Micromechanisms of the phase transformation in NiTi shape memory alloys

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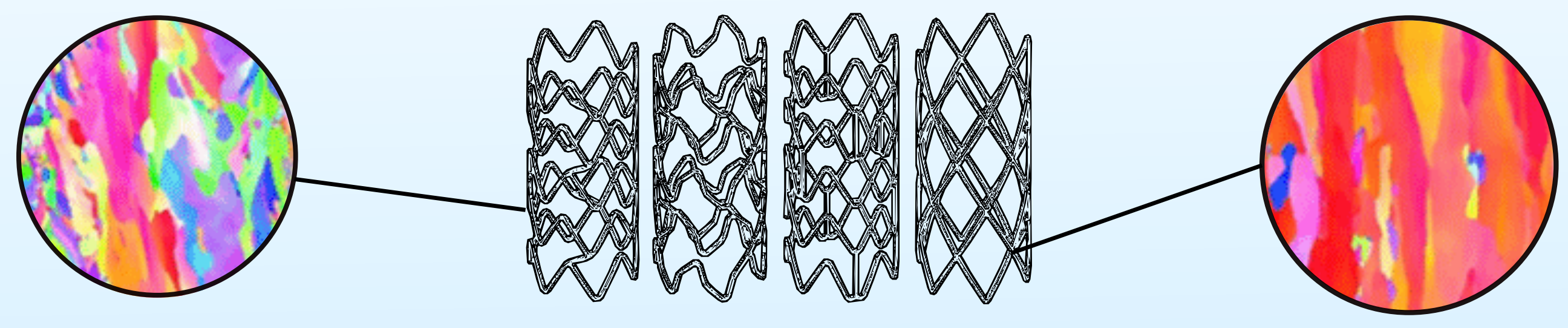
Problem Statement

The combination of geometry freedom in additive manufacturing with tailored transformation behaviour of shape memory alloys provides an infinite design opportunity for customisable functional devices e.g., patient specific medical stents.

However, multiscale design frameworks specific for functional materials like shape memory alloys need to be impletemented combining the relevant physical metallurgy underlying physics, with large deformation continuum mechanics formulations and numerically efficient methodology for design optimization.



Hsiao, Hao-Ming, et al. "Hemodynamic behavior of coronary stents in straight and curved arteries."

Ewald, et al. "Laser powder bed fusion processing of Fe-Mn Al-Ni shape memory alloy—on the effect of elevated platform temperatures."

Objectives

1 - Develop a micromechanical continuum model to predict thermomechanical behavior of SMAs.
2 - Validate that model against typical NiTi examples.
3 - Run different design and material cases to build surrogate models for efficient design evaluation.
4 - Integrate all in a machine learning loop to optimise the stent geometry + SMA material design.

Geometrical and SMA design frammework for additive manufacturing

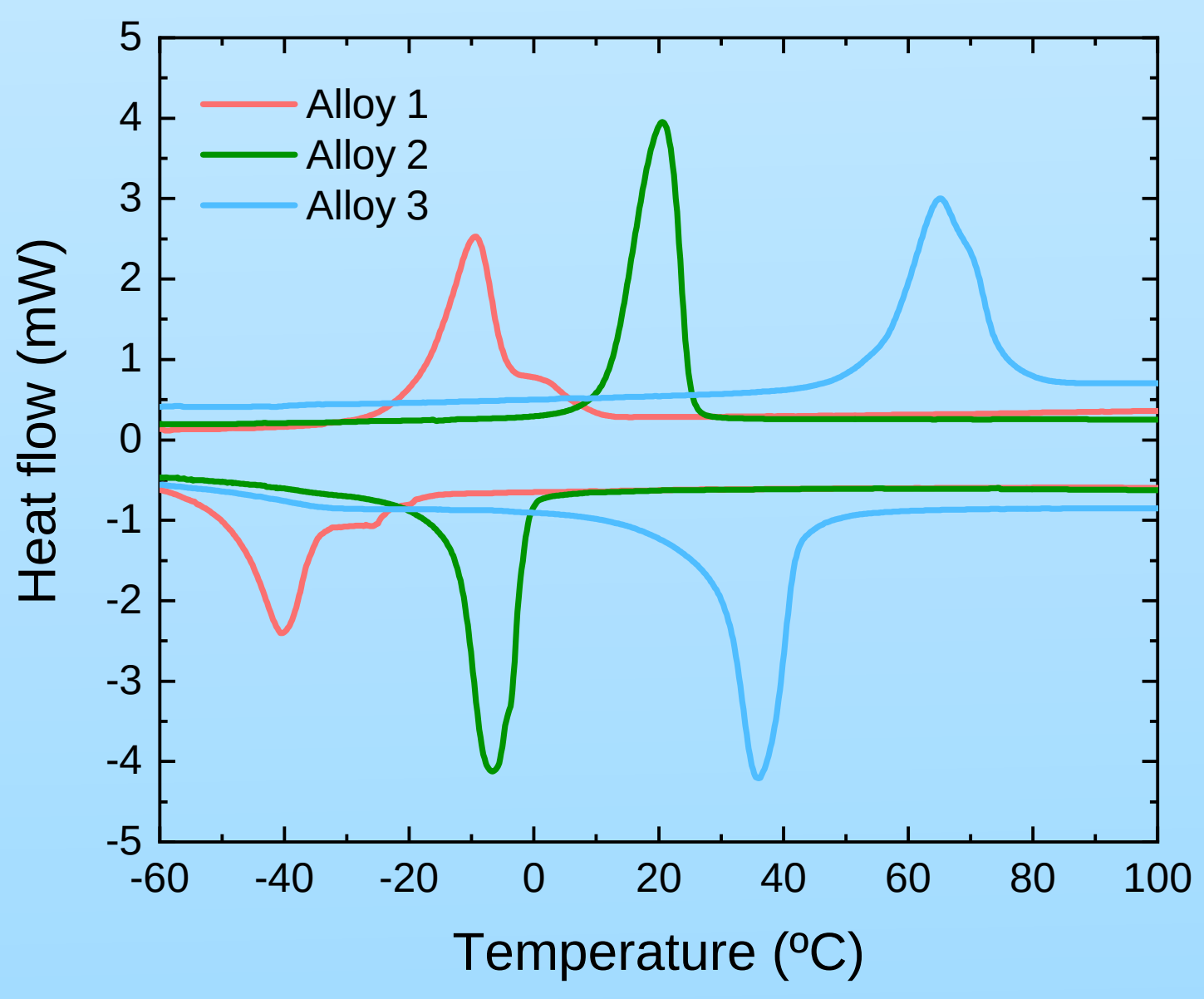
Continuum micromechanical model ▷ Surrogate models + Machine learning ▷ Optimal functional design

Material characterization and model validation

1. Material characterization

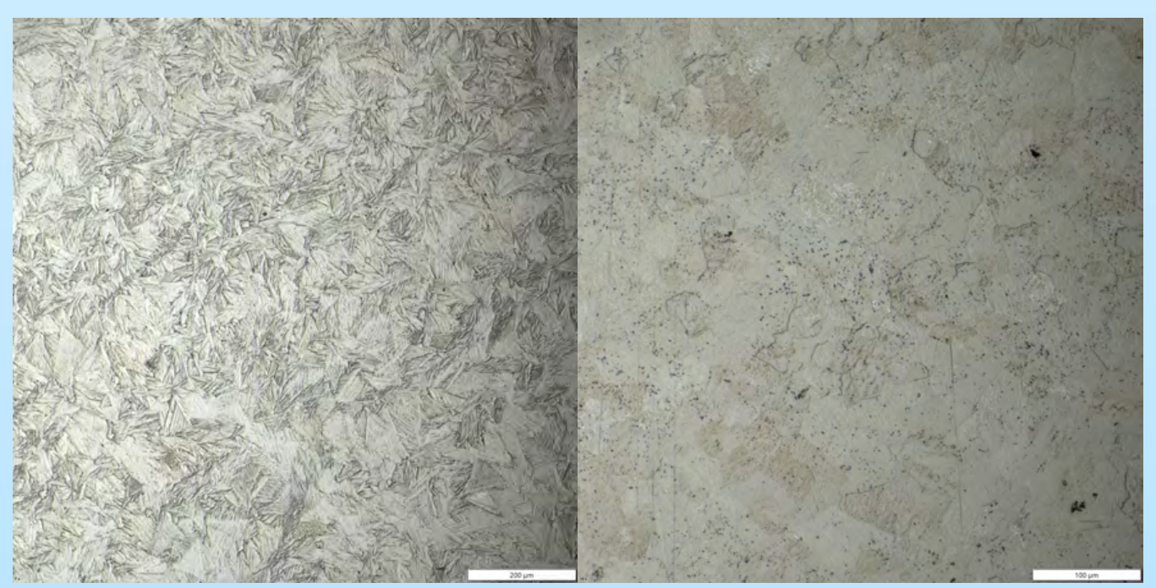
Three different alloys with slight different Ni/Ti ratios (1.09, 1.16, 1.18) have been chosen to study and validate the aplicability of the micromechanical continuum model.

DSC transformation temperatures



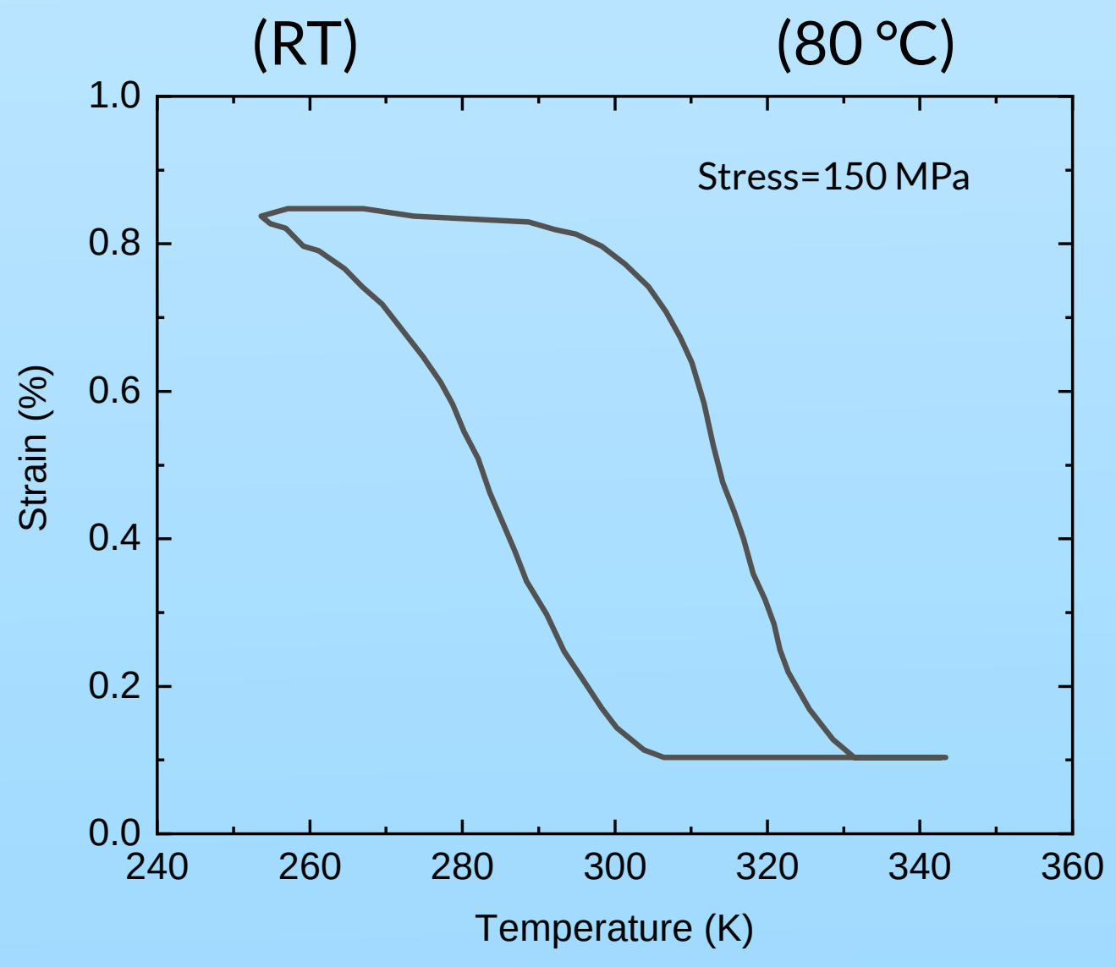
Thermomechanical and transformation behaviour

Microtensile test



Martensite phase (RT)

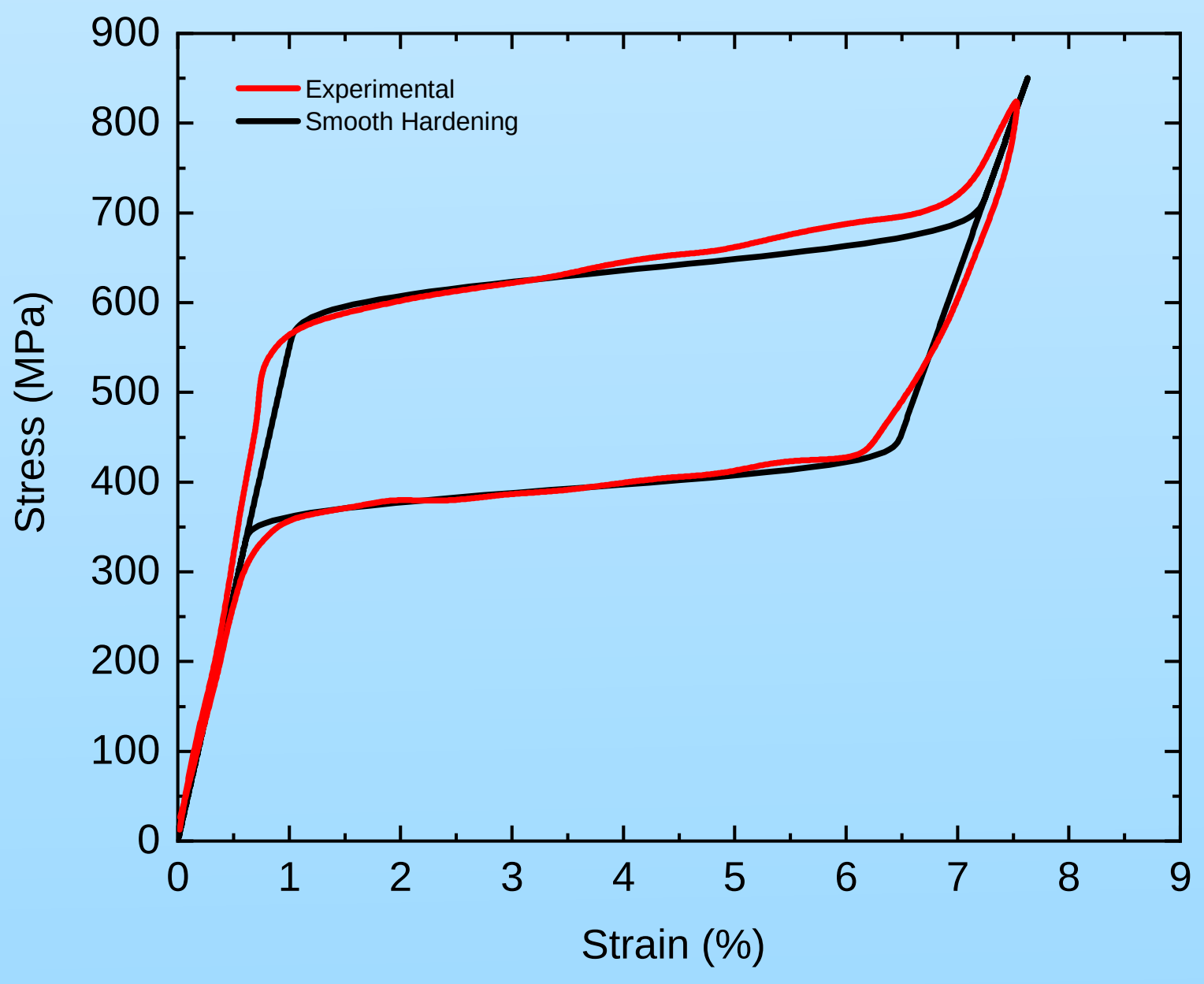
Austenite phase (80 °C)

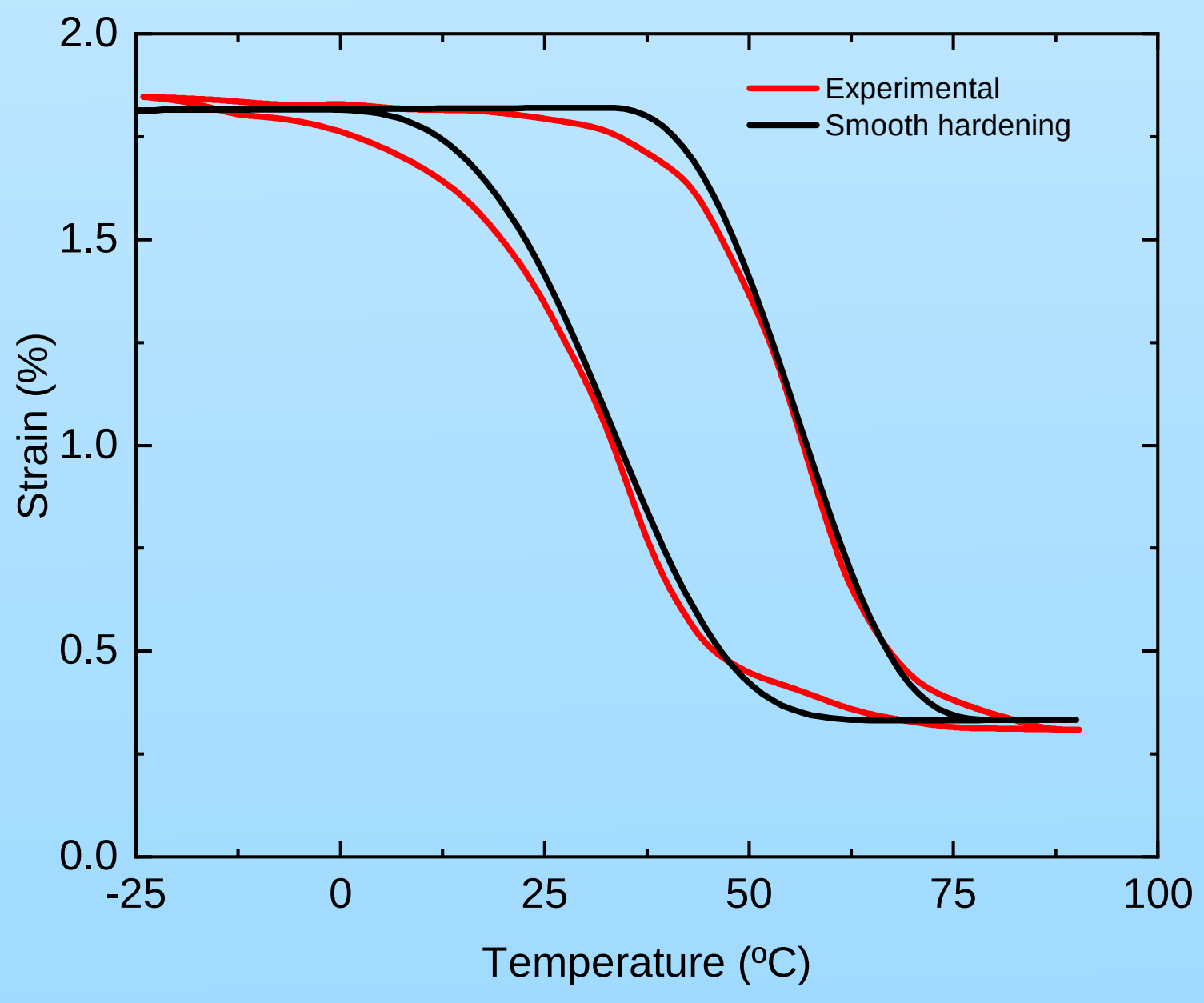


2. Mechanical testing and model validation

A micromechanism-based continuum model formulated in large deformations has been implemented to simulate the thermomechanical transformation behaviour of shape memory alloys derive from previous work of Lagoudas et al. [1]

$$G(\mathbf{S},T,\mathbf{E}^t,\xi) = -\underbrace{\frac{1}{2\rho}\mathbf{S}:\mathcal{S}:\mathbf{S}}_{\text{Elastic energy}} - \frac{1}{\rho}\mathbf{S}:[\underbrace{\alpha(T-T_0)]}_{\text{Thermal energy}} + \underbrace{\mathbf{E}^t]}_{\text{Transformation energy}} + c\left[\underbrace{(T-T_0) - T ln\left(\frac{T}{T_0}\right)}_{\text{Internal energy}}\right] - \underbrace{s_0 T}_{\text{Entropy}} + \underbrace{e_0}_{\text{Internal energy}} + \underbrace{\frac{1}{\rho}f(\xi)}_{\text{Hardening function}}$$

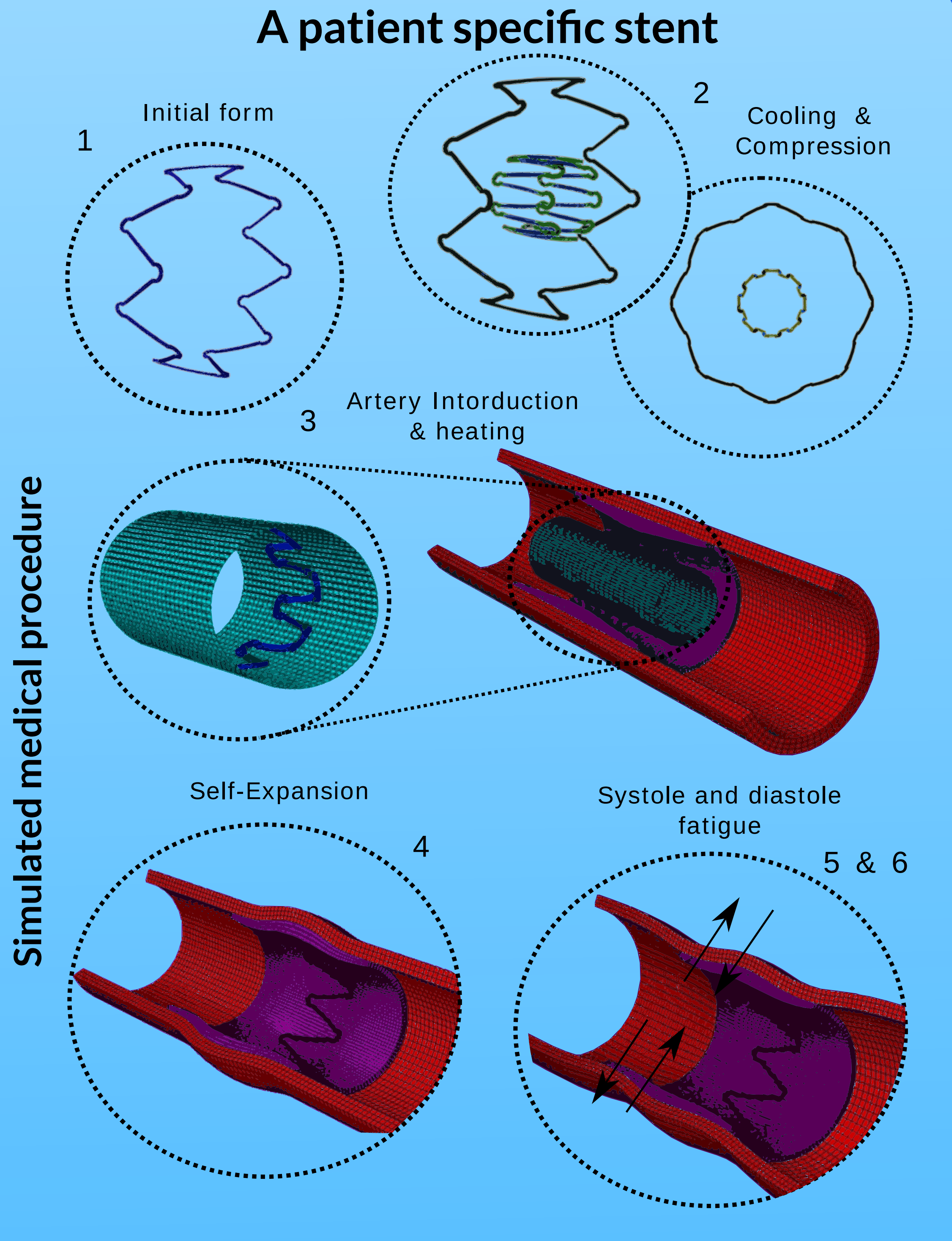




[1] Lagoudas et al.¨User material subroutine for thermomechanical constitutive model of SMA¨

Application to a phase-transformation based functional design

Case of study
A patient specific stent

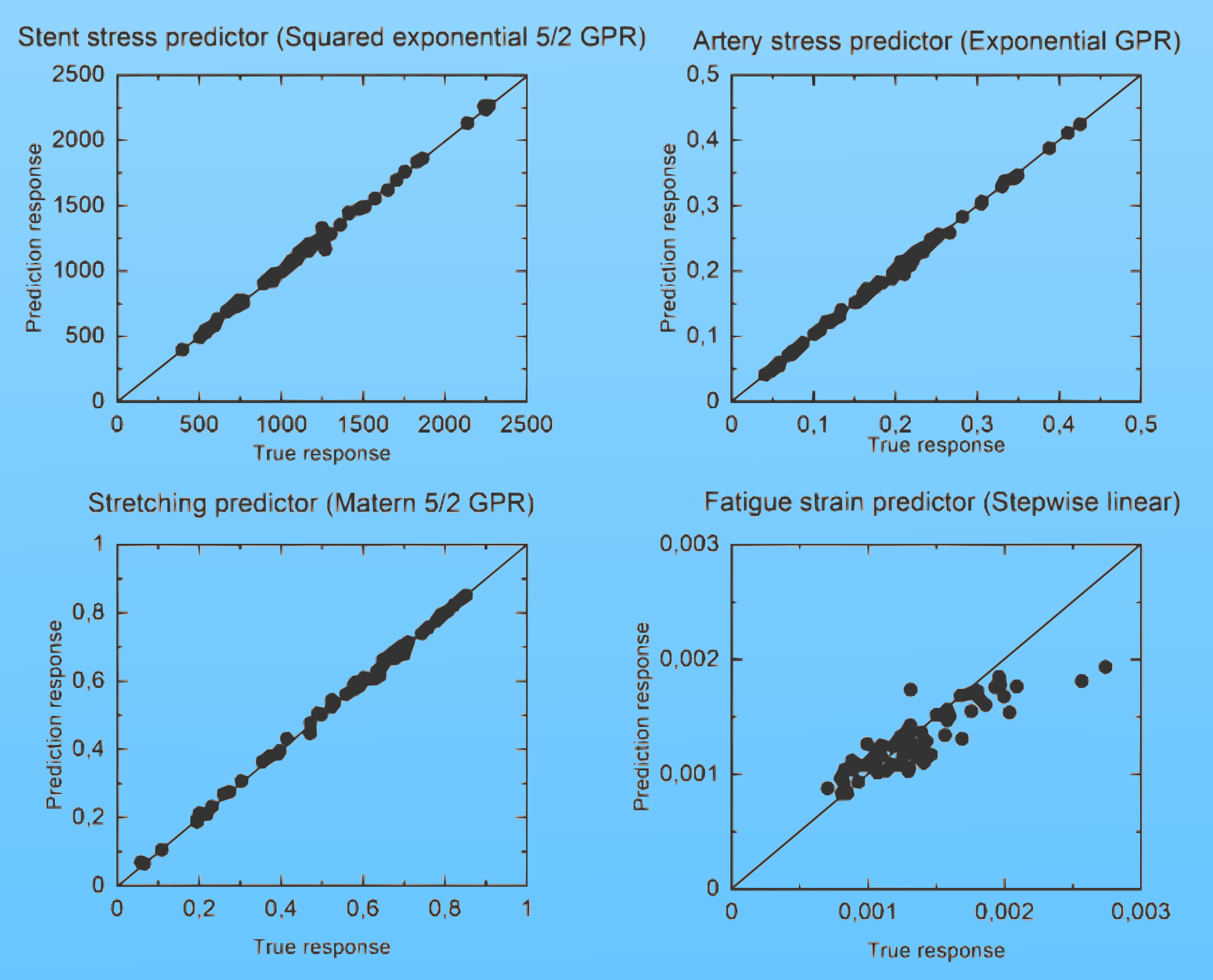


Geometrical design freedom + Tailored transformation
(5 geometrical variables) (12 material parameters)

762 billions possibilities if 5 steps are choosen per variable

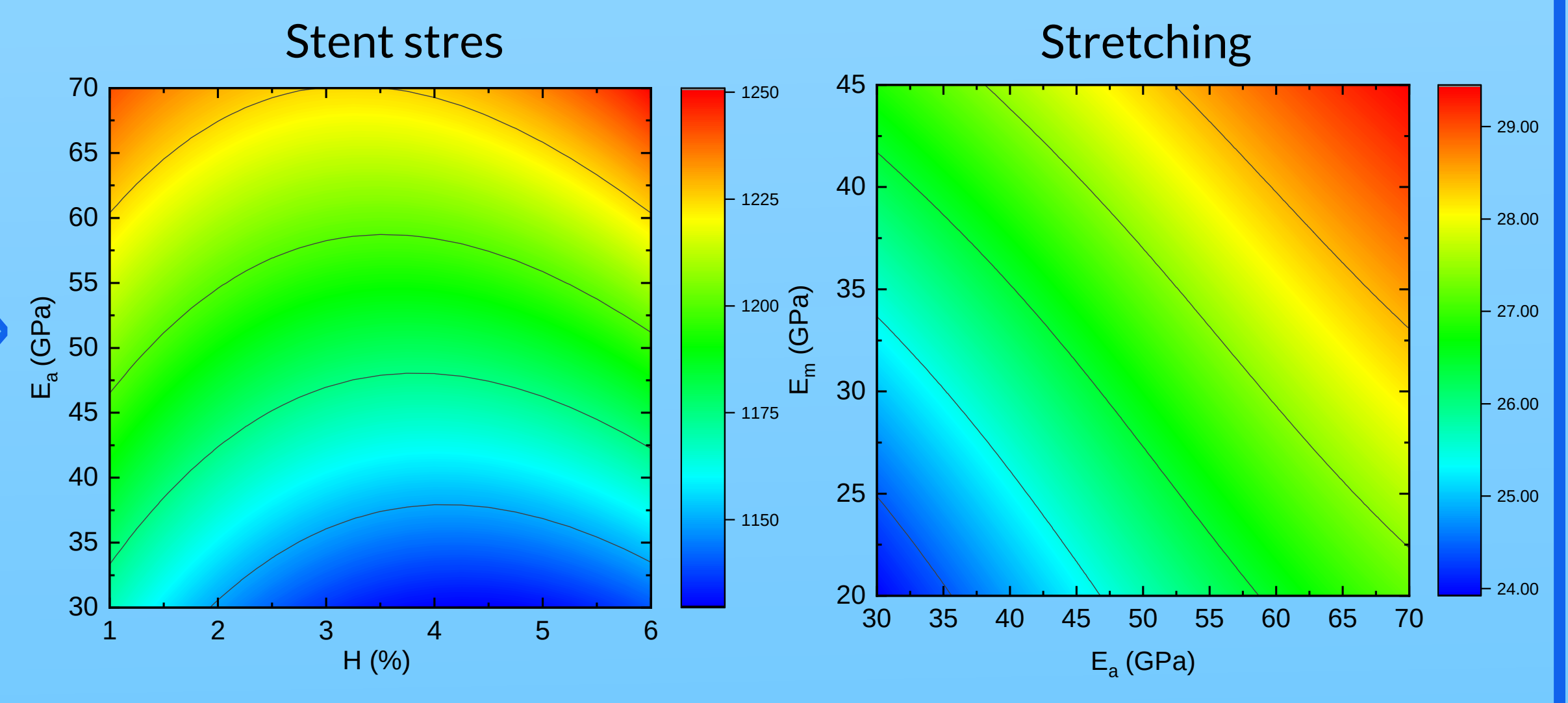
1. Surrograte models of machine learning

81 simulations were conducted to train the machine learning model. 4 outputs were selected:



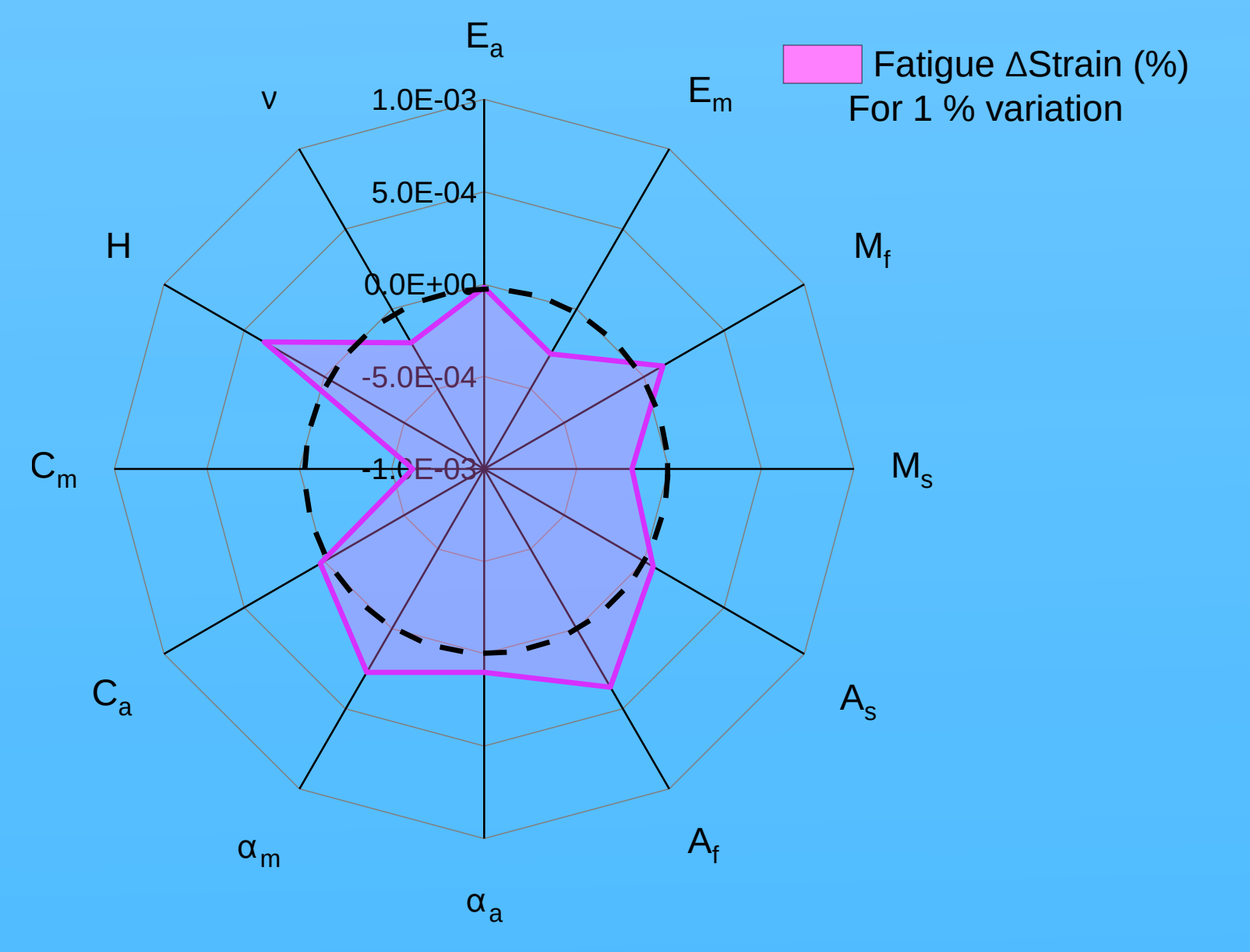
2. Design space study

Prediction functions can be used to calculate output values based on input parameters. This enables a clear understanding of how each parameter influences the outcoming combination with others.



3. Sensitivity study

The equations of the Gaussian model have been linearized to study the dependencies between the variables.



4. Optimized stent vs real stent case

	Reference stent*	Optimal Stent	Design Limits
Stent stress	1270 MPa	510.8 MPa	<1350 MPa
Artery stress	73.8 KPa	89.9 KPa	<1200 MPa
Stretching	0.34 mm	0.46 mm	>0.3 mm
Fatigue strain	0.38%	0.15%	< 0.4%

*M.S. Cabrera et al. ¨Understanding the requirements of self-expandable stents for heart valve replacement¨

Conclusions

- The **thermomechanical and transformation behaviour of three different SMAs with different Ni/Ti ratios** has been studied experimentally. Higher Ti contents lead to higher transformation temperatures in accodance with the literature.
- The **implemented model can describe accurately the thermomechanical and trasnformation behaviour** of the alloys with different transformation temperatures.
- **Surrogate models** for the constitutive response have been built based on the continuum framework response **for computing efficiency**. The results show great accuracy between the full continuum model and the surrogate models.
- The **surrogate constitutive framework has been coupled with machine learning optimisation tools** to optimise the geometrical design and material selection **for a pateient-specific stent**
- The new stent delivers a **superior performance** with an equivalent artery stress and a **60% reduction in maximum stent stress, 35% higher stretching and 60% less fatigue strain.**

Acknowledgments

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Code/Name of the Project:
SMARTALLOYS
(PI: Daniel Barba)