pearlite steel and obtained acceptable cutting forces and chip forms considering the limited data used to calibrate the model parameters. The modeling framework is a first step into the simulation of the cutting process as function of the microstructure using precise CP models and opens the door to study the effect of the raw material texture or dual microstructure in the process. The explicit representation of the microstructure allows to go behind this simulation and investigate in next studies the effect of the microstructure in the tool wear.

The improvement of the model calibration with more experimental data as well as the extension of the model to more accurate CEL or ALE simulation frameworks will improve the accuracy of the simulations. In addition, from a physical point of view, the model can be improved by introducing recrystallization during the cutting process.

CHAPTER 5

Conclusions and Future work

5.1 Summary

Metals and alloys play a crucial role in our society. Due to their importance in industry, an in-depth understanding and accurate prediction of their behavior may lead to notable economic benefits. Theoretical and numerical models have existed for decades now, but accuracy demands from complex manufacturing processes require more sophisticated models than the standard ones. The new models must incorporate precise descriptions of the physics that metals undergo during thermomechanical processes, and provide information about the state at which they end after being subjected to extreme conditions.

Metallic materials usually undergo large strain, high strain rate and high temperature, and their deformation is usually thermally coupled. They also exhibit plastic anisotropy and microstructure heterogeneity. To better describe their behavior, in this work a thermo-mechanically coupled finite element framework incorporating a crystal plasticity constitutive model has been developed to predict the behavior of metallic material during thermo-mechanical processes. This model is physics-based and physics-informed, minimizing the number of parameters that are obtained from experiments. At the same time, it holds much more information than phenomenological plasticity models, thus serving the purpose to feed highly accurate information to analysts and engineers.

Real metallic materials are polycrystalline. Each macroscopic material point represents numerous single crystals. To extract the macroscopic behavior of polycrystalline metals from its associated single crystals in the microstructure, an homogenization approach is usually needed. In this study, a computational homogenization approach is adopted and applied to study the plastic deformation of polycrystalline metals by combining with the previous proposed coupled finite element crystal plasticity framework. This combination can predict the behavior of polycrystals under various initial temperatures and strain rates. It could also

reveal the effect of heat transfer at the grain level on the distribution of stress and temperature field at the microstructural scale.

Finally, we have employed the model developed for the simulation of an extremely complex thermomechanical process, namely, that of high-speed machining. This is one of the most important manufacturing operations in modern industry but so complex that very few true plasticity models have been able to simulate it. In this research, a microstructure informed constitutive model is first developed for low carbon steel C45, based on crystal plasticity theory. Then, it is integrated into a thermo-mechanical coupled Lagrangian framework to study the orthogonal cutting process of C45. The numerical results are in acceptable agreement with experimental observations. In addition, our model captures the heterogeneous distribution of stress, temperature in the chip and the contact force on the rake face of the cutting tool, which may not be observed with the conventional Johnson-Cook model.

5.2 Future Work

In the future, we could extend the work presented in this dissertation with regard to the following aspects:

1. Develop thermo-mechanically coupled frameworks based on other, more efficient alternative approaches, instead of the finite element method. For large scale problems which usually need parallel computing, the finite element method usually exhibits poor parallel efficiency, limiting its application to large scale engineering problems in rapidly advancing supercomputers. There some other numerical approaches that may have good parallel performance, such as the FFT based homogenization and the peridynamics approaches.
2. Improve the numerical framework we have established for the simulation of cutting process of ferrite-pearlite steel. Currently, and for the sake of simplicity, we have taken many assumptions and simplifications. In the future, we could improve the simulation accuracy by finding better material properties for the ferrite and cementite phases, performing curve fitting procedures to obtain parameters in the constitutive models that could reproduce experimental results at much wider range of temperatures and strain rates. In a similar topic, the solutions obtained have been proven to be fairly sensible to the element deletion criterion, and further analysis of the latter might result in overall improvements.

3. Apply the proposed numerical framework to the cutting simulation of other commonly used engineering materials such as Ti6Al4V. Due to the generality of our framework, only minor modifications and extensions are needed to develop a similar microstructure informed constitutive model for this dual-phase metal.
4. Explore the feasibility of using the ALE method and CEL method in the simulation of cutting processes based on our proposed constitutive model. These two approaches could potentially give better simulation accuracy as they do not use the non-physical element deletion criteria that could degrade the accuracy.
5. Introducing the size effect in our constitutive model, study the micro-cutting process of tiny size metallic components, with application in various fields such as the biomedical, optical, and mold/die industries.

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