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**E.T.S. de Ingenieros de Caminos, Canales y
Puertos.**

**Multiscale modeling of junction
processing in FDSOI and FinFET
devices for 10 nm node technology and
below**

A thesis presented by

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in partial fulfillment of the requirements for the degree of Doctor of Philosophy

Supervised by

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To my parents: Lidia and José

A mis padres: Lidia y José

Given for one instant an intelligence which could comprehend all the forces by which nature is animated and the respective positions of the beings which compose it, if moreover this intelligence were vast enough to submit these data to analysis, it would embrace in the same formula both the movements of the largest bodies in the universe and those of the lightest atom; to it nothing would be uncertain, and the future as the past would be present to its eye.

P.S. Laplace

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Contents

List of Figures	ix
-----------------	----

List of Tables	xix
----------------	-----

I	Technological context	1
1	Roadmap of device scaling	2
2	Low thermal budget in junction formation	4
3	The regrowth process	6
3.1	Amorphization	6
3.2	Recrystallization	7
4	Modeling SPER	8
4.1	The needs for multiscale	8
4.2	Ab initio	10
4.3	Molecular Dynamics	11
4.4	Monte Carlo Methods	13
5	Introducing MMonCa	16
6	Goal of this work	17
II	Introduction to the solid phase epitaxial regrowth	19
1	The amorphous to crystalline transition	20
1.1	Atomic structure of crystalline and amorphous phases . . .	20
1.2	On the thermodynamics of the crystalline transition	23
1.3	Kinetics of solid phase epitaxial regrowth	25
2	Anisotropic behaviour	28
3	Defect formation	30
4	Dopants and impurity concentration dependence	31
5	Hydrostatic and non-hydrostatic stress impact	33
6	Summary	34
III	Multidirectional SPER of intrinsic Silicon	37
1	Multidirectional SPER	38
2	Growth interface pinning	39
3	Regrowth of box-shaped amorphous regions	42

3.1	Intrinsic stress pattern: Finite element method calculations	44
3.2	MD simulations of SPER upon stress	45
3.3	Extended LKMC modeling of the defected regrowth	50
4	Regrowth of box-shaped amorphous regions without surface pinning	57
4.1	MD study of the SPER curvature dependence	57
4.2	Extended LKMC modeling in the absence of surface pinning	59
5	Summary	64
IV	Modeling SPER of SiGe alloys	67
1	Introduction to SiGe alloys	68
2	Germanium impact on SPER activation energy	70
2.1	Regrowth of relaxed SiGe alloys	70
2.2	Nudged Elastic Band Calculations	74
3	Defect nucleation during SPER	78
3.1	Simulation details and observations	79
4	Summary	81
V	Strained SiGe channel for FinFET devices	85
1	Incorporation of SiGe alloys as channel material	85
2	Strain compensation by relieving defects	88
2.1	Novel FinFET fabrication process	88
2.2	Simulation details and results	88
3	Summary	93
VI	Concluding remarks and further work directions	97
1	Defect formation dependence on stress	98
2	Two part behaviour of the SPER activation energies in SiGe alloys	99
3	Strain relieving defects in SiGe channel FinFETs	99
4	Further work suggestions	100
4.1	Preliminary results of the study of Boron diffusion in SiGe alloys	100
4.2	OKMC model presentation	102
4.3	Simulation details and observations	104
	Appendices	107
A	Generation of amorphous phase	109

B List of communications	113
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Bibliography	117
--------------	-----

List of Figures

I.1	Evolution of device structures depending on the gate length (blue line) and total number of transistors (red line). Extracted data from [Schwierz <i>et al.</i> 2015].	2
I.2	3D sequential integration flow process. (a) The bottom level transistor is processed with a high temperature budget, (b) then a high quality film is deposited, and (c) finally the top transistor is fabricated with a low thermal budget procedure.	3
I.3	TEM cross-section image of two stacked FDSOI transistors with a gate length of 50 nm and ultra thin interlayer dielectric of 23 nm. Image taken from [Batude <i>et al.</i> 2011].	3
I.4	Hole mobility incremental performance as function of Ge composition for relaxed and strained SiGe PMOSFET along <110> channel direction and (001) wafer orientation. Data extracted from [Cheng <i>et al.</i> 2015].	4
I.5	Low thermal budget design temperatures of the critical steps in 3DMI. Stars represent the target temperatures to preserve the bottom layers. Filled circles are the performed temperatures for standard processes. Data extracted from [Cheramy <i>et al.</i> 2017]	5
I.6	Schematic representation of a single ion collision in the crystalline lattice (a), and the resulting cascade (b). If the implanted ion transfers enough energy to a substitutional atom, it is displaced from its lattice site creating vacancy defects (dotted circles), and becoming interstitial atoms (red and blue circles). If interstitials have enough energy may affect in turn other substitutional atoms, generating damage cascades.	6
I.7	Atomic configuration of the bond defect. The local distortion of the lattice consists of five-fold and seven-fold membered rings. Gray and white atoms represent the plane along <001> direction. Atoms in rotated ion-pair are colored in black.	7

I.8	Stages of the ion implantation after continuous cascades leading to the formation of a complete amorphous layer on the top of the ionized surface. (a) Interstitials (blue circles) and vacancies (dotted circles) are generated, see Fig. I.6. If they do not recombine, amorphous pockets may appear (b) and continue growing until a complete amorphous layer is obtained (c).	8
I.9	Time and length scales of the modeling techniques.	9
I.10	Verlet list approach. Being r_v the second cutoff radius, when a particle moves further than $r_v - r_c$, the Verlet list is update. . . .	13
I.11	Schematic of the procedure for picking reaction pathway to advance the system to the next state in the standard KMC algorithm. Each event with a length proportional to the rate constant for its pathway are placed end to end.	14
I.12	Schematic of the kinetic transition for scape from state A to state B, given by the equilibrium outgoing flux through the dividing surface within the TST	16
I.13	Overall structure of the MMonCa simulator.	17
II.1	Schematic model of the crystalline network structure. (a) Three dimensional view, (b) $\langle 100 \rangle$ direction, (c) $\langle 110 \rangle$ direction and (d) $\langle 111 \rangle$ direction.	21
II.2	Experimental pair correlation function of amorphous Si and Ge, from [Laazari <i>et al.</i> 1999] and [Ethernington <i>et al.</i> 1982], obtained by conventional diffraction methods.	22
II.3	Schematic of the Gibbs free energy for a SPER reaction. Red line represents the structural relaxation taking place before the recrystallization starts.	25
II.4	Schematics of single-dimensional patterned SPER process showing (a) the as-implanted state, (b) partial growth, and (c) completed SPER resulting in a single crystal.	26
II.5	Arrhenius fitting for Si(001) and Ge(001) for temperatures ranging from 500-800° and 315-530°, respectively. Extracted values of activation energy have been obtained from time-resolved reflectivity measurements (TRR) [Olson & Roth 1988, Csepregi <i>et al.</i> 1977b]. .	27

II.6	Normalized regrowth rate at 550°C versus the substrate orientation dependence from (111) direction, extracted from [Csepregi <i>et al.</i> 1978] for Si and [Darby <i>et al.</i> 2013] for Ge. Relative dangling bond density is taken from [Custer <i>et al.</i> 1992].	28
II.7	Atomistic configurations for {110}, {100} and {111} growth planes. Atoms in gray color are attached to the crystalline phase when forming two undistorted bonds, highlighted in gray-dashed line. . .	29
II.8	Schematic drawing of the two possible bonding positions at the {111} planes: Normal (red) and twin (green) configurations. . . .	30
II.9	Cross-sectional TEM images showing a silicon fin (a) after implantation, (b) during annealing where the regrowth is not complete, and (c) once the recrystallization is complete and twin formation can be observed. Extracted from [Duffy <i>et al.</i> 2007].	31
II.10	XTEM images of Ge fins (a) when the recrystallization is not complete, (b) small defects formed in the amorphous Ge, and (c) {111} facets seen at the foot of the fins. Extracted from [Duffy <i>et al.</i> 2011].	32
II.11	SPER rates versus hydrostatic pressure for Ge(001) represented in red and Si(001) in blue, values extracted from [Lu <i>et al.</i> 1991]. . . .	33
III.1	Schematic of two dimensional SPER resulting from implanted mask: (a) the as-implanted state and (b) partial growth during recrystallization proceeding in both vertical and lateral directions.	39
III.2	Cross-sectional TEM images from [Saenger <i>et al.</i> 2007a] of SiO ₂ filled trenches leading to {111} facets formation after annealing at 900 °C in: (a) Si(001), (b) Si(011) substrates with insulator edges aligned with <110> crystal in-plane directions, and (c) Si(011) substrate aligned with <100> directions.	40
III.3	Schematic structure of a FinFET device: (a) plane and (b) cross view after implantation. The 3D structure introduces lateral interfaces with the SiO ₂ present for isolation purposes.	41
III.4	Partial regrowth of trench-bounded <110>-aligned amorphous layer on Si(100): (a) Cross sectional TEM image after 60 s of annealing from [Duffy <i>et al.</i> 2007], and (b) MD snapshot of wide fin structure at t=15 ns. Blue lines indicate the {111} stacking fault formation, which limits the typical form of an arrow tip. Inset in (b) illustrates the formation of {111} twin boundaries highlighted in green.	42

III.5	Snapshots taken during MD annealing at 1800 K of a 4.3 nm wide fin structure aligned along the $\langle 100 \rangle$ direction after (b) 12 ns and (c) 60 ns. Blue lines indicates the lateral facet formation along $\{110\}$ planes at 45° from vertical.	43
III.6	Microscopic configurations indicating how atoms in the α -c interface have to rearrange for Si(100) substrates with SiO ₂ edges aligned with (a) the crystal in-plane $\langle 110 \rangle$ direction, and (b) $\langle 100 \rangle$ direction.	44
III.7	Shear strain patterns generated by volume expansion of α -Si in a box-shaped amorphized structure for (a) MD domain size and (b) LKMC domain size. Taken from [Prieto-Depedro <i>et al.</i> 2015].	45
III.8	Cross sectional schematics of (a) $\langle 110 \rangle$ -aligned shaped regions in (001) Si and (b) $\langle 100 \rangle$ -aligned shapes in (011) Si. Grey slabs represent fixed atoms used as a substrate. Atoms in the top slab are identified with filled trenches. Taken from [Prieto-Depedro <i>et al.</i> 2015]	46
III.9	MD snapshots showing the cross sectional free-stress (a) $\langle 110 \rangle$ -aligned box-shaped in (001) Si and (b) $\langle 100 \rangle$ -aligned box-shaped in (011) Si, after 4 ps annealing at 2000 K. Twinning formation is identified with red-dashed lines. Extracted from [Prieto-Depedro <i>et al.</i> 2015].	47
III.10	Cross sectional MD simulation snapshots of $\langle 110 \rangle$ -aligned box-shaped α -Si regions in (001) Si under compressive stress after annealing at 2000 K for (a) 0.3 ns and (b) 0.5 ns. Dashed-red lines illustrate defected regrowth zones. Published in [Prieto-Depedro <i>et al.</i> 2015].	48
III.11	Cross sectional MD simulation snapshots of $\langle 100 \rangle$ -aligned box-shaped α -Si regions in (011) Si under compressive stress after annealing at 2000 K for (a) 0.6 ns and (b) 1.2 ns. Dashed-red lines illustrate defected regrowth zones. Published in [Prieto-Depedro <i>et al.</i> 2015].	49
III.12	Cross sectional SEM images of $\langle 110 \rangle$ -aligned lin-shaped α -Si regions in (001) Si: (a) as implanted; and after annealing at 550°C for (b) 6 min and (c) 12 min. And $\langle 100 \rangle$ -aligned lin-shaped α -Si regions in (011) Si: (d) as implanted; and after annealing at 550°C for (e) 12 min and (f) 24 min. Extracted from [Saenger <i>et al.</i> 2007b].	49

III.13 Cross sectional images of the complete regrowth of (a) $\langle 110 \rangle$ -aligned box-shaped α -Si regions in (001) and (b) $\langle 100 \rangle$ -aligned box-shaped α -Si regions in (011), under compressive in-plane external stress. Blue lines identify the formed dislocations. Red lines indicate the presence of twins. Taken from [Prieto-Depedro <i>et al.</i> 2015].	50
III.14 Recrystallization of $\langle 110 \rangle / (001)$ at 550 °C: (a) initial structure, after (b) 100 s, (c) 150 s, (d) 200 s, (e) 250 s, and (f) the complete regrowth has been achieved.	53
III.15 Simulation snapshots of recrystallization of $\langle 100 \rangle / (011)$ at different stages of the anneal at 550 °C: (a) initial structure, after (b) 100 s, (c) 150 s, (d) 200 s, (e) 300 s, and (f) the complete regrowth has been achieved.	53
III.16 Recrystallization analysis of [(a)-(e)] $\langle 110 \rangle / (001)$ and [(f)-(j)] $\langle 100 \rangle / (011)$ structures extrated from LKMC simulations. Defected regrowth regions are identified with dashed red lines. The $\{111\}$ faceting and the meeting point of the recrystallization fronts are highlighted for both cases. Extracted from [Prieto-Depedro <i>et al.</i> 2015].	54
III.17 Cross-sectional TEM images of $\langle 110 \rangle$ -aligned α -Si in (a) (001) Si and (b) (011) Si taken from [Saenger <i>et al.</i> 2007b].	55
III.18 Comparison of formed defects observed by XTEM (left) reported in [Saenger <i>et al.</i> 2007b] and predicted by LKMC model (right) for (a) $\langle 110 \rangle$ -aligned box-shaped in (001)Si and (b) $\langle 110 \rangle$ -aligned box-shaped in (001)Si. Taken from [Prieto-Depedro <i>et al.</i> 2015]. . .	56
III.19 Cross-sectional schematics of (a) $\langle 110 \rangle$ -aligned shaped regions in (001) Si and (b) $\langle 100 \rangle$ -aligned shapes in (011) Si. Grey slabs at the bottom represent fixed atoms used as a substrate in MD simulations. Atoms in the top slab, identified in light pink, simulate the presence of Si_3N_4 present in real samples.	57
III.20 MD snapshots of the SPER process in $\langle 110 \rangle$ -aligned box-shaped in (001)Si structure without α -c interfacial pinning at the surface after annealing at 2000 K for (a) 0.3 ns and (b) 0.7 ns. Defected regrowth is highlighted in blue.	58

III.21	XTEM images of the $\langle 110 \rangle$ -aligned shaped structure in (001) Si without interface pinning at the surface: (a) as-implanted, (b) after annealing for 2.5 h, (c) after annealing for 5.0 h and (d) after annealing for 10.0 h. Images (e)-(h) correspond to the level set simulation of the structure evolution. Extracted from [Morarka <i>et al.</i> 2009] . . .	59
III.22	MD snapshots of the SPER process in $\langle 100 \rangle$ -aligned box-shaped in (011)Si structure without α -c interfacial pinning at the surface after annealing at 2000 K for (a) 0.2 ns and (b) 0.7 ns. Defected regrowth is highlighted in blue.	60
III.23	Cross sectional images of the complete regrowth of structures with no interfacial pinning: (a) $\langle 110 \rangle$ -aligned box-shaped α -Si regions in (001)Si and (b) $\langle 100 \rangle$ -aligned box-shaped α -Si regions in (011)Si, under compressive external stress. Blue lines identify the formed dislocations, and red lines the presence of twins.	60
III.24	Simulation snapshots of recrystallization of $\langle 110 \rangle / (001)$ at different stages of the anneal at 550 °C: (a) initial structure, after (b) 100 s, (c) 200 s, (d) 300 s, (e) 400 s, and (f) the complete regrowth has been achieved.	61
III.25	Simulation snapshots of recrystallization of $\langle 110 \rangle / (001)$ at different stages of the anneal at 550 °C: (a) initial structure, after (b) 100 s, (c) 200 s, (d) 300 s, (e) 400 s, and (f) the complete regrowth has been achieved.	62
IV.1	Schematic configuration of the simulation box. First atomic planes are held fixed acting as a substrate. Extracted from [Prieto-Depedro <i>et al.</i> 2017]	69
IV.2	MD simulation snapshots after 20 ns of annealing at 1750 K for different Ge compositions: (a) 0%, (b) 20%, (c) 71% and (d) 100%. Silicon atoms are in red, and Germanium in blue.	70
IV.3	Time evolution of the structure factor $S(y)$ at $T=1800$ K for pure Silicon. For $S(y)=0.5$, the interface position is extracted at each time step.	71
IV.4	Arrhenius fitting for $\text{Si}_{0.89}\text{Ge}_{0.11}$ for temperature ranging from 1750 to 2000 K. Inset: α -c interface position versus the annealing time at 1800 K.	72

IV.5	Activation energy for SPER as a function of Ge concentration. Experimental data from [Haynes <i>et al.</i> 1995] are represented as empty squares, and [Kringhoj & Elliman 1994] as filled circles with error bars. LKMC model [Payet <i>et al.</i> 2016] is presented as a dashed line. MD simulation results are included as filled circles [Prieto-Depedro <i>et al.</i> 2017].	73
IV.6	Energetic reaction pathway between the initial and final states of a solid-solid transformation. The saddle point corresponds to the maximum energy along the MEP. Points represent the system replicas used in the simulation.	75
IV.7	NEB simulation snapshots for the slowest recrystallize configuration in pure silicon when the atom to rearrange into the crystalline phase is (a)-(c) Si, identified in green; and Ge (d)-(f), identified in yellow. Amorphous atoms are in gray, while crystalline in white. Reconnected bonds show how the atom is rearranged for crystal regrowth to proceed in the $\langle 100 \rangle$ direction. Images (a)-(c) are taken from [Prieto-Depedro <i>et al.</i> 2017].	75
IV.8	NEB simulation snapshots for the slowest recrystallize configuration in pure germanium when the atom to rearrange into the crystalline phase is (a)-(c) Ge, identified in yellow; and Si (d)-(f), identified in green. Amorphous atoms are in gray, while crystalline in white. Reconnected bonds show how the atom is rearranged for crystal regrowth to proceed in the $\langle 100 \rangle$ direction.	76
IV.9	Energy along the minimum energy path between the initial state and the final state when an amorphous atom rearranges into the crystalline phase: (a) Si, and (b) Ge atoms in pure Si; and (c) Ge, and (d) Si atoms in pure Ge. Values corresponding to the saddle point are contained in Table IV.1.	77
IV.10	Cross sectional $\langle 110 \rangle$ lattice resolution TEM images showing $\{111\}$ faceting formation, and the subsequent stacking faults and twin nucleation for a $x=0.30$ Ge fraction. Extracted from [Paine <i>et al.</i> 1990].	79

IV.11 MD simulation snapshots of SPER for a Ge content of 53% after anneal at 1800 K for: (a) 15 ps, and (b) after complete recrystallization. Silicon atoms are shown in white, and Ge atoms are in green. $\{111\}$ facet formation is identified in red, twinning formation in yellow (also shown in the inset to clarify), and dislocations are in dark blue.	80
IV.12 Defect free layer thickness depending on the Ge fraction present in the annealed samples shown in blue. The lattice parameter dependence is also reported as a red line.	81
V.1 Schematic drawing of the 3D SiGe finFET structure. An isolation mask is used to protect the top of the substrate. The cross section is also illustrated.	86
V.2 Cross sectional TEM image of FinFET SiGe channel after reveal step, extracted from [Carter <i>et al.</i> 2018]. SiGe relaxation occurs along the Shallow Trench Isolation (STI) edge, acting as a free surface.	87
V.3 (a) Schematic view of coherently strained heteroepitaxial layers with equal lattice parameter for the substrate and the top film ($a_{Si} = a_{SiGe}$), and (b) relaxed structure with a misfit dislocation.	88
V.4 Process flow of the SiGe FinFET manufacturing: (a) void generation in the Si surface, (b) void refilling by SiGe in direct contact with the Si substrate, and (c) after the etching process where the final fin structure with Si S/D is shown.	89
V.5 Schematical view of the simulation box used for modeling SiGe FinFETs structures previous to the fin patterning. Atoms in the bottom slabs are held fixed during the annealing process.	90
V.6 Simulation snapshot of the structure once the annealing is complete. Defected areas are identified with letters: (a) - (c) corresponds to dislocation nucleation at the channel area, while (d) and (e) identify the twinning formation at the $\{111\}$ planes.	91
V.7 For $x = 1.0$, extracted atomistic structure of formed defects in Fig. V.6(b) and (e). Silicon atoms are identified in white, while Ge atoms are in green.	91

V.8	Formation of defects after the annealing process for $x=0.71$. Dislocations and twins are observed in the channel area as shown in the inset identified with (a), where Si atoms are in white, and Ge atoms in green. Defects in (b) and (c) corresponds to a dislocation and a twin, respectively.	93
V.9	TEM image of dislocation nucleation through strained relaxed SiGe buffer layer (SRB) into Si epi-layer, extracted from [Carter <i>et al.</i> 2018].	94
VI.1	Initial concentration profiles of Ge (in $\text{Si}_{0.95}\text{Ge}_{0.05}/\text{Si}$) and B (in Si and $\text{Si}_{0.95}\text{Ge}_{0.05}/\text{Si}$). Boron implantation is simulated according to experimental dose of $1 \times 10^{13} \text{ cm}^{-2}$ at 60 keV done in [Hasanuzzaman <i>et al.</i> 2016].	102
VI.2	Boron diffusion profiles in Si and $\text{Si}_{0.95}\text{Ge}_{0.05}/\text{Si}$ samples annealed at 970°C for 1 hour in N_2 . Ge interdiffusion profile is shown for the $\text{Si}_{0.95}\text{Ge}_{0.05}/\text{Si}$ sample. Initial profiles for both B and Ge are displayed in black.	105
A.1	Local distortion of Si lattice containing of two five-fold and two-seven fold membered rings. Atoms A and B are displaced. Extracted from [Prieto-Depedro <i>et al.</i> 2017].	109
A.2	Radial distribution function for α -Si obtained by the two techniques used in [Prieto-Depedro <i>et al.</i> 2017]. Results of RDF are also compared to experimental data from [Laaziri <i>et al.</i> 1999].	110
A.3	Angular distribution function for the α -Si phases obtained by the bond switching algorithm and the random method. Extracted from [Prieto-Depedro <i>et al.</i> 2017].	111

List of Tables

I.1	Molecular dynamics algorithm.	12
I.2	Residence-time algorithm, also known as Bortz, Kalos and Liebowitz (BKL) algorithm [Bortz <i>et al.</i> 1975].	15
III.1	LKMC parameters: Activation energy and prefactors. Extracted from [I.Martin-Bragado & Sklenard 2012].	51
IV.1	Recrystallization energy barriers calculated by NEB method for different configurations at the interface. The slowest configuration is considered as the limiting rate, highlighted in bold. Activation energies are in eV.	78
V.1	Summary of the found extended defects depending on the Ge fraction.	92
VI.1	OKMC parameters for native point defect and boron diffusion in $\text{Si}_{1-x}\text{Ge}_x$ / Si structures, for $0 \leq x \leq 0.4$. Extracted from [Dopico <i>et al.</i> 2014].	104

Technological context

As microelectronic device dimensions keep scaling for performance enhancement, the conventional planar CMOS technologies face several challenges in terms of gate length. As a consequence, new replacements have to be introduced to ensure low-power and high speed operation capabilities for the current 10 nm level nodes and beyond, such as planar Fully Depleted Silicon on Insulator (FDSOI) or Fin Field Effect Transistors (FinFETs). Moreover, the 3D sequential integration offers an alternative to conventional scaling while improving integration density. Transistor levels are fabricated sequentially over the same substrate, which requires low thermal budget processing in order to preserve underlying transistors from any degradation. The Solid Phase Epitaxial Regrowth (SPER) is the best technological option to meet the junction formation requirements. This technique involves the amorphization and further regrowth of a crystalline substrate, where the solid-solid amorphous to crystalline transitions are modeled by atomistic simulation techniques.

Contents

1	Roadmap of device scaling	2
2	Low thermal budget in junction formation	4
3	The regrowth process	6
3.1	Amorphization	6
3.2	Recrystallization	7
4	Modeling SPER	8
4.1	The needs for multiscale	8
4.2	Ab initio	10
4.3	Molecular Dynamics	11
4.4	Monte Carlo Methods	13
4.4.1	Determining the rates	14
5	Introducing MMonCa	16
6	Goal of this work	17

Figure I.1: Evolution of device structures depending on the gate length (blue line) and total number of transistors (red line). Extracted data from [Schwierz *et al.* 2015].

1 Roadmap of device scaling

The demanding requirements of semiconductor manufacturing have driven the reduction of microelectronic device dimensions in order to achieve more powerful circuits with higher density. According to Moore's law, since 1965 the number of transistors on a chip has doubled roughly every 18 months. Back then, the number of components was 32 and today there are more than half a billion transistors integrated on a single microprocessor, meaning this prediction has been satisfied until recently, while improving device performance and profit margins for every new generation of integrated circuits. The stated evolution is shown in Fig. I.1.

However, the limit of scaling is being approached since transistor dimensions are on pace to reach atomic scale by the end of next decade. As a consequence of this aggressively scaling several problems have arisen, such as the short channel effect (SCE), where the source and drain are brought into proximity and the gate loses the control of channel electric carriers; the expanding external resistance in abrupt junctions or the substantial increasing in leakage currents due to the reduction of threshold voltages, key for low power consumption.

This approach to miniaturization impacts also the device fabrication regarding the photolithography processes for shrinking the size of the components and the etching

Figure I.2: 3D sequential integration flow process. (a) The bottom level transistor is processed with a high temperature budget, (b) then a high quality film is deposited, and (c) finally the top transistor is fabricated with a low thermal budget procedure.

Figure I.3: TEM cross-section image of two stacked FDSOI transistors with a gate length of 50 nm and ultra thin interlayer dielectric of 23 nm. Image taken from [Batude *et al.* 2011].

systems, increasing the cost-per-function. Among others, these facts make the conventional device scaling an extremely challenging technique, and so new alternatives have to be investigated including new device geometries, like ultrathin channel structures or multiple gates, the introduction of non-based silicon technologies, such as III-V materials, and innovative fabrication processes as the extreme ultraviolet lithography (EUV).

Nowadays, promising technologies appear to be an alternative to device scaling in terms of junction formation. For the current 14-10 nm technology nodes, the microelectronic industry best options are the planar fully depleted Silicon on Insulator (FDSOI) devices or multiple gates FETs, offering faster circuits with low power consumption, and excellent SCE and leakage control. Particularly, FinFET devices have

Figure I.4: Hole mobility incremental performance as function of Ge composition for relaxed and strained SiGe PMOSFET along $\langle 110 \rangle$ channel direction and (001) wafer orientation. Data extracted from [Cheng *et al.* 2015].

made an important contribution in the transition from the planar conventional CMOS since the performance is remarkably improved due to high mobility channels where strain engineering is crucial. This novel technique in 3D architectures has renewed the interest in SiGe alloys as a stressor material in source/drain (S/D) regions in Si-based technologies, evidenced as an efficient way for drive current enhancement. The presence of moderate Ge content does not provide relevant short-channel benefit over Si, and consequently the Ge fraction has been increased from 17% to 40% in 90 nm to 22 nm respectively [Ghani *et al.* 2003, Auth *et al.* 2012, Thompson *et al.* 2004a, Mistry *et al.* 2007]. The hole incremental mobility as function of Ge mole fraction for (001) wafer orientation and $\langle 110 \rangle$ channel direction is shown in Fig. I.4. However, the embedded SiGe in S/D areas is significantly challenge for the current gate length, and SiGe has become an attractive channel replacement for advanced FinFETs generations [Ok *et al.* 2010].

2 Low thermal budget in junction formation

As microelectronics scales down facing several challenges, monolithic 3D (3DMI) sequential integration has been explored in recent years as a competitor for sub 22 nm technology nodes, providing an alternative approach to conventional scaling. This technology consists of processing transistor levels sequentially one after the other, and then connect stacked layers at the transistor scale [Batude *et al.* 2011], enabling ultra-high

Figure I.5: Low thermal budget design temperatures of the critical steps in 3DMI. Stars represent the target temperatures to preserve the bottom layers. Filled circles are the performed temperatures for standard processes. Data extracted from [Cheramy *et al.* 2017]

density vertical connections due to the great alignment accuracy ($\sigma \sim 10$ nm [Batude *et al.* 2008] against $\sigma \sim 0.5$ μ m [Topol *et al.* 2005] for parallel integration). Top transistors are subsequently fabricated with a low thermal budget in order to preserve the underlying devices. Limiting temperatures for this preservation of the bottom level from any degradation depend on the considered technology, for 14 nm FSDOI architectures the process temperature is under 500 °C [Micout *et al.* 2017]. The basic integration flow of two transistor levels is shown in Fig. I.2, (a) optimized FSDOI transistor is fabricated on the bottom layer at standard high temperature. Thin interlayer dielectric (ILD) is deposited, followed by low temperature (LT) molecular bonding [Batude *et al.* 2011] of SOI substrate to obtain the top film layer, which enables the full transfer of monocrystalline Si layer (b). Finally, (c) the top transistor is processed at low temperature. Fig. I.3 shows transmission electron microscopy (TEM) cross-section of a 3D sequential structure with two stacked FSDOI transistors [Batude *et al.* 2011].

The desired temperatures of the critical steps for low thermal budget fabrication are shown in Fig. I.5. As represented, the main challenge in thermal budget reduction is the dopant activation process, typically performed at temperatures higher than 1000 °C by spike annealing. To meet the LT requirements, dopants can be activated through solid phase epitaxial regrowth (SPER), enabling the formation of high performance and shallow junctions.

Figure I.6: Schematic representation of a single ion collision in the crystalline lattice (a), and the resulting cascade (b). If the implanted ion transfers enough energy to a substitutional atom, it is displaced from its lattice site creating vacancy defects (dotted circles), and becoming interstitial atoms (red and blue circles). If interstitials have enough energy may affect in turn other substitutional atoms, generating damage cascades.

3 The regrowth process

3.1 Amorphization

Dopant atoms are introduced into the substrate by ion implantation, which consists of the introduction of accelerated ions into the solid surface producing radiation damage when a moving ion transfers enough energy to a target atom and displaces it from its lattice site [Gibbons 1972]. The expelled atoms, due to the transferred kinetic energy after the collision, move through the lattice as interstitial defects and may collide in turn with other lattice atoms, creating the so-called cascades consisted of successive collision events. Also, upon implantation the created defects tend to recombine if there is enough lattice vibration, and their lifetime depends on the dose of implanted species and temperature [Posselt *et al.* 2001]. The entire process is represented in Fig. I.6 for a single ion implantation.

Interstitials (I) and vacancies (V) interact with each other and may annihilate if the energy barrier of the process is overcome (~ 1.23 eV [Tang *et al.* 1997]). These so-called IV pairs are referred as a bond defect, as they induce a local distortion of the lattice creating two five-fold and two seven-fold membered rings packed together, typical of the amorphous state in diamond lattice [Marqués *et al.* 2003], as shown in Fig. I.7. This kind of defect plays a key role in the amorphization process, as it becomes more stable as surrounded by more bond defects, and as a consequence amorphous pockets grow until a continuous amorphous layer on the top of the crystalline surface is formed, as represented in Fig. I.8. At this point, within the LT process, the partial amorphization of the substrate has been achieved as the α/c phase is created according to the implantation dose in selected areas.

Figure I.7: Atomic configuration of the bond defect. The local distortion of the lattice consists of five-fold and seven-fold membered rings. Gray and white atoms represent the plane along $\langle 001 \rangle$ direction. Atoms in rotated ion-pair are colored in black.

The accuracy of the pre-amorphization step is crucial, and it should be pointed out how difficult is controlling such process regarding FDSOI architectures with thicknesses below 30 nm. On the one hand, low amorphization rates imply less active dopants in the substrate, meaning the device may not perform as expected. On the other hand, deep amorphization could impact the crystalline seed at the bottom, and so SPER does not take place in the absence of a proper crystalline seed. In these cases, recrystallization may occur through Random Nucleation Growth (RNG), leading to the formation of agglomerates which evolve into crystallites with a poor electrical performance. Fortunately, RNG does not happen in the LT due to its high activation energy (~ 4 eV) [Olson & Roth 1988].

3.2 Recrystallization

Once the amorphous phase is created, a subsequent layer-by-layer recrystallization process from the α/c interface is carried out by thermal annealing at a temperature below 500 °C for Si and 350 °C for Ge [Johnson *et al.* 2015], and so SPER takes place. During the solid-solid amorphous to crystalline transitions, dopant impurities present in the amorphous regions are incorporated into lattice sites becoming electrically active. The thermal stability of the activated dopant profile is critical in LT regime, as further processing at temperatures greater than the SPER anneal may lead to dopant deactivation, increasing the sheet resistance and so degrading device performance [Duffy 2014].

In addition, another drawbacks arise during SPER, making this process a very complex phenomenon. SPER is well known to have anisotropic behaviour and being strongly dependent on stress and the presence of impurities. And finally, the need to control the formation of defects during the recrystallization, such as point defects,

Figure I.8: Stages of the ion implantation after continuous cascades leading to the formation of a complete amorphous layer on the top of the ionized surface. (a) Interstitials (blue circles) and vacancies (dotted circles) are generated, see Fig. I.6. If they do not recombine, amorphous pockets may appear (b) and continue growing until a complete amorphous layer is obtained (c).

dislocations loops, microtwins and stacking fault concentrations. These defects may cause severe junction leakage when generated in the area beyond the α -c interface, and even dopant diffusion and deactivation [Jin *et al.* 2002].

4 Modeling SPER

The need to optimize the junction formation processes at low temperatures has stimulated the interest in the mechanisms of atomic rearrangement at the epitaxial interface. Indeed during SPER, the movements of adatoms and their corresponding bonding configuration at the interface are responsible for the macroscopic evolution of the growing film, and as a consequence, modeling epitaxial growth has become a challenging multiscale problem. To reach the time and length scales involved in several phenomena, atomistic models have to be used to further describe applications at continuum scale by incorporating such atomistic effects, and finally bridge the gap between these different models. With the advent of powerful simulation techniques and deep understanding of physical phenomena occurring during the regrowth process this goal can be achieved.

4.1 The needs for multiscale

Reducing the large dependence on the costly and time consuming empirical approach of materials development is still a significant challenge. Basic understanding of physical models and the advent in multiscale and computing technology play a key role to support future material discovery and design. The relevance of such increasing interest

Figure I.9: Time and length scales of the modeling techniques.

in multiscale modeling techniques is due to the reliability in predicting properties of these new materials and processes whose performance extends over many scales in time and space.

However, extracting meaningful information from mechanisms taken place at lower scales in order to extend to largers in a consistent manner has inherent issues. To bridge the wide range of time and length scales, it is necessary to deal with a hierarchy of models of physics. This sequential approach could lead to error propagation within the multiscale model, emerging the need for the validation of the physical consistency by comparing to empirical or well established single scale models. In addition, another issue is the availability of tools at the computational level as well as software enviroments, for programming and performing simulations.

Despite all these challenges, multiscale modeling is an actively and widespread approach in most scientific and technological advances, specially on nanotechnology. The nanoscale is an area with relevance in both the physics involved and the large impact on potential applications, especially on novel devices where modern manufacturing techniques require better insight of length/time scales for further performance improvement.

These complex materials exhibit interesting features which are dependent on their low-scale properties, and so models and constitutive relations are required for an accurate description of the behaviour of nanomaterials, as illustrated in Fig. I.9. As a consequence, the needs for multiscale techniques to link the atomic level structure with

the effective properties of these complex systems, in such a way that the microscopic models provide the information to account the influence of atomistic mechanisms on the macroscopic behaviour of the system. To establish such connection, hierarchical handshaking is crucial.

Throughout the present work, different simulation techniques are going to be used aimed at modeling the SPER process. Linking models allows to extend atomistic effects into a continuum and statistical approach, and give a comprehensive description of the phenomena under study.

4.2 Ab initio

Starting from the bottom-up, *ab initio* methods allow to determine fundamental properties of materials based on the laws of quantum mechanics. The underlying core is the resolution of the many-body Schrödinger equation for systems containing from tens to thousands of atoms. Given the position of a set of atom nuclei and the total number of electrons:

$$\mathcal{H}\Psi = E\Psi, \quad (\text{I.1})$$

where $\mathcal{H}$ is the Hamiltonian of the structure, Ψ the wavefunction and E the total energy of the system. The computational complexity grows exponentially with the number of atoms, and so several approaches have arisen to be able to solve it. Non relativistic Born-Oppenheimer approximation assumes that electrons move much faster than nuclei, as they are thousands of times lighter. As a consequence the electronic and nuclei motion are decoupled, and so the problem is reduced to solve the time independent Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{1}{\Psi(r)} \nabla^2 \Psi(r) + V(r)\Psi(r) = E\Psi(r), \quad (\text{I.2})$$

being $\hbar = h/2\pi$ where h is Planck's constant and $V(r)$ the potential energy function.

A well defined theoretical framework are the wavefunction-based approaches. The simplest one is the Hartree-Fock method, which produces reasonable results for many properties, by using the variational theorem to obtain an approximate solution. However it neglects electron correlation in electronic structure calculations, which implies each electron accounts the rest of them as a mean-field. Another drawback is the high computational effort, calculations for a N-system atom scale as N^4 [Leach 2001].

A complementary approach to Hartree-Fock is the density functional theory (DFT), based on the Hohenberg-Kohn theorem [Hohenberg & Kohn 1964] which states that the ground state electronic energy is uniquely determine by the electron density, $E(\rho)$.

Despite several approaches are to be made of the correct functional of energy, DFT calculations are feasible for realistic models and accurately predict material properties. But some care is to be taken, for instance band gap problems of generalized gradient approximation (GGA).

4.3 Molecular Dynamics

Molecular Dynamics (MD) is a well known deterministic technique for computing the equilibrium and transport properties of a classical many-body system. The dynamic evolution of the system containing N particles is followed in time according to laws of classical mechanics by solving the Newton's equations of motion until the properties no longer change with time. For the force calculation an interatomic potential is required to describe the interactions between all constituent particles. There are several types of potentials to be used depending on the demanded accuracy. Fundamental potentials derived from *ab initio* methods describe the system precisely but they are time-consuming in terms of computational costs. In contrast, empirical potentials reduce the computational demand though they need to be carefully fixed to a certain atom type. In fact the choice of the potential to study the physical phenomena depends on its reliability in predicting properties for which it has not been fit to. For crystalline silicon, several empirical potentials have been developed: Tersoff [Tersoff 1989], Stillinger-Weber [Stillinger & Weber 1985] or Bond Order Potential (BOP) [Gillespie *et al.* 2007].

The classical MD computational approach is shown in Table I.1, where position and velocities are obtained forward in time. Once the initial conditions of the run are set (e.g., initial temperature, number of particles, density, time step), for $t=0$, positions and velocities are assigned to each particle in the system. Next step is the force calculation, obtained from the interatomic potential in the system as $F_i = -\partial U / \partial r_i$. This is the most time consuming part of the simulation: the evaluation of the contribution to the force on particle i due to all its neighbors scales as N^2 [Frenkel & Smit 1996]. The most common technique used to speed up the simulation is the *Verlet list*, where only the particles within a cutoff distance (r_c) are considered in the computation of the forces, see Fig. I.10.

Finally, when all the forces between particles have been computed, the Newton's equations of motion can be integrated. In a classical approach the Hamiltonian can be identified with the total energy of the system as:

$$H(\mathbf{r}_i, \mathbf{p}_i) = \sum_{i=1}^N \frac{1}{2m} \mathbf{p}_i^2 + U(\mathbf{r}_i). \quad (\text{I.3})$$

Table I.1: Molecular dynamics algorithm.

call init	Initialize positions and velocities
t=0.0	Set time to 0
do while (t < t _{max})	for t < t _{max}
subroutine force(f,en)	Compute the force (F_i) and energy
subroutine integrate(f,en)	Solve Newton's equations of motion
t=t+deltat	Update time
call sample	Sample the time averages
enddo	If t > t _{max} stop

The equations of motion for a system with $H(r_i, p_i)$:

$$\frac{d\mathbf{r}_i}{dt} = \frac{\partial H}{\partial \mathbf{p}_i} \quad (\text{I.4})$$

$$\frac{d\mathbf{p}_i}{dt} = -\frac{\partial H}{\partial \mathbf{r}_i} \quad (\text{I.5})$$

From Eqs. I.3, I.4 and I.5:

$$m \frac{d^2 \mathbf{r}_i}{dt^2} = -\frac{\partial U(\mathbf{r}_i)}{\partial \mathbf{r}_i}. \quad (\text{I.6})$$

Then, the third law of Newton is obtained:

$$\mathbf{f}_i = m\mathbf{a}_i. \quad (\text{I.7})$$

One of the simplest numerical algorithms used to integrate Eq. I.6 is the Verlet algorithm given by [Verlet 1967, Verlet 1968]:

$$\frac{d^2 \vec{r}_i}{dt^2} = \frac{1}{\Delta t^2} (\vec{r}_i(t + \Delta t) - 2\vec{r}_i(t) + \vec{r}_i(t - \Delta t)) = \frac{\vec{F}_i(t)}{m_i}, \quad (\text{I.8})$$

solving Eq. I.8 for $t + \Delta t$:

$$\vec{r}_i(t + \Delta t) \sim 2\vec{r}_i(t) - \vec{r}_i(t - \Delta t) + \vec{F}_i(t) \frac{\Delta t^2}{m_i}. \quad (\text{I.9})$$

Velocity is not used to compute position in the next step, and it can be derived from Eq. I.9 as:

$$\vec{v}(t) = \frac{\vec{r}_i(t + \Delta t) - \vec{r}_i(t - \Delta t)}{2\Delta t}. \quad (\text{I.10})$$

The choice of the algorithm is crucial, there are several points to consider such as speed, energy conservation or accuracy for long time steps. Verlet algorithm has been evidenced as the simplest and most stable. It is fast, requires only little memory

Figure I.10: Verlet list approach. Being r_v the second cutoff radius, when a particle moves further than $r_v - r_c$, the Verlet list is update.

(useful in large systems simulations) and exhibits little long-term energy drift. Also, trajectories are kept close to the true ones for a time comparable to the duration of the simulation [Frenkel & Smit 1996].

4.4 Monte Carlo Methods

Despite the remarkable range of MD applications, there is an important limitation regarding the high computational cost due to the short time steps required for an accurate integration. As a consequence, the time and size-scale limitations of classical MD do not always allow to simulate conditions similar to real devices. Monte Carlo methods attempts to overcome this limitation.

It first appeared in the late 1940's with its most popular algorithm, Metropolis Monte Carlo [Metropolis & Ulam 1949] focused on studying thermal ensembles. Since then, relying on the use of random numbers, several algorithms have been developed to describe the state to state evolution of a given system, instead of following the whole trajectories through every vibrational period. As a result, large time and size scales are reach, allowing to extend the study into real applications. In the kinetic Monte Carlo method (KMC) [Young & Elcock 1966], the dynamic of a system is given by occassional transitions from one state to another separated by an energy barrier, identified as an event. A simple stochastic procedure is defined to propagate the system, assuming each transition depends only on the rate constants. If those are known *a priori* for every state, the evolution of the system is described over a vast time scale, typically seconds. For a current state, there is a set of pathways with their corresponding rate

Figure I.11: Schematic of the procedure for picking reaction pathway to advance the system to the next state in the standard KMC algorithm. Each event with a length proportional to the rate constant for its pathway are placed end to end.

constant (r), being the probability distribution for the first scape at time t :

$$f(t) = r \times \exp(-rt) \quad (\text{I.11})$$

The reaction pathway is picking up as shown in Fig. I.11. The events are placed end to end with a length proportional to the constant rate. Then a random number (s) is selected on the interval (0,1) multiplied by the total constant rate, $R = \sum_{i=1}^N r_i$, and the event with the rate $R_{n-1} < sR \leq R_n$ is chosen. To keep track of time, a random Δt from the exponential distribution is computed on the system as:

$$\Delta t = -\log(s')/R, \quad (\text{I.12})$$

being s' a second random number on (0,1). The described procedure is known as the residence-time algorithm [Bortz *et al.* 1975], see Table I.2, and it will be used throughout the present manuscript.

4.4.1 Determining the rates

Assuming all the possible pathways are known, the transition state theory (TST) [Laidler & King 1983] is the formalism used in many KMC methods to compute the transition rate constant for each pathway. Within the theoretical framework of TST, the rate constant for escape from state A to state B is approach to the equilibrium flux through the dividing surface between the two states, as shown in Fig. I.12, and expressed as [Glasstone *et al.* 1941]:

$$k^{TST} = \frac{k_B T}{h} \frac{Z_{\ddagger}}{Z_{min}}, \quad (\text{I.13})$$

Table I.2: Residence-time algorithm, also known as Bortz, Kalos and Liebowitz (BKL) algorithm [Bortz *et al.* 1975].

$t=0.0$	Set time to 0
do while ($t < t_{max}$)	for $t < t_{max}$
Listing r_i	Listing all the rates r_i for all possible events e_i
$R_N = \sum_i^N r_i$	Compute the cumulative function
$s \in [0, 1)$	Get a uniform random number
$R_n - 1 < sR \leq R_n$	Find the event e to perform
e_n	Carry out the chosen event
Update e_i and r_i	Update events and rates after transition
$s' \in (0, 1)$	Get a second uniform random number
$\Delta t = -\log s'/R$	
$t = t + \Delta t$	Update time
enddo	If $t > t_{max}$ stop

where $Z_{\ddagger}$ and Z_{min} are the partition function of the initial state and the dividing surface respectively, h is the Planck constant, k_B is the Boltzmann constant and T the temperature. The TST assumes successive crossings through the dividing surface are uncorrelated, however a trajectory may cross it more than once before escaping to state B or falling back to state A. Consequently, the partition function evaluation is not possible in reality and a further approach to TST is performed by most of KMC methods, the so-called Harmonic TST often referred as Vineyard theory [Vineyard 1957]. In HTST, the transition pathway is determined by a saddle point on the potential energy surface, which is well described with a second-order energy expansion leading to:

$$Z_{min} = \frac{\exp(-\beta V_{min})}{\prod_{i=1}^D \beta \hbar \omega_{min,i}} \quad (\text{I.14})$$

and

$$Z_{\ddagger} = \frac{\exp(-\beta V_{\ddagger})}{\prod_{i=1}^{D-1} \beta \hbar \omega_{\ddagger,i}} \quad (\text{I.15})$$

being $\beta = (k_B T)$, V_{min} and $V_{\ddagger}$ the potential energies for the minimum and saddle point respectively, $\hbar$ is the reduced Planck constant, ω is the vibrational frequencies of the

modes and D is total number of vibrational degrees of freedom, but free translations and rotations. From Eq. I.14 and I.15, Eq. I.13 yields the Vineyard expression [Voter 2005]:

$$k^{HTST} = v_0 \times \exp \frac{\Delta V}{k_B T}, \quad (\text{I.16})$$

where

$$v_0 = \frac{1}{2\pi} \frac{\prod_{i=1}^D \omega_{min,i}}{\prod_{i=1}^{D-1} \omega_{\ddagger,i}}, \quad (\text{I.17})$$

is the prefactor (input in KMC simulations), and ΔV is the energy barrier for a given transition, also known as the activation energy, E_a :

$$\Delta V = V_{\ddagger} - V_{min}. \quad (\text{I.18})$$

Figure I.12: Schematic of the kinetic transition for escape from state A to state B, given by the equilibrium outgoing flux through the dividing surface within the TST .

5 Introducing MMonCa

In this section the Modular Monte Carlo simulator **MMonCa** created by Dr. Ignacio Martin-Bragado is presented [MMonCa 2017]. **MMonCa** has been implemented in C++ and integrated with TCL library for user interaction via input script. There are two different modules:

- The lattice kinetic Monte Carlo (LKMC) module can be used independently or linked to the object KMC module. It is based on the "Lattice atom". Depending on the local configuration and other material properties, different events are

Figure I.13: Overall structure of the MMonCa simulator.

performed related to the atom position within the lattice. According to this approach it is mainly used to simulate phase changes such as Solid Phase Epitaxial Regrowth [Martin-Bragado 2011, I.Martin-Bragado & Sklenard 2012] and Solid Gas Epitaxy [Martin-Bragado & Moroz 2011], out of the scope of the present work. This module is used in chapter III.

- The object kinetic Monte Carlo (OKMC) is an off-lattice module and it is used to study the evolution of defects not assigned to specific positions of the lattice [Martin-Bragado *et al.* 2013]. This module is going to be introduced in chapter VI.

The simplified structure of the simulator is shown in Fig. I.13. The user interfaces through input scripts containing TCL commands, which are then internally mapped with MMonCa methods to perform the simulation.

6 Goal of this work

The final goal of this work is to model some of the junction fabrication processes for advanced node technologies of 10 nm and below, where different and critical mechanisms are studied as a multiscale phenomena. As introduced in the present chapter, the Solid Phase Epitaxial Regrowth (SPER) is the best option for the microelectronic industry in terms of dopant activation process in the low temperature regime, required for the formation of high performance and shallow junctions. The concept of SPER itself is introduced in chapter II, to give an overview of the fundamental mechanisms taken place during the regrowth as well as its numerous dependencies. More precisely, given the technological relevance of Si as the dominant material in the semiconductor industry, the multidirectional SPER of Si is studied in detail in chapter III. The great impact of stress in the formation of defects taken place during SPER is analyzed

by using different atomistic simulation techniques: Finite Element Methods (FEM), Molecular Dynamics (MD) and Lattice Kinetic Monte Carlo (LKMC) simulations. The three of them are hybridized to present a comprehensive multiscale description of the defect formation mechanisms during the evolution of SPER. As the downsizing of conventional CMOS technologies continues, new materials and architectures are considered as a potential replacement for Si-based technologies. As an example, current generations of devices are introducing SiGe alloys as a replacement of Si for p-type Metal-Oxide-Semiconductor Field Effect Transistors (p-MOSFET) due to a better hole and electron mobility. As SPER has been evidenced as a suitable technique to grow high quality SiGe layers over a Si substrate, modeling the microscopic mechanisms taking place during SPER of SiGe alloys has gained renewed interest. Consequently, chapter IV is focused on the study of the Ge composition dependence of SPER rates. The anomalous behaviour obtained from simulation results is described by using the Nudged Elastic Band method. Finally, chapter V deals with the strain relieving defects in SiGe channel FinFET technologies. The incorporation of SiGe as channel material has lead to the formation of defects at the interface, which are evaluated by using atomistic simulation techniques in order to determine the threshold Ge content for the nucleation of defective areas.

Introduction to the solid phase epitaxial regrowth

In this chapter the solid phase epitaxial regrowth (SPER) concept is introduced. To understanding the mechanisms of atomic rearrangement taken place during SPER, the atomic structure of the crystalline and the amorphous phases must be described, seen in section 1.1. In section 1.2, the thermodynamics of the recrystallization process is reviewed according to classic theories of nucleation and growth. Moreover, section 1.3 gets insight into the SPER kinetics to present the regrowth rate within the TST as stated in section 4.4.1 in Chapter I. The kinetics of SPER is described also in terms of the microscopic mechanisms taken place during SPER according to reported works in literature. The numerous SPER dependencies are described in sections 2, 3, 4, and 5 to take into account their influence into the physical phenomena studied in the following chapters.

Contents

1	The amorphous to crystalline transition	20
1.1	Atomic structure of crystalline and amorphous phases . .	20
1.2	On the thermodynamics of the crystalline transition . .	23
1.3	Kinetics of solid phase epitaxial regrowth	25
2	Anisotropic behaviour	28
3	Defect formation	30
4	Dopants and impurity concentration dependence	31
5	Hydrostatic and non-hydrostatic stress impact	33
6	Summary	34

1 The amorphous to crystalline transition

As previously described in Chapter I, SPER consists basically on the recrystallization of an amorphous phase which is in direct contact with a crystalline seed at an elevated temperature. This process has been studied for several decades as a single directional phenomena, being the roles of substrate orientation [Drosd & Washburn 1982, Ho *et al.* 1984, Csepregi *et al.* 1978], stress [Rudawski & Jones 2009, Rudawski *et al.* 2008b] and dopant and impurity concentrations [Johnson & McCallum 2010, Csepregi *et al.* 1977a] widely reported in literature. However, regarding the device processing, SPER must be considered as a multidirectional or patterned process due to the different crystallographic feature alignments acting during the front-end process of integrated circuits. To made progress in understanding multidirectional SPER, this section is focused on the kinetics and thermodynamics of its single direction counter part, as well as its numerous dependencies.

1.1 Atomic structure of crystalline and amorphous phases

Before discussing the kinetics of SPER, it is necessary to define the crystalline and the amorphous structures, as well as the interface between them. At ordinary pressure and temperature conditions, the lowest energy phase for crystalline Si and Ge is the diamond lattice, see Fig. II.1 (a). The four valence electrons bond purely covalent to four nearest neighbors at a distance of $a\sqrt{3}/4$ ($a_{Si} = 0.543$ nm and $a_{Ge} = 0.566$ nm), configuring a tetrahedral configuration with an angle of 109.47° . The resulting structure is composed of six-fold rings as shown in Fig. II.1, along [100] (b), [110] (c) and [111] (d) directions.

For SiGe alloys, the crystalline structure is the same as pure Si and Ge, since both atoms have the same electronic structure of sp^3 (as a result of $3s$ and $3p$ orbitals hybridization). Ge is soluble in Si at all compositions and temperatures forming a random alloy, where both types of atoms are placed into lattice sites. However, Ge atoms are bigger and the lattice constant is stated as a linear interpolation between the Si and Ge lattice parameters according to Vegard's law:

$$a_{Si_{1-x}Ge_x} = a_{Si}(1 - x) + a_{Ge}x, \quad (\text{II.1})$$

for $0 < x < 1$, being x the Ge composition. Unless neglected for simplicity, according to [Dismukes *et al.* 1964] and [Kasper *et al.* 1995], the actual lattice parameter differs from Vegard's law by a correction factor:

$$a_{Si_{1-x}Ge_x} = a_{Si}(1 - x) + a_{Ge}x + 0.02733x^2 - 0.02733x. \quad (\text{II.2})$$

Figure II.1: Schematic model of the crystalline network structure. (a) Three dimensional view, (b) $\langle 100 \rangle$ direction, (c) $\langle 110 \rangle$ direction and (d) $\langle 111 \rangle$ direction.

Figure II.2: Experimental pair correlation function of amorphous Si and Ge, from [Laazari *et al.* 1999] and [Ethernington *et al.* 1982], obtained by conventional diffraction methods.

The structure of the amorphous phase is not as easy to define, since both structural and electronic properties depend on the sample preparation (e.g. rapid quenching, ion implantation or low temperature deposition) and the thermal treatments. Several models consider the α - phase as a continuous random network (CNR), where there is a complete absence of translational symmetry [Spaepen 1978a, Saito & i. Ohdomari 1981]. Overall, the density is reduced about 1.8% as shown in experiments in [Custer *et al.* 1994] and the angular distribution presents a standard deviation equal to 10.6° [Djordjević *et al.* 1995].

To characterize such structural features of the amorphous phase a statistical description of the atomic distribution in space is used, the pair correlation function $g(r)$, i.e. the probability to find an atom between the spheres of radius r and $r + dr$ centered on any atom, given by:

$$g(r) = \frac{1}{4N\pi r^2\rho} \sum_{i,j} \delta(r - |R_i - R_j|), \quad (\text{II.3})$$

where $|R_i - R_j|$ is the distance between atoms i and j , ρ the average density and N the total number of atoms. Experimental pair correlation function of amorphous Si and Ge is shown in Fig. II.2, where at least two peaks are distinguishable, corresponding to the distances between first (2.35 and 2.45 Å) and second (3.83 and 4.00 Å) neighbors, respectively. The $g(r)$ analysis reveals only the short range order (SRO) is preserved when comparing to its crystalline counter part, since no peaks are shown further than 4 Å; while in the medium range there is a hierarchy of disorder and the long range order is totally absent. As a measure of the quality of the amorphous phase, the calculation of $g(r)$ is carried out in Appendix A.

In addition, the amorphous phase could be modeled by the presence of structural defects. As an anomaly of the covalent bond present in the SRO, the most general kind of defects are the dangling bonds (i.e. an unpaired electron within a distorted sp^3 orbital), with typical five- and seven- fold membered rings already shown in Fig. 1.7. According to this configuration, the orbital may accommodate a second electron, lost the unpaired electron or capture a hole, meaning the dangling bond may be in three charge states [Knief & von Nielsen 1999].

The interface between both phases is the starting point of the recrystallization process, where atoms are fully coordinated corresponding to a state of lowest energy [Spaepen 1978a]. Topological analysis of the interface evidences the formation of defects as the front advances, for instance the dimer bonds created at the initial stage of recrystallization that may lead to $\{111\}$ stacking fault formation as reported by [Munetoh *et al.* 2001]. The critical point for the formation of such defects among others, is the sharpness of the interface which causes strain accumulation, generating the greater distortion.

As a responsible for the nucleation through the α -c barrier, the interfacial tension has been measured as a relevant quantity to characterize the interface. Values for both Si and Ge are 0.49 J/m^2 [Bernstein *et al.* 1998] and 0.23 J/m^2 [Spaepen 1978a], respectively.

1.2 On the thermodynamics of the crystalline transition

The recrystallization process represents a transition from the amorphous to the crystalline phase, and such transition can be described by thermodynamics using macroscopic quantities according to classic theories of nucleation and growth. The transition is induced by driving forces, leading particles from the initial state to cross the phase boundary allowing the system to approach equilibrium conditions. Due to the lack of long range order, the α - phase has a higher Gibbs free energy per atom than the c-Si or c-Ge. As a consequence, the recrystallization reaction is thermodynamically favourable, since $\Delta G_{ac} > 0$. The total free energy of recrystallization is defined as:

$$\Delta G_{ac} = \Delta H_{ac}(T) - T\Delta S_{ac}(T), \quad (\text{II.4})$$

where ΔH_{ac} and ΔS_{ac} are the crystallization enthalpy and entropy, respectively. Values of ΔH_{ac} have been measured by using novel implantation and differential scanning calorimetry (DSC) techniques. Calorimetric measurements for α -Si and α -Ge reported by [Donovan *et al.* 1983] are $11.95 \pm 0.7 \text{ kJ/mole}$ and $11.66 \pm 0.7 \text{ kJ/mole}$, who evidenced α -Ge to relax continuously to an amorphous state of lower free energy, with a total enthalphy of relaxation of 6.0 kJ/mole before crystallization starts. While for α -Si no

evidence was found of heat release due to relaxation. In contrast, more recent studies show structural relaxation in α -Si as for α -Ge, with a value of total relaxation enthalphy of 5.3 kJ/mole [Roorda *et al.* 1991], determined to be proportional to the point defect concentration. In this approach, structural relaxation is understood as annihilation of network defects as inferred from electron spin resonance (ESR) [Spitzer *et al.* 1983] and luminescence measurements [Street 1981].

As Si and Ge are very similar, in both the amorphous and crystalline phases, structural relaxation in α -Ge may be also controlled by defects, which is the underlaying mechanism for a second approach where the structural relaxation is related to a lowering of the strain energy stored in the distorted bonds in the amorphous network, in agreement with Raman experiments in [Sinke *et al.* 1988]. The strain energy associated with bond-angle distortions is given by [Saito *et al.* 1982]:

$$U_{\Delta\theta} = \sum 6 \left[\frac{1}{2} k_{\Delta\theta} (r \Delta\theta)^2 \right], \quad (\text{II.5})$$

where $k_{\Delta\theta}$ is a constant and r is the atomic distance. The factor 6 is related to the number of bond pairs per atom, and the summation is extended over all atoms in the network.

Depending on the stored potential energy due to elastic deformation, there is a range of relaxation in the amorphous state. This relaxation in the amorphous network involves the rearrangement of bonds mediated by defects to a microscopic configuration where the bond angle distortion is minimum. Values of $\Delta\theta$ have been found to be 7° and 6° for α -Si and α -Ge [Tsu *et al.* 1984], respectively. The temperature dependent strain energy corresponding to $\Delta\theta$ is given by [Sinke *et al.* 1988]:

$$U_{\Delta\theta}(T) = U_0 - U_1 \exp(-E_a/k_B T), \quad (\text{II.6})$$

where U_0 and U_1 are constants, E_a is the activation energy and k_B is the Boltzmann constant. From Eq. II.6, the activation energy for structural relaxation is approximately 0.2 eV for both α -Si and α -Ge.

The second term in Eq. II.4 to determine the Gibbs free energy is the crystallization entropy. Based on the defect-free model to calculate the configurational entropy proposed by [Spaepen 1974], a value of 1.66 J/K/mol is estimated for a fourfold coordinated random network ($\Delta S_{\alpha c}^0$ at 0 K). Above this value, the entropy increases due to structural defects, given for a first order estimation by [Roorda & Sinke 1990]:

$$\Delta S_d = -x k_B \ln(x), \quad (\text{II.7})$$

where the concentration of defects is defined as $x = n/N$, being n the number of

Figure II.3: Schematic of the Gibbs free energy for a SPER reaction. Red line represents the structural relaxation taking place before the recrystallization starts.

defects distributed over N atoms, and assuming $x \ll 1$. The non equilibrium nature of involved defects limits the use of this model.

Another important point concerns the strong influence of density of defects on the melting temperature, [Roura *et al.* 2013] reported the melting temperature to span over a range of 280 K for α -Si. In terms of structural relaxation, the melting temperature is expected to increase when a full relaxation is possible, e.g. slow heating procedures. Experiments in [Grimaldi *et al.* 1991] show that unrelaxed α -Si melts at 115 K below its relaxed counter part. These values allow to conclude that the effect of defects on the melting temperature is more pronounced than the relaxation state.

1.3 Kinetics of solid phase epitaxial regrowth

The amorphous to crystalline transition has been described as a favourable reaction, since the crystalline phase has a lower free energy than the amorphous state and as a consequence atom positions are rearranged into those of the crystal by driving forces. In addition, the structural relaxation taking place before recrystallization decreases the excess of free energy as represented by the red-dashed line in Fig. II.3. However, the recrystallization is a thermal activated process with an energy barrier to overcome (ΔG^*). For high enough temperatures ($T_{Si}=500^\circ\text{C}$ and $T_{Ge}=350^\circ\text{C}$), crystallization occurs with increasing rapidity. The transition of an atom or group of atoms over the

Figure II.4: Schematics of single-dimensional patterned SPER process showing (a) the as-implanted state, (b) partial growth, and (c) completed SPER resulting in a single crystal.

α -c interface is entirely determined by the SPER rate given by the transition state theory (TST) [Olson & Roth 1988]:

$$v = \frac{k_B T}{h} f \lambda \left[1 - \exp\left(-\frac{\Delta G_{ac}}{k_B T}\right) \right] \times \exp\left(-\frac{\Delta G^*}{k_B T}\right), \quad (\text{II.8})$$

where f is the fraction of sites where the atomic rearrangement can occur, λ is the displacement distance of the interface for one rearrangement, and k_B is the Boltzmann constant. According to Eq. II.4, $\Delta G^* = \Delta H^* - T\Delta S^*$, where ΔH^* and ΔS^* are the activation enthalpy and entropy, respectively. Within the framework of the TST [Atkins 1986]:

$$E^* = \Delta H^* + k_B T \quad (\text{II.9})$$

For recrystallization reactions, $\Delta H^* \gg k_B T$, and so the activation free energy can be written as $\Delta G^* = E^* - T\Delta S^*$, where E^* is the activation energy, also identified as E_a . Consequently, Eq. II.8 can be expressed by an Arrhenius equation:

$$v = A \times \exp\left(-\frac{E_a}{k_B T}\right), \quad (\text{II.10})$$

where the prefactor v_0 is given by [Christian 1965]:

$$A = \frac{k_B T}{h} f \lambda \left[1 - \exp\left(-\frac{\Delta G_{ac}}{k_B T}\right) \right] \times \exp\left(-\frac{\Delta S^*}{k_B}\right). \quad (\text{II.11})$$

In the case of SPER, the rate can be measured by extracting the velocity of α -c interface as the layer by layer recrystallization proceeds, see schematics of SPER in Fig. II.4. The regrowth velocity has been measured at different temperatures by using

Figure II.5: Arrhenius fitting for Si(001) and Ge(001) for temperatures ranging from 500-800° and 315-530°, respectively. Extracted values of activation energy have been obtained from time-resolved reflectivity measurements (TRR) [Olson & Roth 1988, Csepregi *et al.* 1977b].

several experimental techniques in order to determine the activation energy for the SPER process, for both Si and Ge with values of 2.6-2.7 eV [Olson & Roth 1988, Roth *et al.* 1990, McCallum 1996] and 2.0-2.2 eV [Csepregi *et al.* 1977b, Johnson *et al.* 2008] respectively. Even for SiGe alloys the composition dependence of E_a has been reported in literature [Kringhoj & Elliman 1994] and will be introduced later in chapter IV.

Rates for Si(001) and Ge(001) as function of $1/k_B T$ are shown in Fig. II.5, extracted from [Olson & Roth 1988, Csepregi *et al.* 1977b]. From the Arrhenius plot, values of $E_a=2.7$ eV and $v_0=4.64 \times 10^6$ m/s for Si and $E_a=2.15$ eV and $v_0=2.6 \times 10^7$ m/s for Ge are obtained. SPER takes place also in the high temperature regime. [Olson & Roth 1988] conducted extensive studies in the regime over 1000°C, where the crystallization kinetics has been evidenced to be controlled by the same mechanisms as at lower temperatures. The single value of the activation energy implies there is only a rate limiting the SPER process at all temperatures.

The kinetics of SPER has been described also in terms of the microscopic mechanisms taken place during the recrystallization process by empirical models. As an example, [Spaepen 1978a] developed a model where the epitaxial regrowth is viewed as a bond rearrangement process occurring at the α -c interface, as the bond breaking

Figure II.6: Normalized regrowth rate at 550°C versus the substrate orientation dependence from (111) direction, extracted from [Csepregi *et al.* 1978] for Si and [Darby *et al.* 2013] for Ge. Relative dangling bond density is taken from [Custer *et al.* 1992].

and reconnection is propagated along a crystalline ledge. Based on the assumption that an atom becomes part of the crystalline phase when at least two neighbors are already in crystalline position, [Csepregi *et al.* 1977b] proposed that the regrowth takes place by lateral spread of {111} terraces at the interface. The kinetics of SPER has been also described by diffusion processes, where the crystallization is mediated by the diffusion of dangling bonds [Germain *et al.* 1983], or even by the diffusion of self-interstitials from the amorphous phase in order to enhance the bond rearrangement at the interface [Narayan 1982].

However, analytical models do not provide a clear picture of the competition of atomistic processes taken place during the recrystallization. Atomistic simulation techniques have been used throughout the present work in order to provide a further insight into the microscopic mechanisms underlying the SPER in Si and SiGe alloys, as will be largely discussed in chapters III and IV.

2 Anisotropic behaviour

The substrate orientation has a great influence on the SPER rate, as well as on the quality of the resulting crystal, for both Si and Ge. Velocity ratios of 24:7:1 for Si and 15:10:1 for Ge, along $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$, respectively have been reported

Figure II.7: Atomistic configurations for $\{110\}$, $\{100\}$ and $\{111\}$ growth planes. Atoms in gray color are attached to the crystalline phase when forming two undistorted bonds, highlighted in gray-dashed line.

by [Csepregi *et al.* 1978, Csepregi *et al.* 1977b]. Despite the relevant anisotropy regarding the SPER rates, activation energies do not vary with the substrate orientation, which suggests the nature of the underlying atomistic process does not change. Fig. II.6 shows the dependence of the SPER rate versus the substrate orientation angle (θ) from (111) direction in Si and Ge.

In order to explain such results, a simple bond-rearrangement model proposed by [Csepregi *et al.* 1978] success at qualitatively explaining the behaviour on $\{111\}$ and $\{100\}$ substrates, however it does not account for $\{110\}$ direction, neither the intrinsic formation of defects related to regrowth. [Drosd & Washburn 1982] presented a model based on the assumption that an atom must have formed two undistorted bonds to add the crystalline phase, where the undistorted bonds have the characteristic length and angle of the crystalline phase ($a_0\sqrt{3}/4$ and 109°). The nucleation of new atomic layers is shown for the three primary crystal surfaces, as shown in Fig. II.7. The regrowth of the $\{100\}$ plane occurs mediated by one single atom forming two bonds to the crystal, while the remaining bonds may be to α -atoms or unsatisfied. When the $\{110\}$ surface is involved, a cluster of two atoms is needed, each of them form two undistorted bonds. And finally, during $\{111\}$ crystallization, nucleation of a new layer requires three atoms to complete the sixfold ring. It should be pointed out that the present model is the basis of the LKMC model used through the present work, as will be shown in next sections.

Figure II.8: Schematic drawing of the two possible bonding positions at the $\{111\}$ planes: Normal (red) and twin (green) configurations.

3 Defect formation

Another important concern is the defective regrowth observed experimentally and confirmed by atomistic models. Due to the relevance in the final device performance, several contributions have been reported to give a further insight into the origin of defects in recrystallized layers [Saenger *et al.* 2007c, Burbure *et al.* 2007, Saenger *et al.* 2007b, Marqués *et al.* 2003, Prieto-Depedro *et al.* 2015].

The nucleation of microtwins in $\{111\}$ planes has been visualized by transmission electron microscopy (TEM) in [Jones *et al.* 1988]. The formation of this kind of defect depends on the two possible bonding positions of the three required atoms, since both keep the first neighbor distance and angles between bonds. Atoms attached in the correct position continue the normal stacking order of $\{111\}$ planes, and those attached with a twin orientation reverse such order as shown in Fig. II.8. As both may occur with the same probability, the resulting regrowth in $\{111\}$ direction is highly defected.

Despite no twin nucleation can be initiated in $\{100\}$ and $\{110\}$ planes, the formation of $\{111\}$ facets as the recrystallization occurs may lead into the formation of defects as they serve as a seed for further defective growth. Cross-sectional TEM images of Si fin field-effect transistors reported by [Duffy *et al.* 2007] show the aforementioned $\{111\}$ local configurations as the main source of twinning formation as regrowth proceeds over (110) direction, further confirmed by the predictive LKMC model presented by [Martin-Bragado 2011].

As in the case of Si, the characteristic $\{111\}$ facets have been observed also in (110) oriented Ge fins by high-resolution XTEM measurements [Duffy *et al.* 2011], leading to the formation of twin boundaries and even small crystallites, as shown in Fig. III.18.

Another complex shapes of recrystallization fronts have been studied, showing

Figure II.9: Cross-sectional TEM images showing a silicon fin (a) after implantation, (b) during annealing where the regrowth is not complete, and (c) once the recrystallization is complete and twin formation can be observed. Extracted from [Duffy *et al.* 2007].

the formation of small triangular edge pockets bounded by $\{111\}$ planes [Saenger *et al.* 2007b]. Moreover, mask-edge defects appear at the meeting point of different recrystallization fronts, which have been determined recently to be Frank partial loops [Shen *et al.* 2012]. This point will be largely discussed in next sections based on the atomistic simulation results obtained in the present work.

4 Dopants and impurity concentration dependence

The presence of electrically active and inactive species has a strong influence on growth kinetics. In the case of dopant impurities incorporated into lattice sites during SPER, these become electrically active and enhance the regrowth velocity in a linear way, as extracted from Rutherford backscattering measurements in [Csepregi *et al.* 1977a] for the case of P in Silicon, and further confirmed for As and B [Johnson & McCallum 2010]. To model such impact of doping impurities, the generalized Fermi-level shifting model (GFLS) first proposed by [Williams & Elliman 1983], accounts for the experimentally observed dopant enhancement of SPER rate in terms of structural changes at the α -c interface to shifts in the Fermi level. [Johnson *et al.* 2012] refined the GFLS model to study the effect of various dopants in Ge, where the presence of As and Al to concentrations greater than 1×10^{19} resulted in enhanced SPER rates [Johnson *et al.* 2008], in agreement with results reported by [Suni *et al.* 1982] where the SPER rate in As implanted α -Ge is 2.5 times faster than the intrinsic rate. However, at high dopant concentrations the regrowth rate does not increase anymore, suggesting

Figure II.10: XTEM images of Ge fins (a) when the recrystallization is not complete, (b) small defects formed in the amorphous Ge, and (c) $\{111\}$ facets seen at the foot of the fins. Extracted from [Duffy *et al.* 2011].

a competition between electrostatic and thermodynamical effects. This reduction may be affected also by the redistribution of the doping profile towards the surface during SPER, as reported for As SPER in Si [Demenev *et al.* 2012]. In the case of SiGe alloys, the effect of boron incorporation into substitutional positions has been studied by [Rodríguez *et al.* 1997]. The presence of B is evidenced to reduce the layer-substrate mismatch, and as a consequence there is a decrease of the average strain relaxation of the grown layers and a relevant increase of the defect-free layer thickness. This fact agrees with the investigations by [Rudawski *et al.* 2008a] where the dopants and stress are suggested to be synergistic in influencing the SPER kinetics. [D'Angelo *et al.* 2007] characterized B and Sb doped $\text{Si}_{0.83}\text{Ge}_{0.17}$ samples, showing an enhancement of SPER rate with no evidence of the final quality and structure of the regrowth SiGe.

The influence of electrically inactive impurities is totally different compared to dopant species, since the regrowth velocity decreases when increasing the impurity content. Extracted results from channeling effect measurements in [Kennedy *et al.* 1977] reveal that the presence of C, N and O in α -Si slows down the regrowth rate. Noble gas ions were also found to retard the velocity, even slower for Ar than for O. Another concern is the presence of water vapor in the annealing ambient, which results in the H infiltration into the substrate through the surface causing a retardation in velocity. The H diffusion does not penetrate as far into α -Ge as in α -Si, since the α -Ge is not able to form a stable native oxide [Johnson *et al.* 2008]. Despite this fact, the H infiltration has been shown to have a greater effect in Ge, where the SPER rate is reduced over 70%.

Another remarkable case is the Ge composition dependence of the SPER rate in

Figure II.11: SPER rates versus hydrostatic pressure for Ge(001) represented in red and Si(001) in blue, values extracted from [Lu *et al.* 1991].

SiGe alloys, that will be further investigated in chapter IV.

5 Hydrostatic and non-hydrostatic stress impact

The relevant effect of stress is an important fact to consider during device fabrication, and as a consequence several works have focused on the stress-influenced SPER. First experimental studies concerned the impact of pure hydrostatic stress (σ) on the recrystallization of Si(110) and Ge(100) [Lu *et al.* 1991], revealing an exponential enhancement of SPER rates under compression ($\sigma < 0$) as shown in Fig. II.11. When introducing the pressure dependent component in Eq. II.4:

$$\Delta G^* = \Delta E^* - T\Delta S^* + P\Delta V^*, \quad (\text{II.12})$$

where ΔV^* is the volume change upon recrystallization, also identified as activation volume and expressed as:

$$\Delta V^* = -k_B T \frac{\partial(\log v)}{\partial P}. \quad (\text{II.13})$$

By dropping the temperature dependence of ΔS^* , from Eq. II.8 the regrowth velocity upon pressure becomes:

$$v = v_0 \times \exp\left(-\frac{\Delta E^* + P\Delta V^*}{k_B T}\right). \quad (\text{II.14})$$

From fitting results in Fig. II.11 to Eq. II.14, extracted values for activation volumes are $\Delta V^* = -0.28\Omega_{Si}$ for silicon and $\Delta V^* = -0.46\Omega_{Ge}$ for germanium, where $\Omega_{Si} = 12.1\text{cm}^3/\text{mol}$ and $\Omega_{Ge} = 13.6\text{cm}^3/\text{mol}$. Negative values are consistent with the increasing SPER rates, since they lead to a decrease of the energy barrier. In addition, hydrostatic results from Eq. II.14, leads to assume SPER is controlled only by nucleation.

The case of non hydrostatic stress is of a great interest, as typical stresses involved during SPER process, even imposed during the device fabrication, are of this nature. The influence of stress on the velocity of a planar interface was first studied by [Aziz 1992], who observed the rate of SPER in Si is enhanced by uniaxial in-plane tension ($\sigma_{11} > 0$), and retarded under uniaxial in-plane compression ($\sigma_{11} < 0$), in contrast to the behaviour observed under hydrostatic pressure. From measurements over the range of ± 600 MPa in Si(001) elastically bent wafers, they extracted an activation strain tensor to determine the effect of an arbitrary stress (σ_{ij}) on v as:

$$v = v_0 \times \exp\left(\frac{\Delta V_{ij}^* \sigma_{ij}}{k_B T}\right), \quad (\text{II.15})$$

where the activation strain tensor (ΔV_{ij}^*) is analogue to the activation volume, and characterizes the kinetic response to nonhydrostatic stress as the volumetric deformation related to the transition from the initial state given by TST. [Rudawski *et al.* 2008a] studied the stressed-SPER up to 1.5 GPa of (001) Si and produced results that can not be explained by the previous model, as the enhancement of v is negligible under tensile stress and there is a rapid retardation with compression stress, approaching saturation at -0.5 GPa. These results suggest the SPER kinetics is mediated by crystal island nucleation with the subsequent island ledge migration. Uniaxial stressed-SPER for Ge substrates remains widely unstudied. Extracted results from [Hong *et al.* 1992] evidenced the presence of compressive stress as a responsible for the increase in the activation energy barrier of SPER for SiGe alloys, and lower when comparing to those of pure Si. In contrast, stress-relaxed alloys have larger rates than Si.

6 Summary

In this chapter a review of the Solid Phase epitaxial regrowth has been presented. Despite SPER is considered as multidirectional process due to the different crystallographic alignments acting during the junction formation process, its single direction counter part has been described in terms of its numerous dependencies to made progress in understanding the influence of external conditions over the process itself.

The atomic structure of the crystalline and amorphous phases is described to shed

light into the atomic rearrangements that may take place at the interface according to the diamond cubic crystal structure where atoms are attached in contact with the amorphous phase. The interface is presented as the starting point of the recrystallization process and it has been characterized for both Si and Ge throughout the present chapter.

Due to the remarkable attention attracted by SPER several experimental and theoretical studies have been carried out to get insight into its kinetics and thermodynamics for more than 50 years. In this chapter, the microscopic mechanisms of recrystallization have been identified according to these classical approaches of nucleation and growth, leading to frame the SPER rate within the TST as a favorable reaction dependent on temperature. Moreover, SPER has been evidenced as a very complex phenomenon due to its several dependencies, which may play an important role in the junction formation of advanced devices. SPER is well known to have anisotropic behaviour, being the SPER rates strongly influenced by the substrate orientation. In contrast, activation energies do not depend on this factor, suggesting the nature of the underlying atomistic process does not change with substrate orientation. Based on these observations, [Drosd & Washburn 1982] presented a model where an atom must have formed two undistorted bonds to attach the crystalline phase. This model will be used within the LKMC approach in chapter III. Another concern is the formation of defects, which has detrimental consequences to the final device performance. Due to its relevance, the nucleation of defects is described in detailed as well as the mechanisms responsible for their formation. In addition, SPER is an attractive technique for dopant activation since it allows the fabrication of highly activated junctions, and consequently the presence of the electrically active and inactive species has a strong influence on growth kinetics. Dopant impurities have been reported to enhance the regrowth velocity, as the case of P in Silicon, or As in Ge. Even the effect of B in SiGe alloys turns out to reduce the layer-substrate mismatch and so the formation of defects, suggesting dopants and stress are synergistic in influencing the SPER kinetics. Assuming all these facts, next chapters account for the SPER dependencies as basis to model the Solid Phase Epitaxial Regrowth as a multidirectional process.

Multidirectional SPER of intrinsic Silicon

During the device front-end processing the solid phase epitaxial regrowth (SPER) exhibits a multidirectional behaviour, and consequently studying this process has a great technological impact. In the present chapter the multidirectional SPER of intrinsic silicon is discussed, being the concept itself introduced in section 1. In section 2, the case of two dimensional SPER extended to multigate FinFET devices is modeled by using molecular dynamics simulations. The regrowth is observed to proceed normally from the bottom, however the presence of bounding materials acting as an insulator inhibits the regrowth at the lateral interfaces and leads to the formation of defects whose character and origin are studied for different crystallographic orientations. Moreover the regrowth of box-shaped amorphized regions is investigated in sections 3 and 4, where the regrowth takes place by competing fronts with different recrystallization rates. The great impact of stress in the formation of defects during the regrowth process is analyzed by using different atomistic simulation techniques. First of all, Finite Element Methods calculations are carried out to determine the strain pattern due to density variation between the amorphous and crystalline phases, and obtained results allows to conclude that defects are enforced by the presence of stress, seen in section 3.1. Next step in section 3.2 is performing MD simulations to obtain the fundamental mechanisms of such defects generation, further extended into LKMC in order to model realistic sample sizes and temperature conditions as seen in section 3.3.1. The three techniques are hybridized to present a comprehensive multiscale description of the defect formation during SPER. The same process is repeated for different mask patterns, see sections 4.1 and 4.2, where the SPER curvature dependence is studied.

Contents

1	Multidirectional SPER	38
2	Growth interface pinning	39
3	Regrowth of box-shaped amorphous regions	42

3.1	Intrinsic stress pattern: Finite element method calculations	44
3.2	MD simulations of SPER upon stress	45
3.3	Extended LKMC modeling of the defected regrowth . . .	50
3.3.1	LKMC model description	50
3.3.2	Modeling defects by LKMC	52
4	Regrowth of box-shaped amorphous regions without surface pinning	57
4.1	MD study of the SPER curvature dependence	57
4.2	Extended LKMC modeling in the absence of surface pinning	59
5	Summary	64

1 Multidirectional SPER

The single directional SPER has been widely discussed in chapter II and introduced as the basis for a further study of multidirectional SPER, where the regrowth is not as straightforward as in planar devices due to the multiple crystallographic orientations of the growth interface. Multidirectional SPER takes place when the amorphous region is directly bonded to a base crystalline substrate in more than one direction, in contrast to unidirectional SPER where the amorphous layer has an infinite lateral extent. Depending on the number of limited directions, multidirectional SPER can be a two- or three- dimensional process, with two or three recrystallization fronts with different rates, respectively. The recrystallization of line-shaped α -Si is expected to proceed with rectilinear fronts meeting at predetermined angles depending on the relative lateral and vertical SPER rates, where atoms in the encompassed amorphous Si are forced to add both sides almost simultaneously. These kind of structures are obtained when the amorphous regions are created by ion-implantation through a patterned mask, as shown schematically in Fig. III.1. In the following, this work makes progress in understanding multidirectional SPER and, more specifically, the underlying mechanisms of defect formation during the regrowth, as well as its relation with the presence of strain.

Figure III.1: Schematic of two dimensional SPER resulting from implanted mask: (a) the as-implanted state and (b) partial growth during recrystallization proceeding in both vertical and lateral directions.

2 Growth interface pinning

The case of two dimensional SPER is extended to multigate devices, where the shapes of recrystallization fronts can be unexpectedly complex due to the presence of lateral free surfaces or interfaces with amorphous SiO_2 for isolation purposes. SPER of trench-bounded α -Si has been addressed by [Burbure *et al.* 2007] for the conventional FET geometry, Si(001) surrounded by oxide-filled trenches aligned with $\langle 110 \rangle$ crystal in-plane directions. Recrystallization proceeds normally at the center, while the growth interface was evidenced to be pinned at the initial points of contact with the trenches. As a result, recrystallization at the edges stops on $\{111\}$ planes, where the regrowth is slow and highly defected as already described in section 3 in the previous chapter.

[Saenger *et al.* 2007a] confirmed the slow-growing at $\{111\}$ planes as the source of the trench-edge defects. Extracted cross-sectional TEM images from this work reveal the presence of defective Si bounded by a $\{111\}$ plane for trench-edges aligned perpendicular to $\langle 110 \rangle$ and $\langle 100 \rangle$ in-plane crystal directions, respectively. In contrast, no defects are found for Si(011) in $\langle 110 \rangle$ directions, as shown in Fig. III.2.

Defective features observed in experiments have been reproduced by using atomistic simulation techniques. [Martin-Bragado 2011] presented a predictive LKMC model that assumes the defective SPER in Si is mainly produced by local $\{111\}$ recrystallization events propagated by further annealing, shown as the source of twin boundary defect formation, also confirmed by MD simulations [Lampin & Krzeminski 2011, Marqués *et al.* 2012]. To get a further insight into the mechanisms leading to the generation of $\{111\}$ facets on nanometric multigate devices, MD simulations have been carried out to model the regrowth of fin structures as the schematic shown in Fig. III.3. SPER simulations considers $\langle 110 \rangle$ -aligned and $\langle 100 \rangle$ -aligned amorphous layers on Si(100) substrates, where a few atomic planes are held fixed at the bottom, acting as a substrate, and next to them crystalline atoms serving as a seed for the recrystallization process are in direct contact with the amorphous phase, created as explained in Ap-

Figure III.2: Cross-sectional TEM images from [Saenger *et al.* 2007a] of SiO_2 filled trenches leading to $\{111\}$ facets formation after annealing at 900°C in: (a) Si(001), (b) Si(011) substrates with insulator edges aligned with $\langle 110 \rangle$ crystal in-plane directions, and (c) Si(011) substrate aligned with $\langle 100 \rangle$ directions.

pendix A. To simulate the influence of surrounding SiO_2 , the atoms belonging to the outer amorphous layer are kept fixed, as they remain amorphous during the annealing step.

For the simulation of fin structures, periodic boundary conditions (PBC) are applied in parallel directions to the α -c interface, while the top surface is left free in order to accommodate volume variations. The annealing of the model nanostructure is simulated using Tersoff interatomic potential in its third parametrization (T3) [Tersoff 1989], which has been already evidenced to accurately reproduce properties of both α - and c - phases [Cook & Clancy 1993], and so it gives a feasible description of the interface [Lampin & Krzeminski 2009]. It should be pointed out a limitation attributed to the T3 potential, as it predicts an excessive high melting temperature of 2400 K [Marqus *et al.* 2001], well above experimental value of 1685 K for Si [Mayer & Lau 1990]. However, this weakness is the key to the observation of SPER using MD, since the phenomenon is fast enough for the technique at ~ 1500 K [Lampin & Krzeminski 2011]. The canonical NVT ensemble (i.e. fixed volume and temperature) is used. The Nose-Hoover thermostat controls the temperature during the initialization stage, where the system is annealed at 1000 K for 20 ps. After equilibration, samples are annealed at 1800 K for several nanoseconds, a temperature high enough to accelerate the system dynamics and keep SPER regime far from melting.

During the annealing regrowth proceeds vertically from the bottom crystalline part to top, but the presence of lateral interfaces retards the crystallization at these areas. As a consequence, crystallization is hindered and soon $\{111\}$ stacking faults are formed

Figure III.3: Schematic structure of a FinFET device: (a) plane and (b) cross view after implantation. The 3D structure introduces lateral interfaces with the SiO_2 present for isolation purposes.

at the sides, as observed in Fig. III.4. Notice that configuration shown in Fig. III.4(b) is a 4.6 nm wide Si fin patterned in $\langle 110 \rangle$ direction, where the total height of 13.8 nm is not shown for the sake of simplicity. These dimensions preserve the aspect ratio of the experimental structure in Fig. III.4(a), while allowing reasonable computer times. The presence of $\{111\}$ stacking faults retards further recrystallization along the regrowth front, where the nucleation of a new layer requires three atoms to complete the six fold ring with two possible bonding positions equally likely [Drosd & Washburn 1982], leading to twin boundary defect formation as shown in Fig. III.4(b). These results are in good agreement with experimental observations of Duffy et al. [Duffy *et al.* 2007] in Fig. III.4(a), who also reported random nucleation and growth events when SPER is significantly retarded. Based on these simulation results, surface proximity is evidenced as a responsible for the defected regrowth, as the limitation of $\{111\}$ stacking faults slows down the recrystallization and leads to twin boundary formation.

A rather different behaviour occurs when the fin is aligned along the $\langle 100 \rangle$ direction. Several snapshots taken during the annealing of a 4.3 nm wide Si fin, with a total height of 11.43 nm, evidence an enhancement in the recrystallization with respect to the $\langle 110 \rangle$ oriented fin. SPER proceeds normally along $\langle 100 \rangle$ direction, while the lateral interfaces are propagated much more slowly, which turns out in the formation of facets at 45° from vertical corresponding to $\{110\}$ planes, see Fig. III.5 (a). Further regrowth is templated by the formed $\{110\}$ plane leading to the defect-free recrystallization of Fig. III.5 (b), where no defects in the stacking sequence are found, in qualitative agreement with XTEM observations of [Saenger *et al.* 2007a].

Finally according to the Drosd and Washburn model [Drosd & Washburn 1982],

Figure III.4: Partial regrowth of trench-bounded $\langle 110 \rangle$ -aligned amorphous layer on Si(100): (a) Cross sectional TEM image after 60 s of annealing from [Duffy *et al.* 2007], and (b) MD snapshot of wide fin structure at $t=15$ ns. Blue lines indicate the $\{111\}$ stacking fault formation, which limits the typical form of an arrow tip. Inset in (b) illustrates the formation of $\{111\}$ twin boundaries highlighted in green.

the observed facet formation for the two fin configurations under study is explained from the atomistic point of view. According to Fig. III.6 (a), on the one hand, for the $\langle 110 \rangle$ -aligned structures the regrowth takes place mediated by a single atom (A) forming two undistorted bonds to its first crystalline neighbors, occurring at center of the fin where the recrystallization proceeds in the $\langle 100 \rangle$ direction. In contrast, atoms at the lateral interface (B) have only one bond with the crystalline phase, and as a result the α -c interface is pinned at the contact points with the trenches resulting in the development of $\{111\}$ facets.

On the other hand as depicted in Fig. III.6 (b), for the $\langle 100 \rangle$ -aligned structures the atomistic configuration is quite different. Far from the interfaces, the recrystallization advances normally (A), while close to the lateral interfaces (B) and indirect mechanism is required. For a (B) atom to recrystallize and (A) atom has to recrystallize first in $\langle 100 \rangle$ direction. As the regrowth is faster in $\langle 100 \rangle$ than in $\langle 110 \rangle$ direction, the formation of $\{110\}$ planes appears.

3 Regrowth of box-shaped amorphous regions

[Cerva & Küsters 1989] were the first to study the regrowth of box-shaped amorphized regions by creating a sharply curved α -c interface under a mask ion-implantation of a

Figure III.5: Snapshots taken during MD annealing at 1800 K of a 4.3 nm wide fin structure aligned along the $\langle 100 \rangle$ direction after (b) 12 ns and (c) 60 ns. Blue lines indicates the lateral facet formation along $\{110\}$ planes at 45° from vertical.

(001) Si wafer with $\langle 110 \rangle$ -aligned SiO_2 lines. The subsequent annealing resulted in the formation of a notch near the initial corner and below the mask-edge, evolving to defect formation in the growth interface and propagated upwards to the surface when the two recrystallization fronts meet. This behaviour has been observed by several researchers, [Saenger *et al.* 2007a] evidenced the formation of downturned edges and their evolution to small triangular edge pockets of α -Si bounded by $\{111\}$ planes. Results from this work were extended into an heuristic model to explain the template of recrystallization in $\langle 110 \rangle$ -aligned α -Si lines in (001) and (011) substrates [Saenger *et al.* 2007c]. The complex shapes of 2D recrystallization fronts have been also modeled by using level set methods based on TEM images [Morarka *et al.* 2009], revealing how the interface curvature significantly affects the regrowth velocity, besides the inherent orientation of the substrate. As per the observations by [Rudawski *et al.* 2008b], it appears to be clear that the mask-edge defects are composed of shear- type or 60° type perfect dislocations with Burger's vector $a_0/2\langle 110 \rangle$ based on g_{220} bright field PTEM analysis. More recently, [Shen *et al.* 2012] determine these defects to be Frank partial loops with Burger vector $a_0/3\langle 111 \rangle$ from MD simulations and from TEM and Inverse-Fast-Fourier-Transform (IFFT) analysis. In addition, the formation of defects can be controlled with the presence of applied mechanical stresses [Rudawski *et al.* 2008b], giving rise to a new kind of Stress Memorization Techniques (SMT) to control the dislocation formation during SPER. As a result, many different types of mask-edge defects have been observed, though their origin remains unclear. The present section is aimed at modeling the defected regrowth of the 2D SPER process to gain a greater insight into the nature of defect formation mechanisms, and their relation with the presence of internal strains that may inhibit the recrystallization rates. To reach this

Figure III.6: Microscopic configurations indicating how atoms in the α -c interface have to rearrange for Si(100) substrates with SiO_2 edges aligned with (a) the crystal in-plane $\langle 110 \rangle$ direction, and (b) $\langle 100 \rangle$ direction.

goal, three different techniques are used within a multiscale approach: finite element method (FEM), molecular dynamics (MD) and lattice kinetic Monte Carlo (LKMC). FEM calculations provide the strain pattern generated by the volume expansion of the α -phase; while MD simulations determine the fundamental mechanisms of defect generation, further extended into LKMC to simulate realistic sample sizes and annealing temperatures.

3.1 Intrinsic stress pattern: Finite element method calculations

As the presence of strain is suspected to inhibit the recrystallization rates, thus inducing the formation of defects, the present study begins with the calculation of the initial strain pattern due to density variation between the α - and c- phases, as basis for the incoming work.

Since the volumetric strain due to α -Si is known (2% as suggested by [Custer *et al.* 1994]), a finite element model of the elastic response is employed to determine the complete elastic fields. As described by [Prieto-Depedro *et al.* 2015], each cell is represented by a standard isoparametric hexaedral element with an elastic constitutive law that includes an eigen-deformation corresponding to the volumetric strain [Hughes 1987]. The energy minimization of the complete body, including its boundary conditions, yields the displacement field in the instantaneous equilibrium, and can be used to derive local gradients like strains, stresses or other quantities of interest.

Fig. III.7 shows the dependence of the sample size on the presence of shear strain computed with the simple FEM model explained before. Fig. III.7 (a) and (b) corresponds respectively, to an α -Si rectangular region of $3.5 \times 13 \text{ (nm}^2\text{)}$ and $40 \times 143 \text{ (nm}^2\text{)}$ embedded in a c-Si template of $4 \times 14.0 \text{ (nm}^2\text{)}$ and $42 \times 146 \text{ (nm}^2\text{)}$. Strains are seen to

Figure III.7: Shear strain patterns generated by volume expansion of α -Si in a box-shaped amorphized structure for (a) MD domain size and (b) LKMC domain size. Taken from [Prieto-Depedro *et al.* 2015].

appear in the near vicinity of the interfaces, where atoms are slightly displaced to accomodate the volumetric expansion of α -Si. As observed, for very small amorphous regions about 10 nm, which can be simulated within reasonable computational time using MD, shear strain is almost negligible. In contrast, for larger sizes within the LKMC domain, the contribution of shear strain due to density variation between both phases is remarkable. It turns out that the effects of internal shear stress can not be studied by MD simulation techniques, but emulating such conditions by applying external in-plane compressions to the nanometric structures, similarly to work in [Rudawski *et al.* 2008b].

3.2 MD simulations of SPER upon stress

To elucidate the defect formation mechanisms and their nature, MD simulations have been carried out to model the regrowth of $\langle 110 \rangle$ and $\langle 100 \rangle$ -aligned structures in (001) and (011) Si, respectively. In this study the Tersoff interatomic potential is used in its third parametrization (T3) [Tersoff 1989], which has been reported to accurately reproduce properties of α - and c- phases in section 2. Moreover, T3 has been shown to be reliable at qualitatively modeling the formation of defects during SPER in Si nanodevices, see [Marqués *et al.* 2012, Lampin & Krzeminski 2009].

SPER simulations are carried out over the schematic structure shown in Fig. III.8, consisted of four different regions. A few atomic planes at the bottom are held fixed in

Figure III.8: Cross sectional schematics of (a) $\langle 110 \rangle$ -aligned shaped regions in (001) Si and (b) $\langle 100 \rangle$ -aligned shapes in (011) Si. Grey slabs represent fixed atoms used as a substrate. Atoms in the top slab are identified with filled trenches. Taken from [Prieto-Depedro *et al.* 2015]

their perfect lattice positions, identified as grey zones in the figure. These frozen atoms act as a substrate, and are in direct contact with crystalline atoms at lined regions, which serve as a seed for further recrystallization. Amorphous atoms to be recrystallized are in the white area, created according to Appendix A. The α -Si region placed at the top of the box acts as a filled trench, where atoms are also kept fixed in their random positions. The total size of the cell is $61 \times 148 \times 38$ ($\text{\AA}^3$) and $76 \times 150 \times 30$ ($\text{\AA}^3$) for $\langle 110 \rangle$ -aligned box-shaped in (001) and $\langle 100 \rangle$ -aligned box-shaped in (011), respectively.

PBC conditions are applied in parallel directions to the α -c interface, while in the normal direction atoms are sandwiched between the α -top slab, simulating the isolation by SiO_2 present in real samples, and the c-substrate at the bottom. As in section 2, the Nose-Hoover thermostat controls the temperature during the initialization stage, where the MD cell is preannealed at 1000 K for 20 ps, and then annealed at 2000 K for 4 ns to recrystallize from the interface. Atomic movements are determined by integrating the Verlet algorithm with a time step of 0.002 ps.

Based on the assumption that the anomalous recrystallization is due to the presence of a strain pattern, MD simulations are carried out under to different set of conditions:

- (a) In the absence of any external stress applied, referred to the pattern in Fig. III.7 (a).
- (b) Under an external uniaxial compressive stress applied to induce the internal strains present in larger sample sizes, as explained in section 3.1, and illustrated in Fig. III.7 (b).

In the second case, MD simulations are performed by compressing the simulation box by 0.5 nm on each side in the y -direction and maintaining the constraint during the whole annealing time. This compression induces an external stress within the range of 5-7 GPa, depending on the orientation of the crystalline substrate, as the threshold stress to generate defects is confirmed to exceed ~ 2 GPa by MD simulations done in the

Figure III.9: MD snapshots showing the cross sectional free-stress (a) $\langle 110 \rangle$ -aligned box-shaped in (001) Si and (b) $\langle 100 \rangle$ -aligned box-shaped in (011) Si, after 4 ps annealing at 2000 K. Twinning formation is identified with red-dashed lines. Extracted from [Prieto-Depedro *et al.* 2015].

present work. In the following, results obtained using the LAMMPS simulator [Plimpton 1995] are presented. According to conditions in (a), the relaxed structures are annealed until the complete recrystallization is reached. The rectangular shape of the amorphous region allows to observe the pinch-off points of the two regrowth fronts. MD snapshots in Fig. III.9 show the formation of twinning for both the $\langle 110 \rangle$ -aligned box-shaped in (001) Si and $\langle 110 \rangle$ -aligned box-shaped in (001) Si. However, the MD model does not catch the slower regrowth at the corners of the box-shaped α -region, hence the mask-edge defects are not formed. These results confirm the suppression of mask-edge defects in the absence of significant strain.

The next step to fully understand the influence of strain on the defect formation is to be carried out MD simulations under conditions in (b), i.e. the generation of defects is enforced by applying external in-plane compression stress. MD snapshots of different stages of the annealing of both structures under study are shown in Figures III.15 and III.14. In both cases, the SPER produces a characteristic $\{111\}$ faceting in the lateral fronts, as a result of the growth front intersect between the upper and lower lateral edges. In contrast, far from surface proximity the recrystallization proceeds normal in the vertical direction along $\langle 110 \rangle$ and $\langle 100 \rangle$ directions respectively, as shown in Figures III.15 (a) and III.14 (a). In particular, the recrystallization of the $\langle 110 \rangle$ /(001) structure shows the presence of the previously mentioned downturned edges, see Fig. III.15 (b). In the case of the $\langle 100 \rangle$ /(011) structure, the deviation of

Figure III.10: Cross sectional MD simulation snapshots of $\langle 110 \rangle$ -aligned box-shaped α -Si regions in (001) Si under compressive stress after annealing at 2000 K for (a) 0.3 ns and (b) 0.5 ns. Dashed-red lines illustrate defected regrowth zones. Published in [Prieto-Depedro *et al.* 2015].

rectilinear shapes is even greater than in $\langle 110 \rangle / (001)$, and as a consequence lateral facet points are well defined due to the prominent angle formed at the meeting point, as seen in Fig. III.14 (b). These situations are in good agreement with cross-sectional SEM observations shown in Fig. III.12. According to the nanofacet model proposed by [Saenger *et al.* 2007c], the SPER of α -Si bounded by two $\{111\}$ planes is free to continue templated by points at which the two $\{111\}$ planes meet at an angle of 70.6° (meeting point on $\{001\}$ growth planes) or 109.4° (meeting point on $\{011\}$ growth planes), which are well matched with MD geometrical predictions. MD goes further by distinguishing the nature of the formed defects, which are analyzed from final structures in Fig. III.13. The regrowth process produced twinning formation from the development of $\{111\}$ planes, identified in red. Again, the rotation angles measured are of 65° for both orientations, in agreement with the twin definition of 60° rotation with respect to one bond in the original tetrahedron, illustrated in Fig. II.8. Another interesting aspect of box-shaped regrowth is the generation of defects due to the slower regrowth at the corner of the amorphous regions clearly observed in Figures III.15 (a) and III.14 (a), resulting in dislocation formation when lateral and vertical fronts pinch-off, identified in blue in Fig. III.13 (a) and (b).

Despite this second mechanism has been identified as Frank Partial loops by contrasting MD simulation results with TEM images [Shen *et al.* 2012], its origin remains unclear. Based on the simulation results, it can be suspected that the density variation between both amorphous and crystalline phases may give rise to strain resulting

Figure III.11: Cross sectional MD simulation snapshots of $\langle 100 \rangle$ -aligned box-shaped α -Si regions in (011) Si under compressive stress after annealing at 2000 K for (a) 0.6 ns and (b) 1.2 ns. Dashed-red lines illustrate defected regrowth zones. Published in [Prieto-Depedro *et al.* 2015].

Figure III.12: Cross sectional SEM images of $\langle 110 \rangle$ -aligned lin-shaped α -Si regions in (001) Si: (a) as implanted; and after annealing at 550°C for (b) 6 min and (c) 12 min. And $\langle 100 \rangle$ -aligned lin-shaped α -Si regions in (011) Si: (d) as implanted; and after annealing at 550°C for (e) 12 min and (f) 24 min. Extracted from [Saenger *et al.* 2007b].

Figure III.13: Cross sectional images of the complete regrowth of (a) $\langle 110 \rangle$ -aligned box-shaped α -Si regions in (001) and (b) $\langle 100 \rangle$ -aligned box-shaped α -Si regions in (011), under compressive in-plane external stress. Blue lines identify the formed dislocations. Red lines indicate the presence of twins. Taken from [Prieto-Depedro *et al.* 2015].

in atom displacement at the lateral front with respect to those in the vertical, leading to dislocation nucleation when the two fronts collapse. As per of the structure sizes, the aforementioned strain is externally applied within the MD simulations domain, evidence of the great influence of strain in the mask-edge defect formation.

3.3 Extended LKMC modeling of the defected regrowth

Despite MD has made progress in understanding SPER microscopic mechanisms, simulation conditions are very different to those in actual devices due to the time and size scale limitations of the technique. Consequently, a LKMC approach fed with the outcome of MD simulations is introduced. The LKMC method, explained in detail in Section 3.3.1 in the present chapter, is integrated with a FEM module for the mechanical calculations, allowing to simulate realistic sample sizes and annealing temperatures and reproducing relevant features of the defected regrowth.

3.3.1 LKMC model description

LKMC describes the Solid Phase Epitaxial regrowth in terms of amorphous to crystalline transitions, where the rate of a recrystallization event corresponds to the probability per unit of time of an atom in the amorphous phase to join the crystalline region. The description of these events taken place at the interface is based on the

qualitative observations of [Drosd & Washburn 1982], and has been implemented in the modular Monte Carlo simulator MMonCa [I.Martin-Bragado *et al.* 2013]. Depending on the local regrowth plane, the model defines three main configurations for $\{100\}$, $\{110\}$ and $\{111\}$ local orientations at the α -c interface, according to the required number of atoms to form two undistorted bonds: 1, 2 and 3, respectively, see Fig. II.7. In the case of the $\{100\}$ configuration, lowly $\{100_l\}$ and highly $\{100_h\}$ coordinated sites are distinguished, according to the number of first and second neighbors [Martin-Bragado & Moroz 2011]. The stress-free recrystallization frequency within the TST is given by:

$$f = K(site) \times \exp(-E_a/(k_B T)), \quad (\text{III.1})$$

where $K(site)$ is the site dependent prefactor, and $k_B T$ has the usual meaning. The rest of the values are summarized in Table III.1 [I.Martin-Bragado & Sklenard 2012].

Table III.1: LKMC parameters: Activation energy and prefactors. Extracted from [I.Martin-Bragado & Sklenard 2012].

Parameter	Si
E_a	2.7
$K(\{100_l\}) (\times 10^{16} \text{ events s}^{-1})$	3.09
$K(\{100_h\}) (\times 10^{17} \text{ events s}^{-1})$	7.42
$K(\{110\}) (\times 10^{15} \text{ events s}^{-1})$	2.08
$K(\{111\}) (\times 10^{12} \text{ events s}^{-1})$	1.62

From MD simulations in Section 3.2, it turns out that there are three important physical mechanisms to be scaled up into LKMC:

1. The formation of twins.

The formation of twins has been implemented according to the model presented by [I.Martin-Bragado & Sklenard 2012], where twins are detected and placed in their lattice positions in order to reproduce realistic configurations further used by the simulator. Once the initial substrate is provided, the model determines the regrowth plane by computing first and second neighbor distances: atoms with two or three first neighbors belong to $\{100\}$, and atoms with only one crystalline first neighbor correspond to either $\{110\}$ or $\{111\}$ configurations. In the last case, if the atom has an amorphous neighbor with one crystalline, it is part of $\{110\}$, if not to $\{111\}$. When the crystallization front is determined, the crystal grows by picking the right match in the configuration table. For $\{100\}$ and $\{110\}$ configurations there is only one match, however for the $\{111\}$ there are actually two of them depending on the two possible bonding positions equally

likely. If the twin configuration is picked the stacking sequence is reversed, and the twin is attached at the α -c interface.

2. The slowed recrystallization near the corners as a consequence of the shear strain.

The presence of strain is included in the calculations by coupling the LKMC model to the FEM module explained in Section 3.1. Both techniques feed back each other iteratively as the structure changes by transforming α -Si into c-Si. At each step, the structure is accounted by the FEM module, which computes the strain associated with the volume expansion of the amorphous phase and transfers the strain back to modify the regrowth rates.

3. The collapse of the two recrystallization fronts induced by the presence of strain and the further dislocation nucleation. This fact is a natural cause of the two previous steps and does not need to be explicitly modeled.

Consequently, a correction factor must be introduced in the activation energy, which is done in two steps. First, the non-shear corrections are accounted by the activation strain tensor to characterize the dependence upon stress state of the phase transition, as described in detail in [Sklenard *et al.* 2013]. Then an extra slow-down produced by the shear strain ϵ_{xy} , as the regrowth Si is at higher energy state with additional strain energy, in agreement with experimental observations in [Shin *et al.* 2007]. Finally the activation energy is given by:

$$E = E_a + \epsilon_{xy}^2 K, \quad (\text{III.2})$$

being $K=9 \times 10^3$ eV, a fitted parameter to properly reproduce experimental observations.

3.3.2 Modeling defects by LKMC

In this section the LKMC model presented in Section 3.3.1 is used to study the regrowth of pattern regions, limited to $\langle 110 \rangle$ -aligned box-shaped amorphous regions in (001)Si and $\langle 100 \rangle$ -aligned box-shaped amorphous regions in (011) Si. Compared to experimental structures in Fig. III.12, simulation sizes have been reduced but the aspect ratio is preserved. The regrowth has been simulated using $42 \times 146 \times 20$ (nm³) boxes, where PBC are applied along z direction. Subsequent annealing takes place at temperatures of 550 °C for a maximum time of 15,000 s. According to the strain pattern reported in Fig. III.7, the size of the amorphous regions is big enough to produce internal strains that impact significantly on the recrystallization, and so external stresses are not applied.

Figure III.14: Recrystallization of $\langle 110 \rangle / (001)$ at 550 °C: (a) initial structure, after (b) 100 s, (c) 150 s, (d) 200 s, (e) 250 s, and (f) the complete regrowth has been achieved.

Figure III.15: Simulation snapshots of recrystallization of $\langle 100 \rangle / (011)$ at different stages of the anneal at 550 °C: (a) initial structure, after (b) 100 s, (c) 150 s, (d) 200 s, (e) 300 s, and (f) the complete regrowth has been achieved.

Figure III.16: Recrystallization analysis of [(a)-(e)] $\langle 110 \rangle / (001)$ and [(f)-(j)] $\langle 100 \rangle / (011)$ structures extracted from LKMC simulations. Defected regrowth regions are identified with dashed red lines. The $\{111\}$ faceting and the meeting point of the recrystallization fronts are highlighted for both cases. Extracted from [Prieto-Depedro *et al.* 2015].

Figure III.17: Cross-sectional TEM images of $\langle 110 \rangle$ -aligned α -Si in (a) (001) Si and (b) (011) Si taken from [Saenger *et al.* 2007b].

Figures III.14 and III.15 present several snapshots at different stages of the SPER process for the two orientations under study. For clarity, only atoms at the α -c interfaces are represented. As clearly observed in Fig. III.14 (b), (c) and (d) for the $\langle 110 \rangle$ -aligned box-shaped in (001)Si, and in Fig. III.15 (b), (c) and (d) for the $\langle 100 \rangle$ -aligned box-shaped in (011)Si, the regrowth is slowed down at the corners due to the presence of strain as shown in Fig. III.7. As a result of the lateral and vertical fronts pinch-off, the development of $\{111\}$ faceting is observed. This faceting leads a trace of defective regrowth in both cases, which is seen to be less defective in the case of $\langle 110 \rangle$ /(001) structures when compared to $\langle 100 \rangle$ /(011). As from the LKMC simulation results, no conclusions are extracted regarding the nature of the formed defects, the upscale technique is used to clarify the origin of the defective regrowth, analysed in detail in Fig. III.16.

Fig. III.16 (b) and (g) shows the formation of $\{111\}$ facets, acting as a template for the progressive recrystallization. The meeting point of the fronts takes place at an angle of 74.23° and 113.03° , for $\langle 110 \rangle$ /(001) and $\langle 110 \rangle$ /(001) respectively, in good agreement with the geometrical approach presented by [Saenger *et al.* 2007c]. For the $\langle 110 \rangle$ -aligned box-shaped in (001)Si, as previously observed in MD simulations, when the vertical regrowth front reaches the $\{111\}$ planes developed at the lateral facets, the expected formation of downturned edges occurs, which evolves into edge triangular pockets as shown in Fig. III.14 (e). These pockets remain after the complete recrystallization has been achieved. For the $\langle 100 \rangle$ -aligned box-shaped in (011)Si, the lateral facet points are well defined due to the prominent angle faces of the two fronts, shown in Fig. III.15 (h). As per of the MD simulations results, the defected regrowth observed by LKMC is concluded to be dislocation nucleation formed at the meeting point of the two ledges.

In general, the agreement with the evolution of similar topologies observed in experiments is remarkable [Morarka *et al.* 2009, Cerva & Küsters 1989, Rudawski *et al.* 2008b, Morarka *et al.* 2008] as seen in Fig. III.17, and evidences how the suc-

Figure III.18: Comparison of formed defects observed by XTEM (left) reported in [Saenger *et al.* 2007b] and predicted by LKMC model (right) for (a) $\langle 110 \rangle$ -aligned box-shaped in (001)Si and (b) $\langle 110 \rangle$ -aligned box-shaped in (011)Si. Taken from [Prieto-Depedro *et al.* 2015].

Successful transfer of meaningful information between MD and LKMC, as well as the hybridization with FEM, provide a reliable technique for simulating realistic experiments. In particular, for the validation of the extended defects predicted by LKMC, simulation results are compared to cross-sectional transmission electron microscopy (XTEM) images reported by [Saenger *et al.* 2007b], seen in Fig III.18.

Overall final structures are well matched, despite some discrepancies are also observed. It is interesting to note that the formation of twins predicted by LKMC, as well as by MD, is not observed in the XTEM images. Nevertheless, these differences may be explained by taking into account that two types of defects (twinning and dislocations) are present in the atomistic modeling, in contrast to the original model of [Saenger *et al.* 2007b]. Only dislocations might be clearly seen at the microscopy images without precluding that twins are also present in the samples in the positions predicted by the current work. According to XTEM images, the lattice resolution does not allow the detailed observation of defects smaller than 2 nm length. Otherwise, the invisibility can be explained by the viewing directions during TEM examinations, not adequate to observe twinning formation at the $\{111\}$ planes.

Figure III.19: Cross-sectional schematics of (a) $\langle 110 \rangle$ -aligned shaped regions in (001) Si and (b) $\langle 100 \rangle$ -aligned shapes in (011) Si. Grey slabs at the bottom represent fixed atoms used as a substrate in MD simulations. Atoms in the top slab, identified in light pink, simulate the presence of Si_3N_4 present in real samples.

4 Regrowth of box-shaped amorphous regions without surface pinning

In the present section, the regrowth of box-shaped amorphous regions where the α -c interface is not in direct contact with the surface and as a consequence not subjected to any surface pinning, is simulated. In the following, this kind of samples is referred to as being without regrowth interface pinning.

As evidenced before, predicting and modeling the evolution of the 2D SPER in patterned amorphized regions is crucial to understand the formation of mask edge defects, and consequently based on these results the influence of stress and the interface curvature have been analysed in structures lacking interfacial pinning. The simulated structures are based on the experimental observations in [Morarka *et al.* 2009], however for computational reasons the sizes have been reduced in both domains MD and LKMC while preserving the aspect ratio.

4.1 MD study of the SPER curvature dependence

First of all, a set of MD simulations have been conducted over the set up for $\langle 110 \rangle$ -aligned amorphous regions in (001) Si and $\langle 100 \rangle$ -aligned box-shaped in (011)Si shown in Fig. III.19. A few atomic planes are held fixed in their perfect lattice positions acting as a substrate. The top slab contains α -atoms, simulating the Si_3N_4 present in real samples, which remain amorphous during the annealing step. Finally, the amorphous region to be recrystallized is created as explained in Appendix A. The total size of the cell is $65 \times 231 \times 38 (\text{\AA}^3)$ and $76 \times 217 \times 30 (\text{\AA}^3)$ for $\langle 110 \rangle$ -aligned box-shaped in (001) and $\langle 100 \rangle$ -aligned box-shaped in (011), respectively. The rest of simulation conditions are the same as those described in Section 3.2.

Figure III.20: MD snapshots of the SPER process in $\langle 110 \rangle$ -aligned box-shaped in (001)Si structure without α -c interfacial pinning at the surface after annealing at 2000 K for (a) 0.3 ns and (b) 0.7 ns. Defected regrowth is highlighted in blue.

Equally to results in Section 3.2, the defect free recrystallization in the absence of stress is confirmed, as the box sizes do not induce intrinsic compressive stress and subsequent mask edge defects. The second step is compressing the simulation box by 0.5 nm on each side in the y -direction and maintaining the constraint during the annealing to enforce the mask edge defects formation. MD simulation snapshots of $\langle 110 \rangle$ -aligned box-shaped in (001)Si under external stress in the range of 5-7 GPa are shown in Fig. III.20.

The recrystallization is slowed down at the corners, where both concave and convex portions of the regrowth interface exists at the same time. After annealing for 0.3 ns as illustrated in Fig. III.20 (a), the concave portion becomes sharp while the convex begins to flatten; further annealing leads a trace of defects as represented in Fig. III.20 (b). These results are in good agreement with experimental XTEM observations in [Morarka *et al.* 2009], where the structure evolution is also modeled in terms of Level Set methods, see Fig. III.21.

Under the same conditions, for the case of $\langle 100 \rangle$ -aligned box-shaped in (011)Si, the propagation of sharp corners of the interface retards also the recrystallization in these areas, as clearly seen in Fig. III.22 (a). After annealing for 0.7 ns, as presented in Fig. III.22 (b), mask edge defects are formed as the corner region of the interface has impinged upon itself. As in the previous case, the convex part of the interface is flatten, however it is defined by $\{110\}$ planes which template further recrystallization. This second case has not been contrasted to other works, since to date there is no experimental study of the regrowth of $\langle 100 \rangle$ -aligned box-shaped in (011)Si structures without surface pinning. Once the complete recrystallization is reached, the formation

Figure III.21: XTEM images of the $\langle 110 \rangle$ -aligned shaped structure in (001) Si without interface pinning at the surface: (a) as-implanted, (b) after annealing for 2.5 h, (c) after annealing for 5.0 h and (d) after annealing for 10.0 h. Images (e)-(h) correspond to the level set simulation of the structure evolution. Extracted from [Morarka *et al.* 2009]

of defects is analysed according to Fig. III.23. Dislocations are nucleated at the pinch off points of the lateral and vertical fronts at the interface for the both type of structures under study, identified in blue in Fig. III.23. The formation and subsequent evolution of twins have been also observed, highlighted in red. For the $\langle 110 \rangle$ -aligned box-shaped α -Si regions in (001)Si the twinning formation takes place due to $\{111\}$ microscopic mechanisms where the SPER is slow and highly defective. In contrast, for the $\langle 100 \rangle$ -aligned box-shaped α -Si regions in (011)Si, the $\{110\}$ microscopic configurations are involved, which generate also larger twins at the edges.

4.2 Extended LKMC modeling in the absence of surface pinning

The LKMC model described in Section 3.3.1 is used again to simulate structures where regrowth interface pinning is not present. The SPER has been simulated using $42 \times 200 \times 20$ and $42 \times 186 \times 20$ (nm^3) boxes for $\langle 110 \rangle / (001)$ and $\langle 100 \rangle / (011)$ respectively, where PBC are applied along z direction. Subsequent annealing takes place at temperatures of 550°C for a maximum time of 15,000 s. The same simulation conditions as in Section 3.3.2 are applied.

Figures III.24 and III.25 show several snapshots at different stages of the SPER process for the two structures under study with an unpinned α -c interface. Again,

Figure III.22: MD snapshots of the SPER process in $\langle 100 \rangle$ -aligned box-shaped in (011) Si structure without α -c interfacial pinning at the surface after annealing at 2000 K for (a) 0.2 ns and (b) 0.7 ns. Defected regrowth is highlighted in blue.

Figure III.23: Cross sectional images of the complete regrowth of structures with no interfacial pinning: (a) $\langle 110 \rangle$ -aligned box-shaped α -Si regions in (001) Si and (b) $\langle 100 \rangle$ -aligned box-shaped α -Si regions in (011) Si, under compressive external stress. Blue lines identify the formed dislocations, and red lines the presence of twins.

Figure III.24: Simulation snapshots of recrystallization of $\langle 110 \rangle / (001)$ at different stages of the anneal at 550 °C: (a) initial structure, after (b) 100 s, (c) 200 s, (d) 300 s, (e) 400 s, and (f) the complete regrowth has been achieved.

only defected atoms and those at the interface are represented.

From Figures III.24 (b)-(d), the recrystallization is observed to be slowed down at the corners. The vertical front advances along $\langle 100 \rangle$ direction, until it collapses to the front advancing at the convex part of the interface resulting in $\{111\}$ faceting. After annealing for 450 s in Fig. III.24 (e), it appears that the lateral front is dissipated, and the regrowth proceeds through the vertical α -c direction leading a trace of defects. The regrowth has finished, but α -Si regions remain at the edges bounded by $\{111\}$ planes. In Fig. III.24 (f) these regions evolve templated by the $\{111\}$ planes where the regrowth is slow and highly defective. Extracted from MD results in Section 4.1, the defects are concluded to be dislocations formed at the corners due to the presence of stress induced by the curvature factor of the interface.

There is a good agreement when compared to experimental observations in [Morarka *et al.* 2009] and presented in Fig. III.21, where the formation of mask edge defects is reported to be formed at the corner regions, as detected also by LKMC simulations. Even the presence of α -Si triangular regions which remain under the mask edge once the recrystallization is complete is validated by the Level Set method used in the same work. The observed behaviour for $\langle 100 \rangle$ -aligned box-shaped α -Si regions in (011)Si is quite different. Fig. III.25 presents simulation snapshots at different stages of the anneal where the $\{110\}$ faceting is observed instead of $\{111\}$. As in the previous case the recrystallization is retarded at the corners, leading a trace of defects. Considering MD simulations results in Section 4.1, these are determined to be dislocations as in

Figure III.25: Simulation snapshots of recrystallization of $\langle 110 \rangle / \langle 001 \rangle$ at different stages of the anneal at 550 °C: (a) initial structure, after (b) 100 s, (c) 200 s, (d) 300 s, (e) 400 s, and (f) the complete regrowth has been achieved.

the previous case.

Finally, the linear dependence of the SPER velocity with interfacial curvature reported in [Morarka *et al.* 2009] is contrasted over the $\langle 110 \rangle$ -aligned box-shaped in (001) Si structures under study in Sections 3.3.2 and 4.2. The normalized regrowth velocity as function of the substrate orientation measured by [Csepregi *et al.* 1978] is extended to include the interfacial curvature dependence as [Morarka *et al.* 2009]:

$$v(\theta, \kappa) = v_{[001]} f(\theta) (a + A\kappa); \quad (\text{III.3})$$

where $v_{[001]}$ is the value of v along [001], $f(\theta)$ is temperature independent, A is a constant with units of length and κ is the curvature factor. Eq. III.3 implies that portions of the regrowth interface with $\kappa > 0$ should enhance the velocity, while $\kappa < 0$ should retard it. From results in Fig. III.14, where the regrowth front is concave type ($\kappa > 0$), Eq. III.3 appears to be valid. In contrast, for the SPER evolution of structures lacking interfacial pinning in Fig. III.24, where both concave and convex portions exist at the same time, the convex part ($\kappa < 0$) is flattened, and the regrowth is evidenced to be retarded at these areas. In particular, after 301 s SPER has finished for the structure studied in Section 3.3.2, while it was not the case for the structure without interface pinning represented in Fig. III.24 in the present section, where SPER takes almost 500 s to finish. Consequently, the curvature significantly influences the amount of localized internal stresses experienced by the α -c interface, which has been evidenced to alter

the kinetics of SPER and affecting the formation of mask edge defects as concluded in Section 3.

5 Summary

The study of the solid-phase epitaxial regrowth (SPER) of Si has been studied as a single directional phenomena for several decades. However regarding the device processing, SPER must be considered as multidirectional since the interface evolves through two- or three- fronts with different crystallographic orientations. Consequently, multidirectional SPER is not as straightforward as its single-direction counter part, and overall the process turns out in the generation of defects which impact the final device performance. The present chapter is aimed at determining the nature of the formed defects and its relation with the presence of stress patterns present during Si-based device fabrication.

First of all, the case of two dimensional SPER has been studied over nanometric multigate devices by using molecular dynamics simulations. During the FinFET fabrication process, devices are isolated by SiO₂, creating trench-bounded amorphous regions which have been shown to give rise to imperfect recrystallization. This anomalous regrowth has been investigated over $\langle 110 \rangle$ -aligned and $\langle 100 \rangle$ -aligned amorphous layers on Si(100) substrates. For the trench edges aligned with the crystal in-plane $\langle 110 \rangle$ direction, regrowth proceeds normally at the center of the structures under study, but the presence of lateral interfaces retards the recrystallization at these areas leading to the formation of $\{111\}$ planes where the regrowth is very slow and highly defected, the so-called trench edge defects. MD simulation results evidenced the formation of twin boundaries at the $\{111\}$ facets, which slows down further recrystallization along the regrowth front. In contrast, when the trenches are aligned along the $\langle 100 \rangle$ direction, an enhancement in the recrystallization is observed. Again, regrowth proceeds normally at the center of the fin structure, while lateral interfaces are propagated much more slowly leading to the formation of facets at 45° from vertical, corresponding to $\{110\}$ planes. Further regrowth is templated by these facets, evolving into a defect-free recrystallization. In both cases, MD results are in qualitative agreement with XTEM observations by [Saenger *et al.* 2007a], and the facet formation is explained in terms of the [Drosd & Washburn 1982] model from an atomistic point of view in order to catch the microscopic rearrangements during SPER of trench-bounded amorphous regions.

The chapter continues with the study of the regrowth of box-shaped amorphous regions, where the presence of two moving fronts creates complex shapes of recrystallization evolving into many different types of mask-edge defects with an unclear origin. To give a further insight into the nature of these defects, a comprehensive multiscale modeling of the process is presented for $\langle 110 \rangle$ -aligned box-shaped in (001)Si and $\langle 100 \rangle$ -aligned box-shaped in (011) Si structures. The study begins with the calculation of the initial stress pattern due to density variation between the α - and c -

phases, as SPER rates are suspected to be inhibited by the presence of strain. The calculations are performed by Finite Element Methods over two sample sizes, one of them within the MD time and space domain, and another realistic sample size. Results allow to conclude that the presence of strain is negligible for small amorphous regions about 10 nm, while strain is clearly observed at the near vicinity of interfaces for samples within the LKMC domain. Consequently, stress must be enforced to study the formation of defects by using MD, where simulations are carried out by applying an external in-plane compression to induce the intrinsic strain present in larger sample sizes. Under these conditions, two types of defects are observed. On the one hand, the formation of twins due to the stability of $\{111\}$ planes. And on the other hand, the nucleation of dislocations at the front meeting point, which have been determined to be produced by the presence of strain due to volumetric expansion of α -Si, since no dislocations are generated in the absence of external strain. MD simulation results feed an extended LKMC model which allows to simulate realistic sample sizes and temperature conditions. The model is hybridized by the FEM module to obtain the strain pattern due to the α -Si. Defects observed by LKMC are compared to XTEM images in [Saenger *et al.* 2007b], confirming the $\{111\}$ planes stability as a responsible for twinning formation as predicted by MD.

Finally, the chapter makes progress in understanding the curvature dependence of SPER by studying the regrowth over structures where the α -c interface is not in direct contact with the surface, and consequently is not subjected to any surface pinning. The annealing of the samples is carried out by MD, allowing to observe a trace of defects once the recrystallization is complete. Again dislocations are observed at the pinch off points of the lateral and vertical fronts, and also the formation and subsequent evolution of twins. The model is extended by using LKMC, where the final structure evolution is well matched with experimental observations by [Morarka *et al.* 2009].

Modeling SPER of SiGe alloys

Current generations of devices have incorporated SiGe alloys for performance enhancement, particularly the presence of Ge induces an uniaxial compressive strain in the channel area which significantly improves the hole mobility. For device manufacturing, the ability to grow strained and relaxed SiGe layers by means of solid phase epitaxial regrowth (SPER) is very attractive for the microelectronic industry and as a consequence SiGe SPER has gained renewed interest. The present work addresses the modeling of SPER in SiGe alloys as well as its underlying mechanisms. In section 2.1, the Ge composition dependence of SPER activation energies is investigated by using Molecular Dynamics simulations. The non-linear behaviour of the extracted profile of SPER activation energies is further analysed by using Nudged Elastic Band (NEB) calculations in section 2.2, where the energy barrier for an atom to attach the crystalline phase is computed to explain the MD observations. In addition, the study of the formed defects during SPER is done in section 3 to determine the influence of the Ge fraction in the evolution of the regrowth process.

Contents

1	Introduction to SiGe alloys	68
2	Germanium impact on SPER activation energy	70
2.1	Regrowth of relaxed SiGe alloys	70
2.1.1	Simulation set up	70
2.1.2	Results and observations	73
2.2	Nudged Elastic Band Calculations	74
3	Defect nucleation during SPER	78
3.1	Simulation details and observations	79
4	Summary	81

1 Introduction to SiGe alloys

As device scaling approaches fundamental limits of miniaturization, semiconductor manufacturing faces several challenges to meet performance requirements below the sub-10 nm gate regime. Although Si has prevailed over several decades as the preferred material for device fabrication due to its great properties, cost effectiveness and mature processing, various novel techniques and materials have been proposed as a potential replacement for Si-based technologies. Improvements in device capability such as mobility-enhancement obtained by strain engineering are of a great interest. In particular, current generations of devices are introducing SiGe alloys as a replacement of Si for p-type Metal-Oxide-Semiconductor Field Effect Transistors (p-MOSFET) due to a better hole mobility. For the 22 nm FinFET technology, selective epitaxial regrowth of SiGe layers has been integrated in the source drain areas to induce a compressive uniaxial strain in the channel region. To further enhance carrier mobility and current drive at the channel, the Ge content has been increased from 17% to 40% in 90 nm to 22 nm node respectively [Ghani *et al.* 2003, Auth *et al.* 2012, Thompson *et al.* 2004a, Mistry *et al.* 2007], as the epitaxial strain depends linearly on the Ge fraction offering a cost-efficient way to control the transport properties. However, for the current 10 nm technology node, the conventional strain engineering at source drain areas is extremely challenging, and consequently FinFETs with SiGe channel have recently drawn significant attention due to its superior hole transport properties [Nanda *et al.* 2015, Hashemi *et al.* 2015], since the presence of strain makes possible to move more current at lower voltages with immunity to short channel effect. For the device manufacturing, the integration of epitaxial SiGe layers in advanced channel structures demands low temperature budget, and SPER is a suitable technique with ability to grow both strained and relaxed SiGe layers. As a result, modeling SPER of SiGe alloys has gained renewed interest.

The case of SPER in pure Si and Ge has been widely modeled, as described in detail in chapter II. However, the SPER in SiGe alloys has not been yet thoroughly studied and the comprehension of the microcopic mechanisms taking place during SPER presents new challenges. The crystallization kinetics of fully relaxed $\text{Si}_{1-x}\text{Ge}_x$ alloy layers have been experimentally studied by [Kringhoj & Elliman 1994]. The extracted results revealed a non-linear activation energy profile depending on the germanium composition. For approximately $x=0.2$, the value exceeds the pure Si SPER activation energy. Accepting the bond breaking event as a responsible for the regrowth as described by the dangling bond model [Spaepen 1978b, Spaepen & Turnbull 1979], further confirmed by [Aziz 1992], the activation energy should decrease monotonically from the pure Si activation energy to the pure Ge value. Based on this assumption,

Figure IV.1: Schematic configuration of the simulation box. First atomic planes are held fixed acting as a substrate. Extracted from [Prieto-Depedro *et al.* 2017]

[Payet *et al.* 2015] presented a comprehensive Lattice Kinetic Monte Carlo model, where the microscopic competition occurring during SPER is also taken into account in order to provide a physical explanation of the dependence of the activation energy profile with the Ge content.

Furthermore, the presence of strain induced by the lattice mismatch during SPER may result in the formation of defects in the regrowth area which may affect the final device performance. Based on TEM observations, [Paine *et al.* 1991] show that only a few nanometers of SiGe regrow in the absence of defects, and how the defect free recrystallized thickness decreases exponentially with increasing the Ge fraction. Another concern is the sharpness of the α -c interface, which increases as it moves from Si to SiGe, leading to strain accumulation and planar defect formation [Lie *et al.* 1995]. As a consequence the defectivity control of SiGe regrown layers is a critical issue, since the lattice distortion induced by strain and the subsequent defect formation may result in dopant diffusion or deactivation. This fact becomes also a major challenge, and modeling the influence of strain and Ge concentration in the assisted dopant diffusion mechanisms has led to several works [Moriya *et al.* 1993, Huang *et al.* 2014, Hasanuzzaman *et al.* 2016]. In the following, this work makes progress in modeling the SPER of SiGe alloys and its underlying mechanisms, as the defect formation.

Figure IV.2: MD simulation snapshots after 20 ns of annealing at 1750 K for different Ge compositions: (a) 0%, (b) 20%, (c) 71% and (d) 100%. Silicon atoms are in red, and Germanium in blue.

2 Germanium impact on SPER activation energy

2.1 Regrowth of relaxed SiGe alloys

As introduced before, the extracted SPER activation energy profile of SiGe alloys does not vary linearly with Ge composition from pure Si to pure Ge values, as asserted by extensive works in literature [Haynes *et al.* 1995, Kringhoj & Elliman 1994, Lee *et al.* 1993]. Several models have been derived from these experimental observations to explain such non-linear behaviour, however they do not account for the atomistic mechanisms taken place during SPER. In the present section, this work addresses the study of the SPER of SiGe alloys by using atomistic simulation techniques. Molecular dynamics simulations are performed to analyse the crystallization of fully relaxed $\text{Si}_{1-x}\text{Ge}_x$ alloys in order to provide an atomistic model of the microscopic mechanisms that may lead to the anomalous Ge composition dependence of the SPER activation energy.

2.1.1 Simulation set up

MD simulations have been conducted to model the planar regrowth of $\langle 110 \rangle$ -aligned box-shaped $\text{Si}_{1-x}\text{Ge}_x$ in (001) Si substrates, as shown in Fig. IV.1. At the bottom, a few atomic planes are held fixed in their perfect lattice positions, acting as a substrate.

Figure IV.3: Time evolution of the structure factor $S(y)$ at $T=1800$ K for pure Silicon. For $S(y)=0.5$, the interface position is extracted at each time step.

Crystalline atoms are next, which serve as a seed for recrystallization, in direct contact with the α -phase created as described in Appendix A. The total size of the cell is $45 \times 100 \times 25$ ($\text{\AA}^3$), being the lattice parameter determined according to [Dismukes *et al.* 1964] depending on the Ge composition of the sample, from 0% to 100%.

Periodic boundary conditions are applied along x and z directions, while the top surface is left free in order to accomodate volume variations. The Nose-Hoover thermostat controls the temperature during the initialization stage, where the system is annealed at 1000 K for 20 ps. After the equilibration approach, the regrowth process starts by coupling the system to a temperature bath ranging from 1750 to 2000 K every 50 K until the complete recrystallization is reached. In order to extract the SPER rate, the interface position during the thermal annealing must be computed at each time step. This calculation requires to distinguish atoms attached to the crystalline phase from those at the amorphous part of the structure. There are several methods used in the literature, as an example [Posselt & Gabriel 2009] define a threshold value for the maximum deviation of the bond angle distribution to declare an atom as crystalline. Another approach to determine whether an atom belongs to the crystalline or the amorphous phase consists of computing a dot product between the atom position and a vector of the reciprocal lattice to the interface, the so-called structure factor:

$$S(y) = \left| \frac{1}{N_y} \sum_{y < y_i < y+dy} e^{j\vec{k} \cdot \vec{r}_i} \right|, \quad (\text{IV.1})$$

where N_y is the number of atoms between y and $y + dy$, r_i is the i atom position and $\vec{k}$ is the reciprocal lattice vector parallel to the α -c interface, which depends on the

Figure IV.4: Arrhenius fitting for $\text{Si}_{0.89}\text{Ge}_{0.11}$ for temperature ranging from 1750 to 2000 K. Inset: α -c interface position versus the annealing time at 1800 K.

substrate orientation as:

$$\vec{k}_{100} = \frac{2\pi}{a_o}(\vec{y} + \vec{z}) \quad (\text{IV.2})$$

$$\vec{k}_{110} = \frac{2\pi}{a_o}(\sqrt{2}\vec{y} + \vec{z}) \quad (\text{IV.3})$$

$$\vec{k}_{111} = \frac{2\pi}{a_o}(\sqrt{2}\vec{y} + \sqrt{6}\vec{z}) \quad (\text{IV.4})$$

The value of dy is chosen as small as possible, also dependent on the orientation with values of $a_0/4$ for (100), and $a_0\sqrt{2}$ for (110) and (111) orientations. This method has been used for the computation of the α -c interface, according to the following criteria: A value of 1.0 indicates the perfect crystal, 0.0 represents the complete disorder, and 0.5 represents the α -c interface, see Fig. IV.3 where the structure factor for $x = 0$ is obtained. From the instantaneous position of the α -c interface versus time, the regrowth rate is calculated, see the inset in Fig. IV.4 for 11% of Ge concentration where the linear evolution of the interface with time is evidenced.

Figure IV.5: Activation energy for SPER as a function of Ge concentration. Experimental data from [Haynes *et al.* 1995] are represented as empty squares, and [Kringhoj & Elliman 1994] as filled circles with error bars. LKMC model [Payet *et al.* 2016] is presented as a dashed line. MD simulation results are included as filled circles [Prieto-Depedro *et al.* 2017].

2.1.2 Results and observations

The MD results for the temperature dependent SPER allow us to obtain from the Arrhenius fitting the activation energy, as shown in Fig. IV.5 for temperatures ranging from 1750 to 2000 K, depending on the Ge fraction. As observed, the activation energy does not vary monotonically between the values for Si and Ge; instead, the activation energy goes through a maximum for approximately $x=0.2$.

According to the dangling bond model, an amorphous atom attaches to the crystalline phase by the rearrangement of bonds at the interface. Regarding this process of breaking and reconnecting bonds in order to propagate the interface, the bonding Si-Ge energy should lie between the values of Si-Si and Ge-Ge, since both the Si-Ge and Ge-Ge bond strengths are lower than that of Si-Si [Pauling 1960]. As the dangling formation energy is expected to decrease with the Ge content, the presence of a second component in the activation energy must be considered. This extra term is identified by [Kringhoj & Elliman 1994] as the defect migration energy at the interface. However, continuous models do not provide information about the atomic processes taking place during SPER, and with this purpose [Payet *et al.* 2016] presented their LKMC

model, where an intermediate rate is introduced, as first hypothesized by [Haynes *et al.* 1995]. Based on these assumptions, the activation energy obtained for Si-Ge bonds is suggested to come from the linear interpolation of pure Si and Ge SPER activation energies and a local strain due to the bond length difference in the alloy, and consequently this second term would explain the maximum. To confirm this point, the NEB method is introduced in the next section to compute the energy barrier for an atom to attach the crystalline phase.

2.2 Nudged Elastic Band Calculations

Considering SPER as a thermal activated process, the rate for an atom to recrystallize within the Transition State Theory can be approximated as:

$$v = v_0 \exp\left(-\frac{E_a}{k_B T}\right), \quad (\text{IV.5})$$

where v_0 is the pre-exponential factor, E_a is the activation energy, and k_B is the Boltzmann constant. According to this approach, the optimal transition state becomes a search for the lowest saddle point at the edge of the potential energy basin corresponding to the initial state. A path connecting the initial and final states is the minimum energy path (MEP), whose maxima are saddle points on the potential energy surface. Assuming a Boltzmann population is reached for the intermediate stable configurations, the overall rate is determined by the highest saddle point [Henkelman *et al.* 2000b]. Many different methods have been proposed for finding MEPs and saddle points [Henkelman *et al.* 2000a, Henkelman *et al.* 2000b]. NEB first proposed by [Mills *et al.* 1995] is an efficient and widely used method for calculating reaction pathways of atomic-scale solid-solid transformations through sampling a minimum energy path. The NEB uses N-replicas of the system obtained by linear interpolation between these two mentioned states as depicted in Fig. IV.6, connected by harmonic springs to ensure continuity of the path, thus mimicking an elastic band [Espinosa & Bao 2013].

The present work addresses the challenge of finding the minimum reaction pathway, i.e. E_a , for solid phase regrowth transitions. These calculations provide information on the energy of different regrowth pathways in SiGe alloys. Focused on the bonds at the interface, where the bond breaking process is a plausible mechanism for the regrowth, four different cases have been taken into account: Si-Si, Ge-Ge, Si-Ge, and Ge-Si. Each bond type has its own activation energy, which will be estimated along the MEP connecting the initial and final states for the atom-dominated mechanism. Simulations are performed by using the set-up described in section 2.1 in the present chapter, re-scaled for a total number of 320 atoms. On the one hand, for $x=0$ and $x=1$, considering a Si atom forming stable bonds at the interface, the MEP is computed,

Figure IV.6: Energetic reaction pathway between the initial and final states of a solid-solid transformation. The saddle point corresponds to the maximum energy along the MEP. Points represent the system replicas used in the simulation.

Figure IV.7: NEB simulation snapshots for the slowest recrystallize configuration in pure silicon when the atom to rearrange into the crystalline phase is (a)-(c) Si, identified in green; and Ge (d)-(f), identified in yellow. Amorphous atoms are in gray, while crystalline in white. Reconnected bonds show how the atom is rearranged for crystal regrowth to proceed in the $\langle 100 \rangle$ direction. Images (a)-(c) are taken from [Prieto-Depedro *et al.* 2017].

Figure IV.8: NEB simulation snapshots for the slowest recrystallize configuration in pure germanium when the atom to rearrange into the crystalline phase is (a)-(c) Ge, identified in yellow; and Si (d)-(f), identified in green. Amorphous atoms are in gray, while crystalline in white. Reconnected bonds show how the atom is rearranged for crystal regrowth to proceed in the $\langle 100 \rangle$ direction.

and so activation energies for Si-Si and Si-Ge bonds are extracted. On the other hand, this process is repeated for a Ge atom attaching the crystalline phase for $x=0$ and $x=1$, where bond types involved are Ge-Ge and Ge-Si. It should be pointed out that this is the less favorable situation, and it is considered in order to simulate the limiting conditions during SPER. In SiGe alloys, recrystallizing atoms as well as their first neighbors could be different, e.g., a Si atom surrounded by 2 Si and 2 Ge atoms, and so on.

To confirm the conclusions extracted in section 2.1, where the activation energy for Si-Ge bonds is obtained from the linear interpolation of pure Si and Ge SPER activation energies and a local strain due to the bond length difference in the alloy, the NEB method is introduced to compute the energy barrier for an atom to rearrange into the crystalline phase. In the process, the involved atom encounters many types of configurations at the interface with their own recrystallization probability. Consequently, several structures have been considered, since SPER is limited to the attachment rate of the slowest crystallizing configuration. The obtained values for the four cases under study are summarized in Table IV.1, where considered energy barriers are the highest values, in well agreement with values reported in [Payet *et al.* 2016].

Figure IV.9: Energy along the minimum energy path between the initial state and the final state when an amorphous atom rearranges into the crystalline phase: (a) Si, and (b) Ge atoms in pure Si; and (c) Ge, and (d) Si atoms in pure Ge. Values corresponding to the saddle point are contained in Table IV.1.

Highlighted activation energies in Table IV.1 correspond to the slowest crystallizing configurations extracted from NEB simulations shown in Fig. IV.7 for the pure Si structure, when the atom to rearrange is Si (a)-(c), and Ge (d)-(f); and Fig. IV.8, for pure Ge being the atom to rearrange a Si atom (a)-(c), and Ge (d)-(f). As shown in all cases, bonds are broken to make topological changes in the structure, and then the loose ones are reconnected. From MEP computation, the activation energy for a particular Si atom recrystallizing in Si is 2.60 eV, in good agreement with the SPER activation energy for pure Si. For pure Ge, the calculated energy barrier is 2.01 eV, giving satisfactory results when compared to pure Ge SPER activation energy. Whether the atom to attach is Ge in Si or Si in Ge, the limiting configuration has been found to be different. The presence of Ge in the Si lattice, and the opposite, induces a local strain due to differences in bond length, and as a consequence the energy barrier is found to be higher than the Si-Si and Ge-Ge bond energies, with values of 2.960 and 2.961 eV, respectively. The corresponding energies along the MEP are shown in Fig. IV.9.

According to NEB results, it can be confirmed that some of the intermediate config-

Table IV.1: Recrystallization energy barriers calculated by NEB method for different configurations at the interface. The slowest configuration is considered as the limiting rate, highlighted in bold. Activation energies are in eV.

Bond	E ₁	E ₂	E ₃	E ₄
Si-Si	2.370	2.443	2.600	2.606
Si-Ge	2.041	2.379	2.943	2.961
Ge-Ge	0.722	1.074	2.000	2.010
Ge-Si	1.289	1.574	2.251	2.960

urations require an extra strain for the propagation of the loose bond. This extra strain explains the difference between the bonding formation energy and the SPER activation energy, allowing this work to provide an explanation to the non-linear behaviour of the SPER activation energy of SiGe alloys.

3 Defect nucleation during SPER

Successful regrowth of strained $\text{Si}_{1-x}\text{Ge}_x$ alloys by SPER requires to identify when strain induced by the lattice mismatch is elastically accommodated rather than relieved by the introduction of defects. For an accurate modeling it is important to take into account that the presence of point defects depends on the Ge fraction present in the alloy. [Paine *et al.* 1990] showed that strained $\text{Si}_{1-x}\text{Ge}_x$ alloys were successfully regrowth when $x < 0.16$, and for alloys with a greater Ge content SPER results in a high density of planar defects, clearly observed by cross-sectional TEM images in Fig. IV.10, where the morphology of the α -c interface is described as adjacent V-shaped features limited by $\{111\}$ planes leading a trace of stacking faults bounded by partial dislocations. Further investigations has lead to the incorporation of substitutional B on the SiGe layers in order to reduce the strain-relieving defects density, as reported by [Rodríguez *et al.* 1997] where the strain compensation is clearly enhanced by the presence of B dopants.

Another concern regarding the formation of defects is the defect-free layer thickness starting from the Si/SiGe interface, already reported by [Paine *et al.* 1991], which involves a critical issue when fabricating high quality strained SiGe layers for micro-electronic devices. This layer is probably coherent with the Si substrate which is contacted, and decreases exponentially with increasing the Ge content. Several attempts have been performed to increase the defect free layer by incorporating P, Sb or C implants, but only C success in this sense [Lie *et al.* 1995, Hong *et al.* 1992, Antonell *et al.* 1996]. In the present section, the nucleation of defects during SPER of

Figure IV.10: Cross sectional $\langle 110 \rangle$ lattice resolution TEM images showing $\{111\}$ faceting formation, and the subsequent stacking faults and twin nucleation for a $x=0.30$ Ge fraction. Extracted from [Paine *et al.* 1990].

strained $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ alloys is reported. Compared to structures used in Section 2.1 in the present chapter, simulation sizes have been increased to investigate the crystalline quality of regrown layers. The total size of the simulation box is $92 \times 155 \times 38 \text{ (\AA}^3\text{)}$, varying the lattice parameter according to [Dismukes *et al.* 1964] for $0 < x < 1$. The rest of simulation conditions are equal to those described in Section 2.1. However in this case, MD simulations have been carried out only at a temperature of 1800 K.

3.1 Simulation details and observations

Based on the literature review reported here, a set of MD simulations have been carried out in order to determine the threshold Ge content to observe the nucleation of defects during SPER. For a Ge fraction lower than $x=0.15$ the SPER proceeds in the absence of defects, not shown for the sake of simplicity. However, it should be pointed out that during the equilibration approach taking place before the anneal, the underlying Si substrate is damaged by the presence of Ge atoms in the lattice, which induce stress due to their larger size in comparison with Si.

As the Ge fraction increases, the formation of defects appears due to the accumulation of strain during SPER, which is probably determined by the competition of regrowth and defect nucleation. SPER simulation snapshots of $\text{Si}_{0.47}\text{Ge}_{0.53}$ are shown in Fig. IV.11. After annealing at 1800 K for 15 ps the α -c interface presents facet par-

Figure IV.11: MD simulation snapshots of SPER for a Ge content of 53% after anneal at 1800 K for: (a) 15 ps, and (b) after complete recrystallization. Silicon atoms are shown in white, and Ge atoms are in green. {111} facet formation is identified in red, twinning formation in yellow (also shown in the inset to clarify), and dislocations are in dark blue.

allel to {111} planes as illustrated in Fig. IV.11 (a), which evolve into planar defects lying parallel to the facets, identified as microtwins in (b). This anomalous morphology is preserved as the planar defects left behind the α -c interface affect further regrowth, and once the complete recrystallization is achieved not only microtwins are observed, also dislocations have nucleated relieving strain as shown in Fig. IV.11 (c). These results are well matched to the features experimentally observed by [Paine *et al.* 1990], consisting of stacking faults parallel to {111} planes bounded by partial dislocations to produce strain relaxation. Analysis for a Ge content of $x=0.20, 0.31, 0.40$, and 0.71 have led to the same results, after a defect free layer a highly defective regrowth takes place, where microtwins and dislocations are nucleated. The density of strain-relieving defects is determined to increase with the Ge fraction, which is in good agreement with experimental observations by HREM images reported in [Rodríguez *et al.* 1997].

A defect-free region is observed at the initial stage of the regrowth and it extends a few layer as shown in Fig. IV.11 (c). It is thought to be strained by the incorporation

Figure IV.12: Defect free layer thickness depending on the Ge fraction present in the annealed samples shown in blue. The lattice parameter dependence is also reported as a red line.

of Ge atoms into the lattice, and to be fully coherent with respect to the Si substrate. Once the critical thickness of the defect-free regrown layer is overcome, dislocations begin to nucleate, leading to conclude that the competition between regrowth and dislocation nucleation determine the final thickness of the coherently regrown layer. Measured thicknesses in all the analyzed samples depending on the Ge composition are shown in Fig. IV.12. The larger the Ge content, and so the lattice parameter of the $\text{Si}_{1-x}\text{Ge}_x$ alloy to be recrystallized, the greater the strain induced by the lattice mismatch, which turns out in the reduction of the defect-free layer thickness. The observed exponential decrease of the defect free layer is in good agreement with experimental observations in [Paine *et al.* 1991, Hong *et al.* 1992].

4 Summary

As device scaling approaches fundamental limits of miniaturization, novel materials and techniques have been recently introduced as potential replacement of Si-based technologies. As an example, current generations of devices are incorporating SiGe alloys as strain-induced mobility boosters, integrated in S/D regions or even as channel material. Within the fabrication process, the integration of epitaxial SiGe layers requires low thermal budget processing, and SPER has been demonstrated as a suitable technique with ability to grow both strained and relaxed SiGe layers. Consequently, the SiGe SPER has gained renewed interest. However, the SPER of SiGe alloys has

not been as widely studied as for pure Si and Ge, and modeling the underlying mechanisms taken place during SPER presents new challenges. In the present chapter, the Ge composition dependence of SPER activation energies has been investigated by using atomistic simulation techniques. Molecular Dynamics simulations have been performed in order to compute the activation energy of a range of strain-relaxed SiGe alloys. The activation energy profile has been determined to have an anomalous behaviour. It does not vary monotonically between values of pure Si and Ge as expected, since according to the dangling bond model the bonding Si-Ge energy should lie between Si-Si and Ge-Ge values, as they both Si-Ge and Ge-Ge have lower bond strengths than Si-Si. As a result, if the activation energy does not decrease with the Ge content, a second term is postulated: the energy needed to attach a new atom into the crystalline phase consists of the SPER energy and an extra term due to the elastic work performed in straining the alloy to overcome the bond length. To confirm the previous assumption, Nudged Elastic Band calculations have been performed to compute the energy barrier in four different cases: Si-Si, Si-Ge, Ge-Si, and Ge-Ge. Extracted values turn out to be in good agreement with SPER activation energies for pure Si and pure Ge configurations. In contrast, when the atom to rearrange into the crystalline phase is not as the same type as the bulk, i.e. the recrystallized atom is Ge in pure Si and Si in pure Ge, values have been found to be higher than the bonding energies in Si-Si and Ge-Ge. These results confirm the presence of the second strain component required to propagate the crystalline phase when the presence of Si and Ge induces a mismatch in the lattice configuration.

Furthermore, the defect nucleation during SPER of SiGe alloys have been analysed by using Molecular Dynamics simulations. Varying the Ge fraction present in the alloy, the formation of defects as well as their nature is evaluated. As the Ge fraction increases the strain induced by the larger size of the atoms starts to be relieved by the nucleation of defects. The evolution of the interface leads a trace of facets parallel to $\{111\}$ planes as observed for a wide range of Ge compositions. This shape evolves into planar defects lying parallel to the faces, identified as microtwins. The nucleation of dislocations have been also observed once the recrystallization is complete. These results are in good agreement with experimental observations reported by [Paine *et al.* 1990], where the formed stacking faults are bounded by partial dislocations to produce strain relaxation. It should be pointed out that the density of defects decreases when decreasing the Ge content. Another concern during the SPER of strained-relaxed SiGe layers is the defect-free layer coherent with the Si substrate observed once the regrowth is complete. This layer thickness has been measured, and determined to decrease exponentially with increasing the Ge content, also in good agreement with experimental results in [Paine *et al.* 1991]. Once the critical thickness is overcome, dislocations and point defects

begin to nucleate, allowing to conclude that the competition between regrowth and dislocation nucleation determine the final thickness of the defect-free layer.

Strained SiGe channel for FinFET devices

Current generations of *FinFET* devices are incorporating Silicon-Germanium alloys as channel material, ensuring the competitiveness of this technology by significantly increasing the device performance. In contrast, the presence of SiGe as stressor material in channel regions involves critical issues during the fabrication process, such as the strain relaxation or defectivity control, that may impact the final quality of the strained SiGe channel. In consequence, this chapter presents the study of the defect formation during the optimized integration of SiGe *FinFET*s for 10 nm nodes technology. The fabrication process is simulated for a wide range of Ge compositions, aimed at determining the threshold Ge content for the nucleation of defects as well as their nature. Due to the novelty of the process presented herein, simulation results are compared to experimental observations at this scale.

Contents

1	Incorporation of SiGe alloys as channel material	85
2	Strain compensation by relieving defects	88
2.1	Novel <i>FinFET</i> fabrication process	88
2.2	Simulation details and results	88
3	Summary	93

1 Incorporation of SiGe alloys as channel material

As introduced in detail in chapter I, according to Moore's law CMOS technology has been continuously scaled down for more than 40 decades driven by the microelectronic

Figure V.1: Schematic drawing of the 3D SiGe finFET structure. An isolation mask is used to protect the top of the substrate. The cross section is also illustrated.

industry demands for more powerful transistors with low power consumption. To overcome downscaling difficulties beyond Silicon, in chapter IV strained SiGe alloys are introduced for further performance enhancement as stressor material in S/D regions coupled with multi-gate non-planar architectures such as FinFET devices. FinFETs have been evidenced to extend the gate limit beyond planar transistors, while still offering superior performance. However, FinFET devices face critical issues when competing with other technological options, such as its high access resistance due to the thin body structure, or the strain boosters implementation. Consequently for FinFET architectures, strain engineering is crucial to improve the transistor performance. Strain techniques developed for planar architectures have been applied into FinFET technology. As an example, selective epitaxial regrown SiGe layers have been incorporated as stressor material in source / drain (SD) regions of Si-FinFET devices. The induced uniaxial stress has been reported to significantly increase the hole mobility, drive current and channel conductivity [Sinha *et al.* 2015]. Moderate Ge content and no strain do not provide relevant short-channel benefit, and so the higher the amount of required stress, the larger the Ge content which has been increased from 17% to 40% in 90 nm to 22 nm, respectively [Ghani *et al.* 2003, Auth *et al.* 2012, Thompson *et al.* 2004b, Mistry *et al.* 2007].

However, for the current 10 nm technology nodes and beyond further mobility boost-

Figure V.2: Cross sectional TEM image of FinFET SiGe channel after reveal step, extracted from [Carter *et al.* 2018]. SiGe relaxation occurs along the Shallow Trench Isolation (STI) edge, acting as a free surface.

ing techniques are required, as the conventional strain engineering using S/D SiGe epitaxial growth becomes significantly challenging due to the small substrate and the 3D device architecture itself [Nanda *et al.* 2015]. To ensure the competitiveness of technology at this scale, material innovation explores SiGe as an attractive channel candidate for advanced FinFETs generations, schematically shown in Fig. V.1 and extended in Fig. V.2, where the cross-section TEM image of a SiGe FinFET is shown. [Ok *et al.* 2010] reported an increase of SiGe FinFETs performance of 16% over the Si fin, which evidences that SiGe FinFETs allow both low power and high performance devices, as strain makes possible to move more current at lower voltages (~ 200 mV lower than the Si threshold voltage) with immunity to short channel effects.

In contrast, the main concern of SiGe FinFETs is the strain relaxation throughout the entire integration process, as the channel may lose strain during thermal annealing processes for dopant activation or by fin cut processes [Tsu *et al.* 1984]. Along with strain retention, defect control is also a critical issue when fabricating SiGe FinFETs. The lattice mismatch ($\sim 4.17\%$) between the $\text{Si}_{1-x}\text{Ge}_x$ channel and the Si substrate is accommodated by lattice distortion or generation of misfit dislocations as illustrated in Fig. V.3, and as a consequence maintaining the required defect level for manufacturing is a major technical challenge. The present work addresses the evaluation of defect formation during the optimized integration of SiGe FinFETs for 10 nm technology nodes, in order to determine the Ge threshold content for the nucleation of defects that may impact the device performance, by reducing the carrier mobilities and also increasing the leakage currents.

Figure V.3: (a) Schematic view of coherently strained heteroepitaxial layers with equal lattice parameter for the substrate and the top film ($a_{\text{Si}} = a_{\text{SiGe}}$), and (b) relaxed structure with a misfit dislocation.

2 Strain compensation by relieving defects

2.1 Novel FinFET fabrication process

The fabrication process referred in the present work is schematically shown in Fig. V.4. Over a Si substrate the channel area is defined by removing a portion of the total volume, generating trenches which are further refilled with a second semiconductor material to form the co-integrated FinFETs. Once SiGe is epitaxially regrowth and implanted on the rendered areas over the Si, the whole structure is subjected to selective etching techniques for the fin patterning process. The study presented herein is focused on the step illustrated in Fig. V.4 (b). After the SiGe deposition, the presence of larger Ge atoms into the lattice made of smaller Si atoms creates a lattice mismatch inducing strain which is expected to be relieved by defect formation. Atomistic simulations are performed to determine the nature of the formed defects for a Ge content of $x=0, 0.12, 0.27, 0.43, 0.71$, and 1.0 .

2.2 Simulation details and results

Molecular Dynamics simulations have been carried out to study the formation of defects over the structure shown in Fig. V.5. A few atomic planes at the bottom are frozen in their perfect lattice positions to fix the whole structure. The cavity contains the $\text{Si}_{1-x}\text{Ge}_x$ alloy with a total volume of 843 nm^3 , while the rest of the box is filled by Si atoms. Dimensions of the entire $\langle 110 \rangle$ -aligned box-shaped in (001) Si are

Figure V.4: Process flow of the SiGe FinFET manufacturing: (a) void generation in the Si surface, (b) void refilling by SiGe in direct contact with the Si substrate, and (c) after the etching process where the final fin structure with Si S/D is shown.

$622 \times 434 \times 7 (\text{\AA}^3)$, containing 88452 atoms, where periodic boundary conditions are applied in the x and z directions, and dimension y is left free. As the whole structure is defined by the Si lattice parameter, the SiGe refilling the void requires to be relaxed in order to accommodate the lattice mismatch, and so an energy minimization of the system is performed using the Conjugate Gradient Method (CGM). After the equilibration approach, the entire system is annealed at 2200 K for 1.4 ns by using a canonical fixed volume dynamics (NVT, i.e. fixed volume and temperature). Once the annealing has finished, the system is subjected to a second energy minimization step. It should be pointed out that simulations have been performed from two to three times using different seeds for the velocity initialization to take into account statistical factors.

During the strain relaxation process of the SiGe alloy present in the annealed samples, the generation of defects reaching the channel region has been observed for a range of Ge compositions. The plastic relaxation mechanisms require mainly the formation of misfit dislocations as introduced already in Fig. V.3, which are expected to

Figure V.5: Schematic view of the simulation box used for modeling SiGe FinFETs structures previous to the fin patterning. Atoms in the bottom slabs are held fixed during the annealing process.

appear at the interface where the lattice mismatch between both materials is accommodated. These misfit dislocations acts by decreasing the total energy of the system being thermodynamically favored. For $x=1.0$ the strain compensation is drastically enhanced by the nucleation of misfit dislocations at the lateral of the structure, identified with letters (a), (b) and (c) in Fig. V.6. As an example, dislocation nucleated in (b) is observed in detailed in Fig. V.7(b), where the missing atomic planes are highlighted in red. The annealing process turns out also in the development of twins at $\{111\}$ planes marked with letters (d) and (e) in Fig. V.6 and extended in Fig. V.7(a) where the stacking fault is identified as 60° rotation with respect to one bond in the original tetrahedron. In addition, the Si substrate is damaged in several points of the simulation box, which have been neglected as the main concern is the defected pattern in the channel area. As the Ge content decreases, the density of defects is reduced. For $x=0.71$, the presence of dislocations and twins is also detected but in a minor quantity, as shown in Fig. V.8. The inset shows the formed dislocation and stacking fault identified in (a), while defects in (b) and (c) are not shown, being a dislocation and twin respectively.

For $x=0.43$, only twinning formation is observed once the annealing process is finished. For lower Ge concentrations examined in the present work, $x=0$, 0.12, and 0.27, no defects have been generated at the end of the annealing, not shown for the sake of simplicity.

According to the simulation results summarized in Table V.1, the larger the Ge fraction the higher the density of the nucleated defects. The presence of a great number of Ge atoms tends to create a local compressive strain in the Si lattice which is finally relieved by the formation of extended defects identified as twins created at

Figure V.6: Simulation snapshot of the structure once the annealing is complete. Defected areas are identified with letters: (a) - (c) corresponds to dislocation nucleation at the channel area, while (d) and (e) identify the twinning formation at the $\{111\}$ planes.

Figure V.7: For $x = 1.0$, extracted atomistic structure of formed defects in Fig. V.6(b) and (e). Silicon atoms are identified in white, while Ge atoms are in green.

Table V.1: Summary of the found extended defects depending on the Ge fraction.

Ge (%)	Defects
0.0	Defect free
0.12	Defect free
0.27	Defect free
0.43	Twinning - Stacking faults
0.71	Two 60° misfit dislocations / Two twins
1.0	Three 60° misfit dislocations / Two twins

{111} planes and misfit dislocations. These results are in good agreement with experimental observations by [Schulze *et al.* 2017], where the formation of 60° misfit dislocations have been identified as a result of half-loops dislocation glide over {111} planes, thereby acting as strain relieving points. Furthermore, the introduction of SiGe as a strained relaxed buffer layer for nFET devices has been also turned out in dislocation formation as reported by [Carter *et al.* 2018], and illustrated in Fig. V.9. Even atomistic simulations have been used to determine the complex atomic rearrangements during strain relaxation, [Maras *et al.* 2017] obtain also the formation of 60° misfit dislocations for highly strained SiGe films, where the most likely nucleation responsible agrees with such half-loop gliding mechanism. Nudged elastic band calculations performed by [Trushin *et al.* 2016] reveal two intermediate states for strain relief at the interface. On the one hand, a half-loop 60° dislocation is nucleated lowering the total energy of the system, and on the other hand a second 60° complementary dislocation is formed in a mirror glide plane. Finally these two dislocations may react to form a 90° dislocation. However this general agreement for the half-loop nucleation mechanism is in contrast with investigations reported by [Maree *et al.* 1987], where the misfit dislocation formed via half-loops is enhanced in the presence of tensile strain, which is the opposite situation.

The existence of the identified defective areas involves a critical issue when fabricating high quality strained SiGe channels for FinFET devices, and so determining the threshold Ge content for the defect free processing is critical as the distortions created in the lattice may seriously affect the carrier mobility. As the maximum strain must be ensured in the channel with very low defectivity, a balance needs to be found between introducing strain by the incorporation of larger Ge content and avoiding the nucleation of defects in the channel area. Results reported in the present work suggest such limiting Ge fraction to be $x=0.27$.

In addition, the influence of the step order within the fabrication process has been also accounted in the present work. To determine the effect of the fabrication flow

Figure V.8: Formation of defects after the annealing process for $x=0.71$. Dislocations and twins are observed in the channel area as shown in the inset identified with (a), where Si atoms are in white, and Ge atoms in green. Defects in (b) and (c) corresponds to a dislocation and a twin, respectively.

in the nucleation of defects, two set of simulations have been performed in order to confirm the stability of the formed defects after the etching process. On the one hand, for $x=0.71$ where the channel area is clearly damaged, once the annealing has finished the structure is cropped according to Fig. V.4 (c) and is subjected again to the same annealing conditions described before. On the other hand, for $x=0.27$ where no defects have been observed, the same procedure is carried out. Simulation results after this second annealing process of the etched structures reveal the formed defects do not dissapear in the first case. While the channel area in the absence of defects remains after the annealing of the etched structure. From this behaviour emerges the annealing step as a trigger for the nucleation of strain relieving defects, which are stable in further processing.

3 Summary

Once the SiGe layers have been regrown by SPER, these are deposited as stressor material in FinFET channel areas. However, during further fabrication processes such as

Figure V.9: TEM image of dislocation nucleation through strained relaxed SiGe buffer layer (SRB) into Si epi-layer, extracted from [Carter *et al.* 2018].

dopant activation or etching techniques, the quality of the layers may be affected and so the final device performance. Regarding the entire integration flow, the strain retention and defectivity control are major challenges, and consequently throughout this chapter, the strain relieving defects in the $\text{Si}_{1-x}\text{Ge}_x$ channel area has been investigated by using Molecular Dynamics.

As Ge atoms are incorporated into the Si lattice, a large misfit strain is induced due to the great difference in the lattice constant which may be relieved by the generation of dislocations. The strain is required for mobility enhancement and therefore the need to prevent strain compensation by the nucleation of defects, as well as the control of the density and their nature are critical issues during the device fabrication process. Varying the Ge fraction present in the alloy, this work determines the threshold Ge content for the nucleation of defects to be $x=0.27$. For lower Ge content, the structure remains defect free once the annealing is complete. Molecular Dynamics simulations provides also the character of the formed defects, which have been determined to be twinning developed at $\{111\}$ planes and 60° misfit dislocations. These results are in close agreement with experimental observations reported in [Schulze *et al.* 2017, Carter *et al.* 2018].

Finally, the stability of the formed defects is confirmed by performing a second set of MD simulations. The etching process for the fin cut is carried out in two annealed samples, $x=0.27$ and $x=0.71$, a defect free and a defective structure, respectively. The samples are then subjected to a second annealing step, and the extracted behaviour suggests the annealing as a responsible for the strain relieving defects. After the etching process and the subsequent annealing, the structure remains in the absence of defects

for $x=0.27$, while defects formed in the first stage are still present in the sample for $x=0.71$.

Concluding remarks and further work directions

The present manuscript addressed the study of the underlying and fundamental mechanisms taken place during the Solid Phase Epitaxial Regrowth (SPER) of Si and SiGe alloys. SPER has been evidenced as the best option for the microelectronic industry to form abrupt and highly activated junctions, very suitable for advanced devices. Furthermore, this technique is crucial for the dopant activation process within the low temperature regime, required for the 3D sequential integration process, which has become a potential alternative to device scaling in the last few years in terms of junction formation. Consequently, this work was mainly focused at giving a comprehensive description of the SPER process in terms of the atomistic mechanisms taken place at the regrowth interface. For that purpose several atomistic simulation techniques have been used, allowing to cover a wide range of time and size scales. In this final chapter, the research performed during this PhD is summarized, concluding with suggestions and guidelines for future work.

Contents

1	Defect formation dependence on stress	98
2	Two part behaviour of the SPER activation energies in SiGe alloys	99
3	Strain relieving defects in SiGe channel FinFETs	99
4	Further work suggestions	100
4.1	Preliminary results of the study of Boron diffusion in SiGe alloys	100
4.2	OKMC model presentation	102
4.3	Simulation details and observations	104

1 Defect formation dependence on stress

Modeling multidirectional SPER has been evidenced to turn out into highly defective areas affecting the final device performance. The study of the formed defects has lead to a great number of contributions aimed at giving a further insight into the mechanisms responsible for such defect formation [Saenger *et al.* 2007c, Marqués *et al.* 2003, Morarka *et al.* 2009], however their origin remained unclear. This work addressed the study of the effect of stress patterns in the formation of defects by introducing a comprehensive multiscale modeling where three different techniques were used: Finite Element Methods (FEM), Molecular Dynamics (MD) and Lattice Kinetic Monte Carlo (LKMC) [Prieto-Depedro *et al.* 2015].

As the SPER rates are thought to be suppressed by the presence of strain, the study begins with the computation of the initial stress pattern due to the density variation between the α - and c- phases. FEM calculations are performed over two different size and time domains: MD and LKMC. Results revealed a negligible effect of stress in amorphous regions smaller than 10 nm, while strain is clearly observed in the near vicinity of interfaces of the simulation box for larger sample sizes within the LKMC domain. According to these results, MD simulations were performed in the same box size and the regrowth took place in the total absence of defects. Furthermore, the influence of strain was then accounted by enforcing the stress with an external application of in-plane compression within the range of 5-7 GPa depending on the orientation of the crystalline substrate. Under these realistic conditions, two type of defects were observed. On the one hand, the formation of twins due to the stability of $\{111\}$ planes. And on the other hand, the nucleation of dislocations at the pinch-off point of the recrystallization fronts, which had been determined to be produced by the presence of strain due to the volumetric expansion of the α -Si, since no dislocation were observed in the absence of external strain.

Due to the size and time scale limitations of MD, these results had been extended into LKMC model allowing to simulate realistic sample sizes and annealing conditions. The LKMC model was fed also with a FEM internal module, which accounted the strain pattern due to the α - phase at each time step. Defects observed in larger samples were compared to data reported in literature, where there was found a general agreement with experimental XTEM images published by [Saenger *et al.* 2007c]. This extended application allowed us to conclude *the presence of strain as responsible for the dislocation nucleation at the regrowth interface, as well as the stability of $\{111\}$ planes as the origin mechanism for the twinning formation predicted by MD.*

2 Two part behaviour of the SPER activation energies in SiGe alloys

As device scaling is in pace to approach fundamental limits of miniaturization, new architectures and materials have been introduced in the last few years as a potential replacement of conventional Si-based technologies. As an example, SiGe alloys have been introduced as strain induced mobility boosters in source drain regions of FinFET devices for further performance enhancement. Within this frame, SPER has been evidenced as suitable technique to grow high quality strained SiGe layers, and consequently modeling SPER of $\text{Si}_{1-x}\text{Ge}_x$ alloys has gained renewed interest. The present work addressed the study of the Ge composition dependence of SPER activation energies.

MD simulations were performed to compute the SPER activation energy profile for a wide range of Ge compositions. Extracted results revealed an anomalous behaviour, since it did not vary monotonically between values of Si and Ge as expected, instead a maximum is observed for approximately $x=0.2$. According to the dangling bond model, the Si-Ge bond energy should lie between values of Si-Si and Ge-Ge, since they both have lower bond strenghts than Si-Si. In contrast, the activation energy was observed not to decrease with increasing the Ge content, leading to hypothesize that there was a second term in the activation energy. This second component was postulated as an elastic work performed to straining the alloy to overcome the bond length, further confirmed by Nudged Elastic Band (NEB) calculations. NEB computed the energy barrier for an atom to attach the crystalline phase in four different cases: Si-Si, Si-Ge, Ge-Si and Ge-Ge. Extracted values turned out to be in good agreement with SPER activation energies for Si-Si and Ge-Ge. However, for Si-Ge and Ge-Si, energies were found to be higher than the bonding energies for Si-Si and Ge-Ge, concluding there was a second component in the SPER activation energy as suspected at the beggining of this study: *the SPER activation energy comes from the linear interpolation of pure Si and Ge SPER activation energies and a local strain due to the bond length difference in the alloy.*

3 Strain relieving defects in SiGe channel Fin-FETs

The conventional strain engineering using SiGe as stressor material in S/D regions faces critical challenges for the current 10 nm node technology and beyond. To ensure the competitiveness of devices at this scale, SiGe has been recently explored as channel

material for FinFET devices. Recent studies reported an increase of SiGe FinFETs performance of 16% over the Si fin [Ok *et al.* 2010]. In contrast, the main concern are the strain relaxation and the defect control, both critical issues when fabricating high quality $\text{Si}_{1-x}\text{Ge}_x$ layers as they seriously impact the final device performance by reducing carrier mobilities and increasing the leakage currents. This work studied the formation of defects within the novel fabrication process introduced in chapter V for a great range of Ge compositions. As Ge atoms are incorporated into the Si lattice, a large misfit strain is induced due the lattice mismatch. The strain was observed to be released by the nucleation of defects, which were determined to be twinning developed at $\{111\}$ planes and 60° misfit dislocations. *This work concluded the threshold Ge content for the nucleation of defects to be $x=0.27$.*

4 Further work suggestions

The work presented in chapter V is about to be submitted, pending on a second set of simulations to finish. Statistical factors should be taken into account by modifying different simulation parameters, such as the random seed used to modify the fraction of the SiGe alloy present in the sample, or the one used to generate the ensemble of velocities at the specified temperature. Another important concern is to account the influence of the size of the samples, as well as the total volume of the Si substrate and the implanted SiGe alloy in the voids. This is in fact an ongoing work.

4.1 Preliminary results of the study of Boron diffusion in SiGe alloys

During this PhD the study of the retardation of B diffusion in SiGe alloys has been addressed. At this point, some preliminary results are introduced, despite some efforts have to be made in order to explain the results we have got so far, and extend the conclusions to the further work proposed herein.

As introduced in chapter IV, the SiGe alloys have been used in recent years for carrier enhancement mobility due to the presence of strain induced by lattice mismatch between Si and Ge. During the thermal processing required for the junction formation process, the Ge interdiffusion may lead to reduce the required strain, affecting the carrier confinement. Even the dopant diffusion mechanisms can be dependent on the Ge fraction along the sample. Consequently, modeling the influence of strain and Ge concentration in the assisted dopant diffusion processes is a major challenge.

Incorporation of Ge is expected to increase the equilibrium point defect concentrations due to changes in formation energy, and dopant diffusivity is well known to

be proportional to the concentration of interstitials and vacancies [Pakfar 2002]. In SiGe alloys the most widely used p-type dopant is Boron, which has been reported to diffuse by interstitial assisted mechanisms and retarded by vacancy injection [Fahy *et al.* 1989, Yan *et al.* 1983]. The suppressed B diffusivity in strained $\text{Si}_{1-x}\text{Ge}_x$ compared to pure Si has raised great discussion about the impact of both strain and Ge concentration. [Carroll *et al.* 2008] hypothesized the lower equilibrium of self-interstitial at the $\text{Si}_{1-x}\text{Ge}_x$ surface as a responsible for the retarded B diffusion, where B diffusivity (D_B) was found to be two times slower than in Si samples. Higher activation energies for the D_B when increasing Ge concentration have been argued to reduce B diffusivity [Carroll *et al.* 2008, Rajendran & Shoenmaker 2001, Uppal & Willoughby 2001]. First-principles calculations by [Wang *et al.* 2004] reported a substantial increase in the interstitial migration energy barrier with the presence of Ge content, leading to decrease the available interstitials for B diffusion. Similar results supported the increase of the migration energy barrier when increasing the Ge fraction for retarded B diffusivity [Bang *et al.* 2007]. [Bang *et al.* 2007] also evidenced how small is the binding energy of Ge-B pairs, concluding Ge atoms are not effective traps to immobilize B atoms, also supported by results published by [Edelman *et al.* 2008]. In contrast, Ge-B cluster formation has been reported as a responsible for retarded B diffusivity [Peterström & Svensson 1992, L.Radic *et al.* 2006]. Ge atoms are expected to create a local compressive strain when introduced in the Si structure, while B atoms due to its smaller size compared to Si atoms generate a local tensile strain. The attraction between Ge and B atoms in order to release stress energy leads to Ge-B pairing formation [Villanueva *et al.* 2001].

Regarding the influence of strain, a few publications have made efforts in determining the effect of strain in the B diffusion process [Kuo *et al.* 1995, Pakfar 2002, Zangenberg *et al.* 2003, Lin *et al.* 2005]. Tensile strain is known to increase the equilibrium concentration of interstitials and decrease the vacancies, while compressive strain acts in the opposite way [Pakfar 2002]. The analysis of B diffusion in compressive and tensile strained $\text{Si}_{1-x}\text{Ge}_x$ structures [Zangenberg *et al.* 2003] showed the decreasing and increasing value of D_B , respectively. Even no stress dependencies have been hypothesized by [Kuo *et al.* 1995], who confirmed the B diffusivity is affected only by the amount of Ge present in the sample. Their study of B diffusion in $\text{Si}_{1-x}\text{Ge}_x$ ($x \approx 0.10$ and $x \approx 0.20$) under compressive and tensile strain resulted in negligible amount of Ge interdiffusion through the $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ interface, and so no interactions between B and Ge atoms. The role of Ge interdiffusion on B diffusivity has been further analyzed by [Hasanuzzaman *et al.* 2016]. Extracted results of retarded B diffusion profiles in $\text{Si}_{1-x}\text{Ge}_x$ reveal the influence of Ge when reaching the B implanted layer by self-diffusion. When Ge content does not reach the B peak, similar profiles are obtained compared to pure Si.

Figure VI.1: Initial concentration profiles of Ge (in $\text{Si}_{0.95}\text{Ge}_{0.05}/\text{Si}$) and B (in Si and $\text{Si}_{0.95}\text{Ge}_{0.05}/\text{Si}$). Boron implantation is simulated according to experimental dose of $1 \times 10^{13} \text{ cm}^{-2}$ at 60 keV done in [Hasanuzzaman *et al.* 2016].

Given the contradictions reported in the literature, it is obvious that there is no agreement on the mechanisms responsible for the retarded B diffusion in $\text{Si}_{1-x}\text{Ge}_x$. The ongoing work consists of confirming the self-diffusion of Ge as a responsible for the suppressed B diffusivity in $\text{Si}_{1-x}\text{Ge}_x$ alloys by performing Object Kinetic Monte Carlo (OKMC) simulations.

4.2 OKMC model presentation

The OKMC computational model of B diffusion in Si and SiGe alloys implemented in [Dopico *et al.* 2014, Castrillo *et al.* 2011] is used to elucidate the effect of Ge self-diffusion on dopant profiles during the annealing. The model is fully implemented in MMonCa [I.Martin-Bragado *et al.* 2013], and it has been already validated by comparison with relevant experiments [Carroll *et al.* 2008]. This model is an off-lattice KMC model where the evolution of defects not assigned to specific site positions is studied. In the case of SiGe alloys, B dopants diffuse typically by interstitial mediated mechanisms:

1. The break-up, when the defect breaks and form two isolated defects, (B^- , I^0).
2. Pairing substitutional B and self-interstitial (I), occuring when particles are within the capture radius of each other. An atom in a substitutional position in the lattice exchanges its site with an adjacent interstitial, raising the atomic diffusion.

Assuming substitutional boron is always immobile and ionized (B^-), the microscopic diffusivity to be simulated is given by:

$$B^- + I^0 \rightleftharpoons B_i^- . \quad (\text{VI.1})$$

From Eq. VI.1, the total number of broken B_i^- per unit time and volume is $[B_i^-]\nu_{bk}(B_i^-)$, and the new formed is given by $[B^-][I^0]\nu_m(I^0)v_{capt}$. As a result, the breaking-up mechanisms determine the concentration in local equilibrium conditions as:

$$\frac{[B_i^-]}{[B^-]} = [I^0] \frac{\nu_m(I^0)}{\nu_{bk}(B_i^-)} \nu_{capt}, \quad (\text{VI.2})$$

Being ν_{capt} the effective capture volume for pairing reaction. And ν_m and ν_{bk} the migration and break-up frequency, respectively:

$$\nu_m = \nu_{0,m} \times \exp(-E_m/k_B T), \quad (\text{VI.3})$$

$$\nu_{bk} = \nu_{0,bk} \times \exp(-E_{bk}/k_B T), \quad (\text{VI.4})$$

Boron diffusivity $D(B)$ considers the contribution of all mobile particles, being the known charged states B_i^- , B_i^0 and B_i^+ [Watkins 1975]:

$$D(B) = D(B_i^-) \frac{[B_i^-]}{[B^-]} + D(B_i^0) \frac{[B_i^0]}{[B^-]} + D(B_i^+) \frac{[B_i^+]}{[B^-]}. \quad (\text{VI.5})$$

As the most frequent break-up reaction occurs for B_i^- , from Eqs. VI.2 and VI.5, diffusivity turns out to increase when increasing the migration rate or decreasing the break-up frequency, meaning it depends on the B_i^- hopping distance before breaking up, and also on how fast it moves [Martin-Bragado *et al.* 2005].

In the present model for SiGe alloys, the effective configuration of interstitials is accounted by an overall transport capacity, which is given by the product of the corresponding diffusivity and the concentration of the point defect, DC_I . Notice there is no general agreement in the values of diffusivity and concentration reported in literature, while the discrepancies between experimental values of transport capacities are much lower. The interaction with traps has been suggested as a responsible of such differences, since they are able to immobilize intrinsic point defects [Pichler 2004]. To cross the SiGe/Si interface the point defect has to overcome an energy barrier, being the probability for a diffusing particle to jump from region 1 (Si) to region 2 (SiGe):

$$P_I^{1 \rightarrow 2} = \frac{DC_{I,2}}{DC_{I,1}}. \quad (\text{VI.6})$$

The influence of stress and chemical dependencies have been also included by adding a local term to the formation and migration energies [Martin-Bragado 2011, Castrillo *et al.* 2011]. To account all these facts, the set of parameters used in the present model are summarized in Table VI.1, extracted from [Dopico *et al.* 2014]. Where E_{fI} and E_{mI} are the formation and migration energy for pure Si, respectively. And D_{0I} and C_{0I} are respectively the diffusion and concentration prefactors in:

$$D_I = D_{0I} \exp\left(\frac{-E_{mI}}{k_B T}\right), \quad (\text{VI.7})$$

and

$$C_I = C_{0I} \exp\left(\frac{-E_{fI}}{k_B T}\right). \quad (\text{VI.8})$$

In the case of boron, E_{fB} and E_{mBi} are respectively the formation and migration energies. The formation energy enhancement is given by $E_{fBi} - E_{fB}$, and it should account for the effective volume for boron diffusion in strained $\text{Si}_{1-x}\text{Ge}_x$ alloys over Si substrates, despite not included in the present model. Finally D_{0Bi} is the diffusion prefactor and C_{0Bi}/C_{0B} is the relative concentration prefactor.

Table VI.1: OKMC parameters for native point defect and boron diffusion in $\text{Si}_{1-x}\text{Ge}_x$ / Si structures, for $0 \leq x \leq 0.4$. Extracted from [Dopico *et al.* 2014].

Interstitial	Boron
$C_{0I} = 6 \cdot 10^{26} \cdot 4^x \text{ cm}^{-3}$	$C_{0Bi}/C_{0B} = 920 \cdot 10^x \text{ cm}^{-3}$
$D_{0I} = 5 \cdot 10^{-2} \text{ cm}^2/\text{s}$	$D_{0Bi} = 5 \cdot 10^{-3} \cdot 10^x \text{ cm}^2/\text{s}$
$E_{fI} = 4 + 0.2x \text{ eV}$	$E_{fBi} - E_{fB} = 2.9 + 0.8x \text{ eV}$
$E_{mI} = 0.8 \text{ eV}$	$E_{mBi} = 0.77 + 0.5x \text{ eV}$
	$E_{fB} = -0.5x \text{ eV}$

4.3 Simulation details and observations

Boron is implanted in $\{100\}$ Si and $\{100\}$ Si capped with a 60 nm $\text{Si}_{0.95}\text{Ge}_{0.05}$ epilayer ($\text{Si}_{0.95}\text{Ge}_{0.05}/\text{Si}$). B implantation profile is defined according to [Hasanuzzaman *et al.* 2016], where the implanted dose allows the material to remain intrinsic at the selected annealing temperatures such that the diffusion is expected to be concentration independent, see Fig. VI.1 where the B peak of the As-implanted B is clearly formed inside the Si substrate. Notice that also the initial concentration profile of Ge in $\text{Si}_{0.95}\text{Ge}_{0.05}/\text{Si}$ samples is shown. Both samples with a total size of $650 \times 80 \times 80 \text{ (nm}^3\text{)}$ are annealed at 970°C for 1 hour in N_2 . Figure VI.2 shows the final B diffusion profiles for Si and $\text{Si}_{0.95}\text{Ge}_{0.05}/\text{Si}$ structures, as well as the interdiffusion of Ge for the

Figure VI.2: Boron diffusion profiles in Si and $\text{Si}_{0.95}\text{Ge}_{0.05}/\text{Si}$ samples annealed at 970°C for 1 hour in N_2 . Ge interdiffusion profile is shown for the $\text{Si}_{0.95}\text{Ge}_{0.05}/\text{Si}$ sample. Initial profiles for both B and Ge are displayed in black.

$\text{Si}_{0.95}\text{Ge}_{0.05}/\text{Si}$ sample, after annealing at 970°C for 1 hour. According to experimental observations by [Hasanuzzaman *et al.* 2016] no remarkable differences of B diffusion between Si and $\text{Si}_{0.95}\text{Ge}_{0.05}/\text{Si}$ samples are expected, as the Ge interdiffusion does not reach the B peak. However, from simulation results we observe how the B diffusion is reduced in $\text{Si}_{0.95}\text{Ge}_{0.05}/\text{Si}$ in comparison to diffusion in Si.

According to the extracted results next questions arise:

1. The model neglects the effect of the compressive strain induced by the presence of Ge atoms in the Si lattice, which is expected to decrease the equilibrium concentration of interstitials, and consequently the dopant diffusivity of B. If this dependence would have been accounted, how would be the diffusion profiles?
2. Both B and Ge diffusion profile suggest there are no damage accumulation or even cluster formation through the sample, as they should be significantly affected by the presence of such effects, and they are not.
3. Based on the previous point, the simulations may be performed again by incorporating the implantation damage through the Binary Collision approximation (BCA) module already included in MMonCa .
4. Assuming the presence of Ge affects locally the equilibrium concentration of interstitials, why is the diffusion suppressed at the tail of the profile where there is no B?

Once the points above would be clarify, simulation results may be compared to experimental observations by [Hasanuzzaman *et al.* 2016], and conclude if the Ge interdiffusion is responsible for the suppressed B diffusivity in SiGe alloys.

Appendices

Generation of amorphous phase

Amorphous regions are introduced by ion implantation during device manufacturing, and so simulating this process should be the best approach to reproduce SPER and to mimic the experiment. However, the description of this process is not realistic by means of MD since the large number of implantations required and the subsequent relaxation of the box would make the process infeasible, in terms of computing resources and CPU time consumed.

Figure A.1: Local distortion of Si lattice containing of two five-fold and two-seven fold membered rings. Atoms A and B are displaced. Extracted from [Prieto-Depedro *et al.* 2017].

According to [Prieto-Depedro *et al.* 2017], the present work introduces an alternative and faster method to generate suitable amorphous phases. To create computational structures to be used in simulations, the exact number of c-Si atoms contained in the region to be amorphized must be known, and then those are added to the system at randomly generated coordinates. Once introduced, atoms are highly overlapped and so an energy minimization is performed by using the Conjugate Gradient method (CGM). As the initial random positions vary with the seed, regrowth simulations are repeated from two to three times and extracted activation energies should converge, being the final value an average of all obtained before.

Figure A.2: Radial distribution function for α -Si obtained by the two techniques used in [Prieto-Depedro *et al.* 2017]. Results of RDF are also compared to experimental data from [Laaziri *et al.* 1999].

This method is validated against the generation of the amorphous phase by introducing bond defects by means of *ab initio* and the subsequent relaxation of the supercell containing 216 atoms. The bond defect introduces a local distortion of the lattice creating two five-fold and two seven-fold membered rings packed together, typical of the amorphous state, as shown in Fig. A.1 from [Prieto-Depedro *et al.* 2017]. This kind of defects is involved in the crystalline to amorphous transition under irradiation [Marqués *et al.* 2003, Motooka 1994]. Indeed, during ion implantation, pairs of interstitial-vacancies are created due to cascades, the so-called IV pairs. Tight binding simulations of [Tang *et al.* 1997] reported that under certain circumstances, the IV-pair creates a metastable defect structure with an annihilation energy of 1.1 eV. [Cargnoni *et al.* 1998] further confirmed the energy barrier and also that IV-pair defect and the bond defect are closely related.

To create a bond defect, two atoms are displaced and their relaxed positions are determined by using density functional theory (DFT) methods, described within the generalized gradient approximation (GGA) by the PBE functional [Perdew *et al.* 1996] with a 245 cut-off energy, $2 \times 2 \times 2$ k-point mesh, and 0.01 eV/Å force tolerance. The displacement of atoms with respect to their perfect lattice position is tracked, while all possible symmetries are taken into account by expressing the displacement vector according to a third non-moving atom, which could be either C or D, as seen in Fig. A.1. To create the amorphous structure, three crystalline neighbour atoms are randomly chosen and two of them are displaced as stated by the displacement vector obtained

Figure A.3: Angular distribution function for the α -Si phases obtained by the bond switching algorithm and the random method. Extracted from [Prieto-Depedro *et al.* 2017].

before. A bond defect is created, and the two atoms that have been displaced are not considered crystalline anymore and cannot be chosen again for displacement. The bond-switching algorithm is repeated until 25 % of the crystalline atoms have been displaced, and the final structure is fully relaxed. The radial distribution function of the amorphous phase constructed by the two methods explained before are shown in Fig. A.2, where data obtained agree with experimental results reported by [Laaziri *et al.* 1999]. To further confirm the quality of the amorphous structures, the angular distribution is measured for both type of structures, where the agreement between them is also shown in Fig.A.3. As a result, the artificial method proposed in the present work has been evidenced to yield high quality amorphous structures, very suitable to reproduce SPER processes.

List of communications

Book Chapters:

- **M. Prieto-Depedro**, J. Segurado, and I. Martin-Bragado. "Kinetic Monte Carlo modeling of shear-coupled motion of grain boundaries". Book chapter in: "Multiscale Materials Modeling: Approaches to Full Multiscaling". Edited by Siegfried Schmauder and Immanuel Schäfer. De Gruyter, 2016. Journal of Applied Crystallography

Journals:

- **M. Prieto-Depedro**, I. Romero, and I. Martin-Bragado. "Multiscale modeling of defect formation during solid-phase epitaxy regrowth of silicon". Acta Materialia 82 (2015) 115-122.
- **M. Prieto-Depedro**, I. Martin-Bragado, and J. Segurado. "An atomistically informed kinetic Monte Carlo model of grain boundary motion coupled to shear deformation". International Journal of plasticity 68 (2015) 98-110.
- **M. Prieto-Depedro**, A. Payet, B. Sklénard, and I. Martin-Bragado. "Atomistic modeling of the Ge composition dependence of solid phase epitaxial regrowth in SiGe alloys". Journal of Applied Physics 122 (2017) 105702.
- **M. Prieto-Depedro**, and I. Martin-Bragado. "Strain compensation by relieving defects in SiGe channel for FinFET technologies". To be submitted.

Conferences:

- **M. Prieto-Depedro**, B. Sklénard and I. Martin-Bragado. "Atomistic simulations of solid phase epitaxy regrowth of silicon amorphized via ion implantation". In the 12th International Conference of Computer Simulation of Radiation Effects in Solids. June 2014, p. 28.
- **M. Prieto-Depedro**, I. Martin-Bragado, and J. Segurado. "Multiscale modeling of grain boundary motion coupled to shear deformation". In the 24th International Workshop of Computational Micromechanics of Materials. October 2014, p. 6.

- **M. Prieto-Depedro**, and I. Martin-Bragado. "Atomistic modeling of the Ge composition dependence of solid phase epitaxial regrowth of SiGe alloys". Internal seminar at Polytechnic University of Madrid, E.T.S. Ingenieros de Caminos. November 2017.

Other contributions:

- **M. Prieto-Depedro**, J. Segurado, and I. Martin-Bragado. "Atomistic simulations of dynamics of grain boundary motion coupled to shear deformation". Poster in the 10th NanoSpain Conference. March 2014, p. 14.
- **M. Prieto-Depedro**. "Atomistic modeling of grain boundaries in Ni". First Year Assessment at IMDEA Materials. April 2014.

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Multiscale modeling of junction processing in FDSOI and FinFET devices for 10 nm node technology and below

Abstract:

As device downscaling is on pace to reach the physical limits of miniaturization, new problems and challenges arise during the fabrication process. Consequently, potential replacements for conventional Si-based technologies have to be explored, such as 3D architectures (FinFETs) or the introduction of strain engineering techniques for further performance enhancement due to high mobility channels (SiGe as stressor material). Their manufacturing requirements involve highly activated and abrupt junction formation at the low temperature regime, and the Solid Phase Epitaxial Regrowth has been evidenced as the best option for processing advanced technology nodes of 10 nm and below. Relying on this context, the present manuscript is mainly focused at modeling the SPER of Si and SiGe alloys using a multiscale approach including: ab initio, Molecular Dynamics (MD), Lattice Kinetic Monte Carlo (LKMC), Object Kinetic Monte Carlo (OKMC) and Finite Element methods (FEM). The defect formation dependence on stress in Si is accounted by computing the strain pattern due to the volumetric expansion of the α -phase by using FEM methods, which are then evidenced as responsible for nucleation dislocation at the pinch off point of the two moving fronts during recrystallization by using MD simulations. Extracted results are finally extended into a LKMC model allowing to simulate realistic sample sizes, providing a physical explanation of the defect formation mechanisms and their strong dependence on the presence of strain patterns. Moreover, SiGe alloys are considered, and the Ge composition dependence of SPER activation energies is modeled by using MD, extracting an anomalous behavior as the profile does not vary monotonically between values of pure Si and Ge. Nudged Elastic Band calculations are performed to confirm the two-part behavior of the SPER activation energies: the SPER rate itself and a second extra term due to the bond length difference present in the alloy. Finally, as a novel application of strained SiGe layers, SiGe channel FinFET devices are modeled in terms of defect formation when increasing the Ge content in the alloy.

Keywords: Solid Phase Epitaxial Regrowth, Silicon, Silicon-Germanium alloys, Kinetic Monte Carlo, Molecular Dynamics