

Process simulation for advanced stress and junction engineering

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ESSDERC/ESSCIRC Tutorial 2008: Characterisation for the nanoelectric era

Process simulation for advanced stress and junction engineering

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France







Tutorial objectives

"Process simulation for advanced stress and junction engineering »

»Large topic and only 45 minutes !

»and 53 slides

» Why Simulation in a characterisation tutorial ?

»Complementary...

»Not a so good idea to go deeply in the modeling aspect

»Overview of the field: the challenge (Part I), status (Part II), progress (Part III & IV) and perspectives (Part V) »No equation















Outline

Part I: Introduction: Challenge and solution for downscaling

Part II: Process simulation ?

Part III: Recent progress in the modeling of stress

Part IV: Recent progress in the modeling of junction engineering

Part V: Perspectives in Atomistic TCAD: towards some atomistic experiment ?

















Part I Introduction: Challenge and solution for downscaling















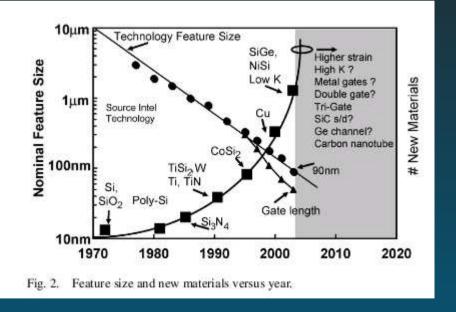


Downscaling (→ 90 nm)

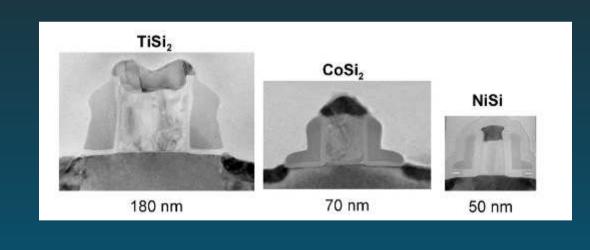
IEEE TRANSACTIONS ON SEMICONDUCTOR MANUFACTURING, VOL. 18, NO. 1, FEBRUARY 2005

In Search of "Forever," Continued Transistor Scaling One New Material at a Time

Scott E. Thompson, Senior Member, IEEE, Robert S. Chau, Senior Member, IEEE, Tahir Ghani, Kaizad Mistry, Sunit Tyagi, Member, IEEE, and Mark T. Bohr, Fellow, IEEE



26



S. E. Thompson et al., IEEE Trans. On Semiconductor Manufacturing, Vol. 18, n°1, 2005











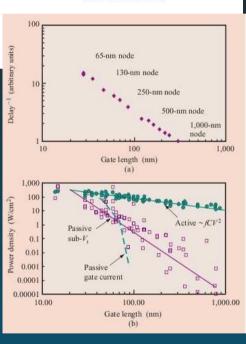




Downscaling (→ 90 nm)

Silicon CMOS devices beyond scaling

To a large extent, scaling was not seriously challenged in the past. However, a closer look reveals that early signs of scaling limits were seen in high-performance devices in recent technology nodes. To obtain the projected performance gain of 30% per generation, device designers have been forced to relax the device subthreshold leakage continuously from one to several $nA/\mu m$ for the 250-nm node to hundreds of $nA/\mu m$ for the 65-nm node. Consequently, passive power density is now a significant portion of the power budget of a high-speed microprocessor. W. Haensch E. J. Nowak R. H. Dennard P. M. Solomon A. Bryant O. H. Dokumaci A. Kumar X. Wang J. B. Johnson M. V. Fischetti



W. Haensch et al., IBM J. Res&Dev, Vol. 50, n°45, 2006















Table 1 Relationships for constant-field scaling and for generalized field scaling, α is the scaling factor for dimensions, and $E = V/\alpha$ is the normalized electric field.

Parameter	Constant-field scaling	Generalizea field scaling	
Physical dimensions,			
L, W, T_{ox} , wire pitch	$1/\alpha$	1/x	
Body doping concentration	α	E/α	
Voltage	$1/\alpha$	E/α	
Circuit density	$1/\alpha^2$	$1/\alpha^2$	
Capacitance per circuit	$1/\alpha$	1 /x	
Circuit speed	α	α (goal)	
Circuit power	$1/\alpha^2$	E^2/α^2	
Power density	1	E^2	
Power-delay product (energy per operation)	$1/\alpha^2$	E^2/α^3	

Stress Engineering approach

• (90nm→ **?)**



Mohta et al., IEEE Circuits and Magazine 2005

L. Peters," Options Narrow at 45nm", Semiconductor International,2006

Main idea: Strain engineering for enhanced mobility and drive current









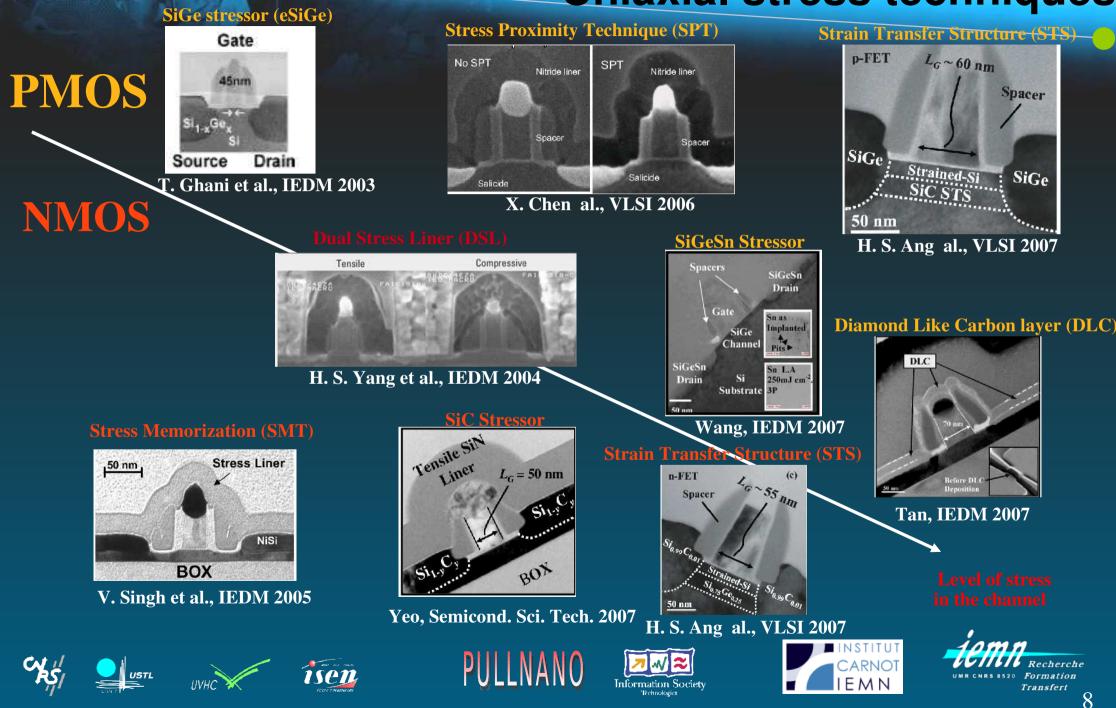




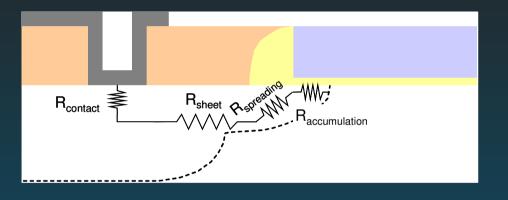


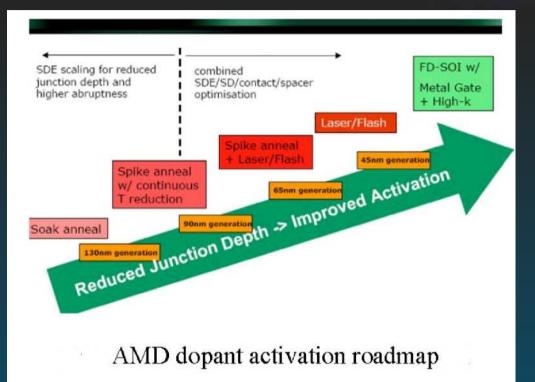
MOBILITY-ENHANCEMENT ROADMAP 130 nm HOT, FDSOL novel materials 120 100 90 nm **Technology** scaling 80 **Multigate FETs** 65 nm 60 **Uniaxial stress** 40 32 nm 22 pm **Biaxial stress** 20 15 am 200 mm 300 mm 2012 2000 2004 2006 2008 2010 2002 2014 Year of introduction by leading-edge companies

Uniaxial stress techniques



Junction optimisation





R_{Sheet}: Conductivity of high doped region J. O. Borland, « 32 nm NODE USJ Implant& Annealing, RTP 2007 High activation: complex techniques













Challenges for 32 & 22 nm

Challenges and Opportunities for High Performance 32 nm CMOS Technology

J.W. Sleight, I. Lauer, O. Dokumaci, D. M. Fried, D. Guo, B. Haran, S. Narasimha, C. Sheraw, D. Singh, M. Steigerwalt, X. Wang, P. Oldiges, D. Sadana, C.Y. Sung, W. Haensch, and M. Khare IBM T. J. Watson Research Center, 1101 Kitchawan Road, Yorktown Heights NY 10598 sleight@us.ibm.com (914) 945-1876

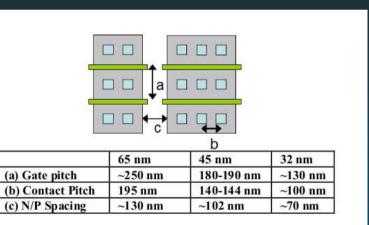


Fig. 1: Selected critical dimensions for different technology nodes.

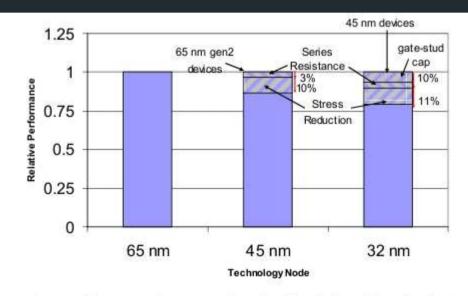


Fig. 2: Performance loss associated with pitch scaling for the 45 nm and 32 nm nodes. The performance loss associated with parasitics and stress loss is likely exacerbated at the 32 nm node.

J. W. Sleight et al., IEDM Tech. Dig., 2006















Challenges for 32 nm

<u>Scalability:</u>

- -11% stress reduction compared to 65nm (decreasing gate pitch) [Sleight06]
- ITRS Junction target (extension depth, abruptness& sheet resistance) challenging

• <u>Yield</u>:

- ITRS[07] : integration of multiple sources of local and global stress
- Not exceeding the local critical shear stress
- <u>Design</u>
 - Pitch and layout dependent
 - "Strain adds new challenges from a design perspective" [Lammers08]

→ TCAD have a role to play to provide key information (process => design)

















PART II: Process Simulation ?







UVHC







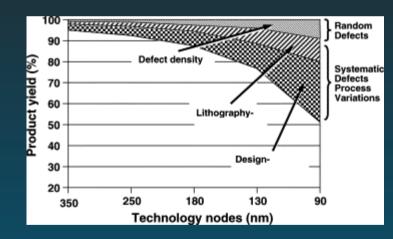


TCAD ?

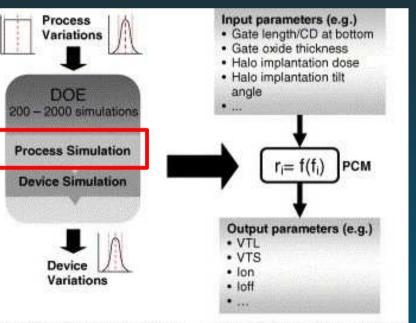


Materials Science and Engineering B 124-125 (2005) 81-85

Trends, demands and challenges in TCAD Ingo Bork*, Victor Moroz, Lars Bomholt, Dipu Pramanik Swopsys, Inc., 700 E. Middlefield Rd., Mountain Yaew, CA 94043, USA



<u>TCAD :</u> → Technology cost development (40% ITRS) *>* Yield



MATERIALS SCIENCE & GINEERING R

www.elsevier.com/.ocate/mseb

Numerical TCAD Model: o(1hr) ----> Process Compact Model: o(1ms)







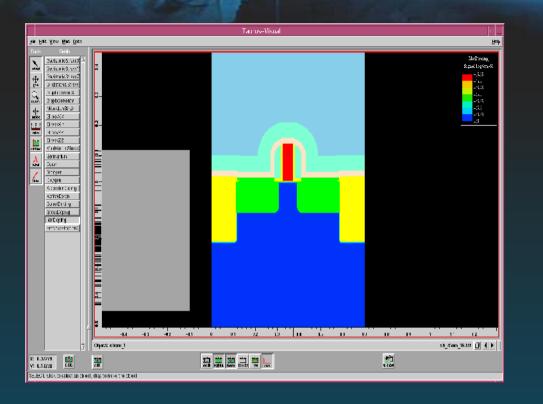


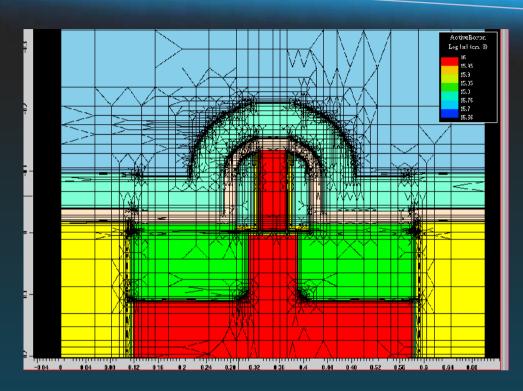






Process Simulation





Standard process simulation:

- Transistor Building (finite elements)
- Simulation of the various process step (implantation, diffusion, oxidation, silicidation
- « Physical » modeling with partial differential equations (PDE)

- Knowledge of the various physical parameters (topology, dopant distribution, stress field) for electrical simulation









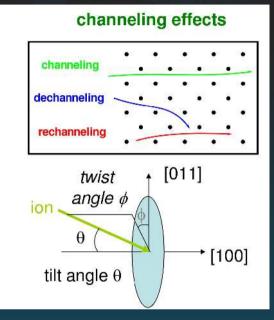






Implantation modeling

Implantation modeling : Implant tables or Monte-Carlo Simulation



Series of consecutive binary collisions of the projectile with the lattice (BCA MC):

Nuclear scattering (Coulomb pair potential) Semi empirical model for the electronic energy loss of particles Phenomenological models for damage probability

M. Posselt, private communication



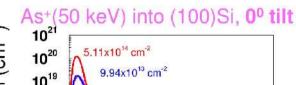




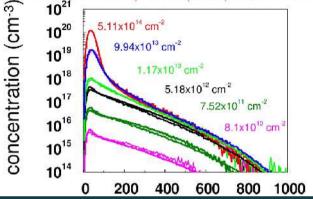




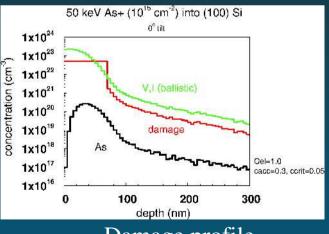




simulation results vs. exp. data:



Range distribution of implanted ions



Damage profile

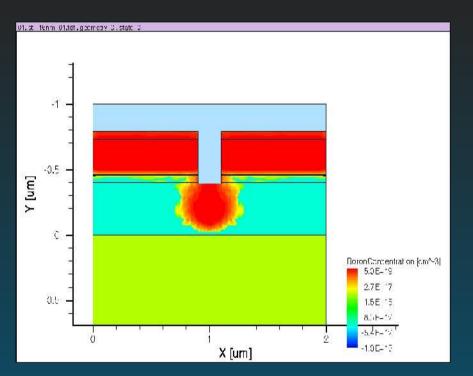
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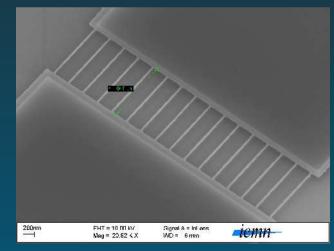
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Implantation Modeling Example

• 2D Implant modeling for nanowire fabrication



200mm EHT = 5.0 kV May - 21.44 K X Signal A = InLens WD - 9 rm



Creation of Silicon nanowire by anisotropic etching with a damage gradient Optimisation (Dopant, Dose, Energy) with simulation

Vikram Passi et al., UCL, NANOSIL WP 2.1 (unpublished results)













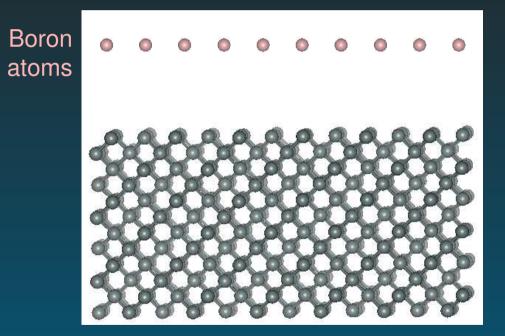


Diffusion modeling (1)

Junction Fabrication

Standard Technology

Ionic implantation for the dopant with various energy& dose



After implantation:

Dopants in an interstistial position electrically inactive
Defects created : interstitials, vacancies,

aggregate, amorphous pocket

 \rightarrow Annealing step mandatory











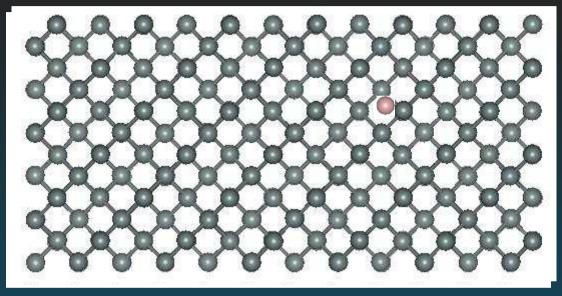




Diffusion Modeling (2)

Boron Kick-out

What's going on during annealing? Example for boron



- Interstitial Boron mobile form
- Immobile Boron impurity (electrically active) and creation of Si interstitial
- Diffusion and recombinaison of Si interstitial.
- Kick-out of a boron atoms by an another Si interstitial
- The junction depth and the activated dose results from the contribution of all these mechanisms
- Standard process simulator used Fick law and diffusion- reaction equations to describe the the intreaction with point defects and mechanism like kick-out









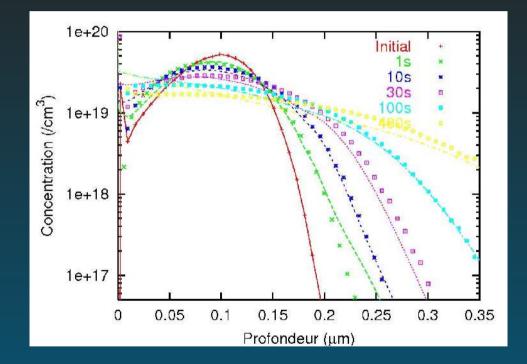




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Diffusion Modeling (3)

 Application: Evolution of doping profile during annealing critical for electrical properties (see also slide 44)



Example of Boron diffusion profile diffusion













Oxidation and stress modeling (1)

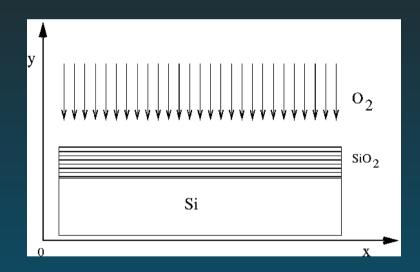
IOURNAL OF APPLIED PHYSICS

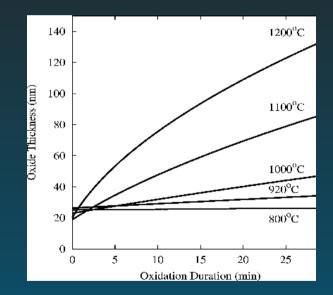
VOLUME 36, NUMBER 12

DECEMBER 1965

General Relationship for the Thermal Oxidation of Silicon

B. E. DEAL AND A. S. GROVE Fairchild Semiconductor, A Division of Fairchild Camera and Instrument Corporation, Palo Alto, California (Received 10 May 1965; in final form 9 September 1965)





Process simulator : generalised Deal& Grove oxidation model (diffusivity & and reaction rate stress-dependent) to take into account the stress (volume expansion)









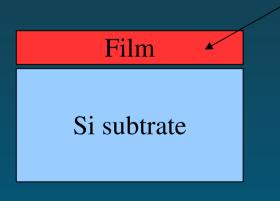


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Various source of stress

Stress sources	Technical Process
Thermal Stress	Thermal variation during various processing step
Topological induced Stress	Thermal growth (oxidation, silicidation), etching
Intrinsic Stress	Film deposition process (nitride, polysilicon, metals)
Extrinsic stress	Structural modifications of films
High doping induced stress	Steep doping gradients

Example : modeling of stress generated by deposition of thin film introduction of an extrinsic stress and mechanical equilibration















σ

extrinsic



Example: Oxidation and stress modeling

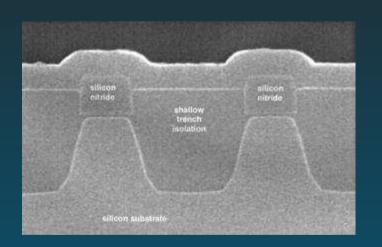
JOURNAL OF APPLIED PHYSICS

VOLUME 94, NUMBER 9

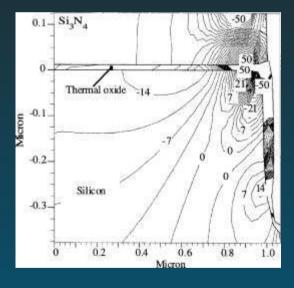
1 NOVEMBER 2003

Strain determination in silicon microstructures by combined convergent beam electron diffraction, process simulation, and micro-Raman spectroscopy

Vincent Senez^{a)} IEMN-ISEN, UMR CNRS-8520, Avenue Poincaré, B.P. 69, 59652 Villeneuve d'Ascq cédex, France



STI (Shallow stress Isolation structure)

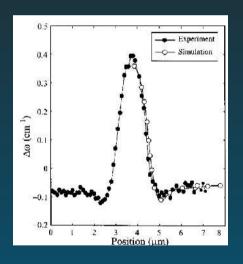


Stress field (TCAD)

Information Society

Technologie

PULLNANO



 μRS (experiment vs simulation)

but for Large structure

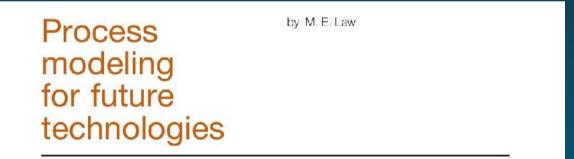




Recherche CNRS 8520 Formation Transfert 22



- These different examples => process modeling promising
- Reality is/was more complex (2002)
 - Example taken from different or academic softwares
 - Difficulty to describe TED Boron, segregation effects, ultra-thin oxidation, silicidation....
 - No real stress modeling capabilities (commercial tool)
- The Mark Law definition: « TCAD : yesterday's technology modeled tomorrow»



M. E. Law, IBM J. Res. Dev., Vol. 46, n°2/3, March 2002















- « TCAD : yesterday's technology modeled tomorrow» still true ?
- No:
 - Large progress have been performed in diffusion modeling (Support by the EC: European project Rapid, Frendtech, PullNaNo,Atomics)
 - Progress have been done for « simple » stress modeling
 - The merging of the major TCAD firms (Avant!, ISE, Synopsys) ~ market 80%
 - DIOS (meshing, numerical stability), TAURUS (3D capabilities, Implantation, stress) and TSUPREM-IV (oxidation modeling) to the FLOOPS-ISE (new diffusion modeling)
 - More contribution and more insight with atomistic modeling
 - There is also a part of « dream »: simulation can not replace characterisation
 - Script models speed up the pipeline (M. Law) : University (models)=>TCAD company (software) => Semiconductor Company ? No but more
- Yes:
 - Complexity increase : Stress Engineering (Slide 8), New material (Ge), Laser Annealing & Solid Phase Epitaxy.....















Recent progress in the modeling of stress

















Modeling SiGe S/D stress field

APPLIED PHYSICS LETTERS 86, 023103 (2005)

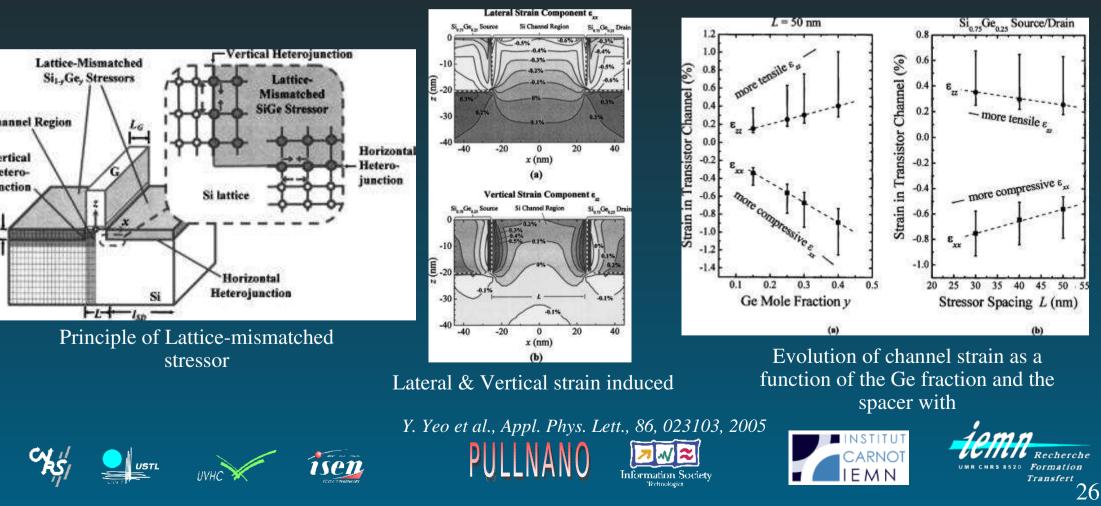
Finite-element study of strain distribution in transistor with silicon-germanium source and drain regions

Yee-Chia Yeo^{a)}

Silicon Nano Device Laboratory, Department of Electrical and Computer Engineering, National University of Singapore, 119260, Singapore

Jisong Sun

Agency for Science, Technology, and Research, Data Storage Institute, DSI Building, 5. Engineering Drive 1, 117608, Singapore



SiGe S/D scalability

IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 53, NO. 7, JULY 2006

Scalability of the $Si_{1-x}Ge_x$ Source/Drain Technology for the 45-nm Technology Node and Beyond

Geert Eneman, Peter Verheyen, Rita Rooyackers, Faran Nouri, Senior Member, IEEE, Lori Washington, Robert Schreutelkamp, Victor Moroz, Lee Smith, Member, IEEE, An De Keersgieter, Malgorzata Jurczak, and Kristin De Meyer. Senior Member, IEEE

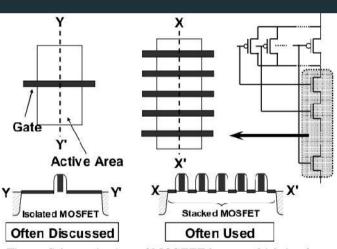
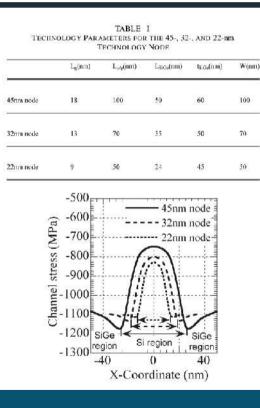
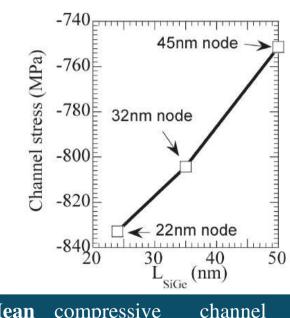


Fig.1 Schematic view of MOSFET layout which is often used and often discussed. Stacked MOSFET which is often used in actual products should be discussed.





Mean compressive stress does not decrease with downscaling

G. Eneman et al., IEEE Trans. on Electron Device, Vol. 86, 023103, 2005















16/7

Modeling CESL stress

Multi-Layer Model for Stressor Film Deposition

K.V. Loiko, V. Adams, D. Tekleab, B. Winstead, X.-Z. Bo, P. Grudowski, S. Goktepeli, S. Filipiak, B. Goolsby, V. Kolagunta, and M.C. Foisy

> Austin Silicon Technology Solutions, Freescale Semiconductor, Inc. 3501 Ed Bluestein Blvd, Austin, TX 78721 Email: loiko@freescale.com

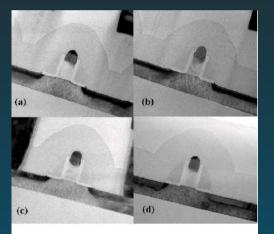


Figure 1. TEMs of 35nm gates with highly stressed ESL films as a function of gate poly pitch: (a) 0.26 µm. (b) 0.38 µm. (c) 0.63 µm. (d) 1.04 µm.

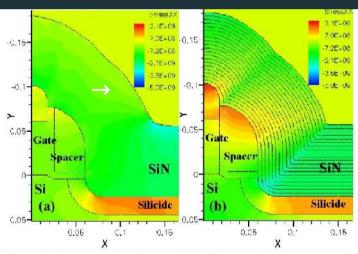


Figure 7. Contours of lateral stress (Pa) in 35nm transistor structures with 20nm source/drain recess simulated using (a) single-layer and (b) 20-layer deposition of nitride with compressive intrinsic stress.

Large difference between mono and multi step deposition

K. V. Loiko et al., SISPAD 2006





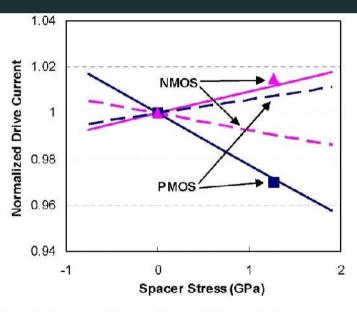


Figure 8. Experimental data (symbols), multi-layer (solid lines) and singlelayer (dashed lines) simulation results on NMOS (tensile ESL) and PMOS (compressive ESL) drive current vs. spacer stress.

Opposite experimental trends with mono step deposition !





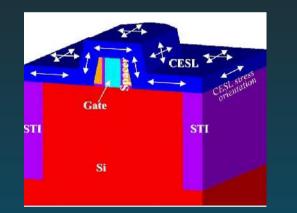
Engineering the CESL stress

814

IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 54, NO. 4, APRIL 2007

Method for Managing the Stress Due to the Strained Nitride Capping Layer in MOS Transistors

Stéphane Orain, Vincent Fiori, Davy Villanueva, Alexandre Dray, and Claude Ortolland



3D Ansys Simulation

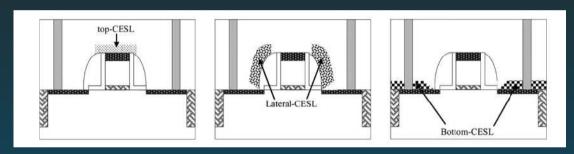


TABLE I SUMMING UP THE IMPACT OF ALL THE CESL EFFECTS (C = CORNER, D = DIRECT, AND I = INDIRECT) FOR EACH CESL ZONE (TOP, LAT. – LATERAL, AND BOT. – BOTTOM)

		Corner	Тор	Lat.	Bot.	LEGEND:
Long	Sx	C*	D-	0	D*	C : Corner effects D : Direct effects I : Indirect effects - : Compressive stress + : tensile 0 : no or low impact
	Sy	C+	D-	0	D+	
	Sz	0	I- /D-	0	0	
Short	Sx	C+	0	D	D*	
	Sy	C+	0	D.	D*	
	Sz	0	1-	I-/ D-	D-	

Which part of the CESL influence the channel stress ?

-Complex answer (Long<>short device) !

-Such table provide guidelines for device optimisation

-Geometry of the spacer (L or D shape) important













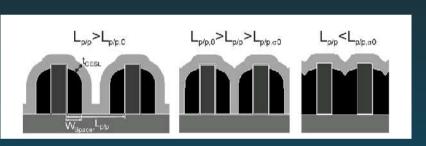


Scalability of CESL

IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 54, NO. 6, JUNE 2007

Scalability of Stress Induced by Contact-Etch-Stop Layers: A Simulation Study

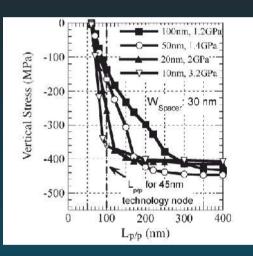
Geert Eneman, Peter Verheyen, An De Keersgieter, Malgorzata Jurczak, and Kristin De Meyer, Senior Member, IEEE



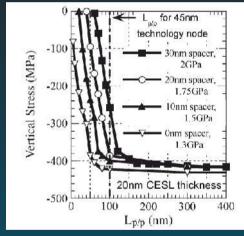
1446

Poly to Poly Distance: Lp/p

 $L_{\rm p/p} > L_{\rm p/p,0} = 2 \cdot t_{\rm CESL} + 2 \cdot W_{\rm Spacer}$



For large CESL thickness, decreasing Lp/p leads to stress reduction



Influence of spacer width on vertical stress for decreasing Lp/p

↘ CESL thickness is no sufficient, spacer dimensions must be scaled

G. Eneman et al., IEEE Trans. on Electron Device, Vol. 54, N°6, June, 2007





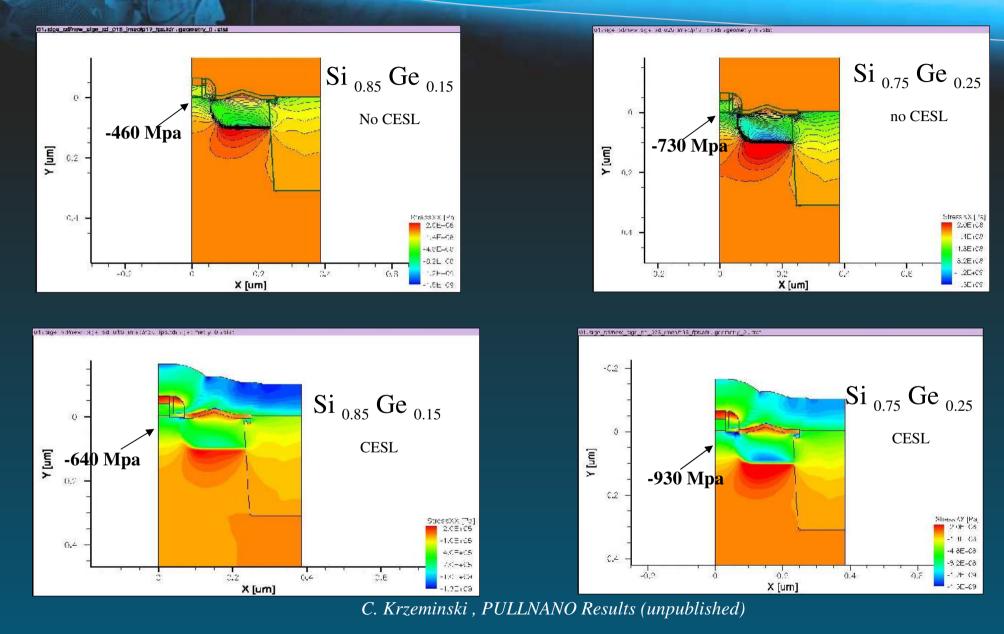








S/D SiGe & CESL modeling with SProcess

















Conclusion

- Large progress have been performed in the stress modeling with the support of experimental development, study of topography influence, evaluation of scalability (SiGe S/D or Stress Liner)
- There was one issue :

Journal or major proceedings conferences Publications (2001-2008)	Number	Proprietary simulator	"Old" simulator Taurus/ Tsuprem-IV	Mechanical simulator (Ansys/ FEMLAB)	Sentaurus Process
TCAD&stress	14	30%	40%	30%	0%

- But large progress have been performed recently in the last version of Sentaurus Process as shown by the last PullNANO Results
- Still a lot of work: Stress Memorization, SiC stressor.....

















Progress in diffusion modeling









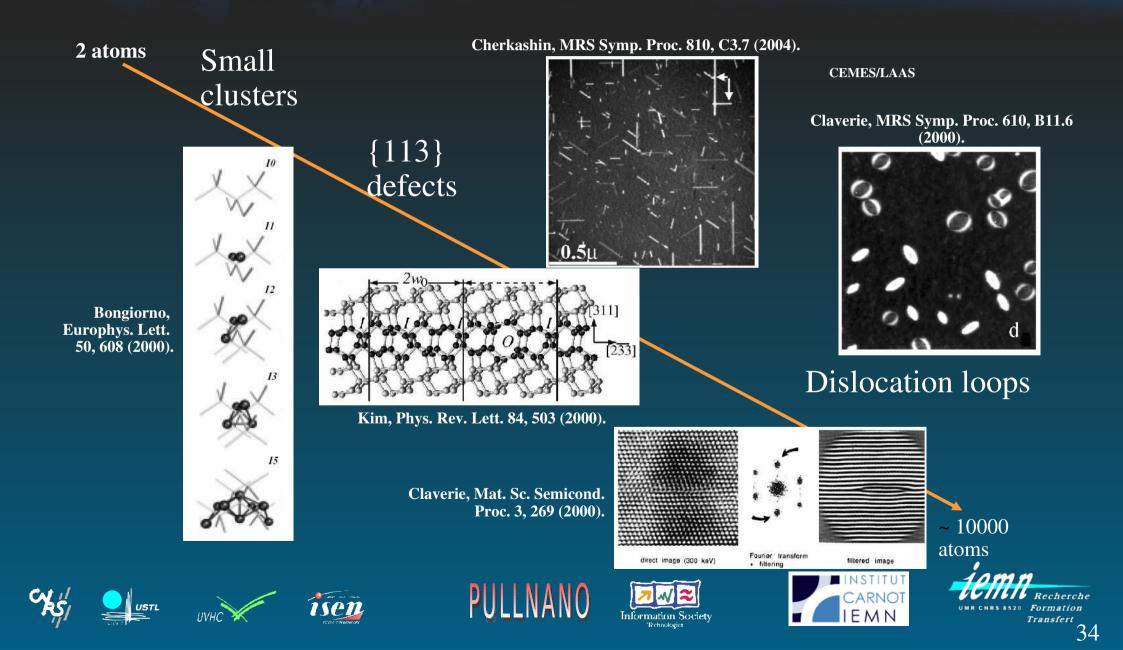






Extended defects

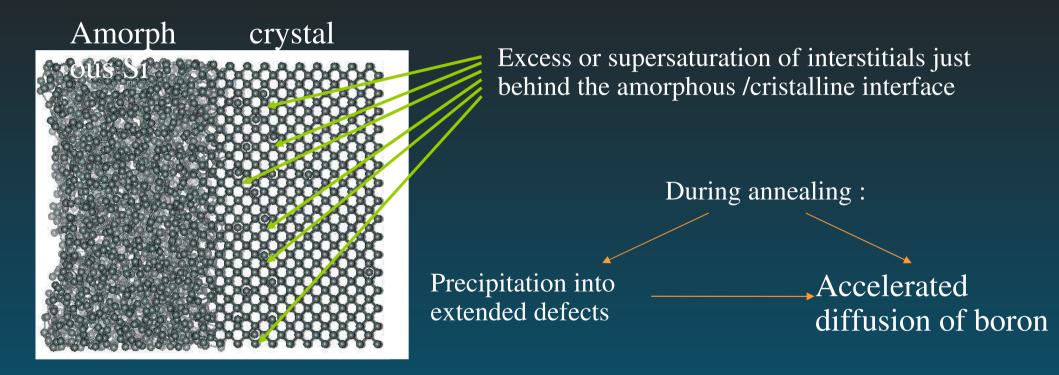
Role on extended defects formed after ion implantation of dopants



Boron Transient enhanced diffusion (TED) & extended defects

 \rightarrow Common origin : the supersaturation of interstitials formed by the implantation step

Ex in the case of a preamorphisation :



 \rightarrow Need to couple a model of extended defects to conventionnal packages of dopant diffusion







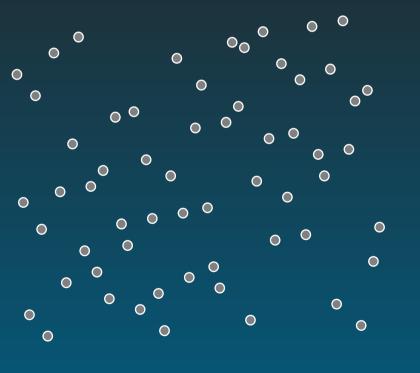






nucleation, pure growth and Ostwald ripening of defects

Nucleation of extended defects – reduction of the system energy



Precipitation

















nucleation, pure growth and Ostwald ripening of defects

Nucleation of extended defects – reduction of the system energy

• Growth of the nuclei by absorption of the residual interstitials

 \rightarrow pure growth



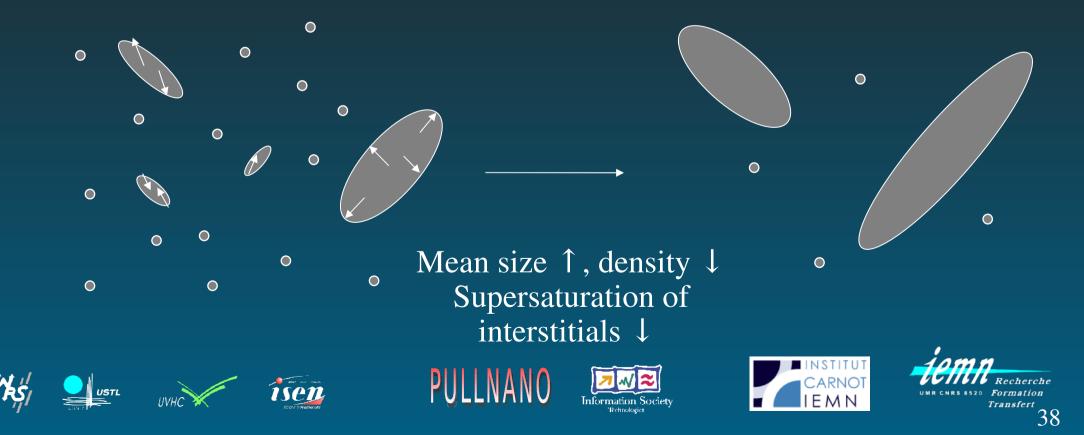
Nucleation, pure growth and Ostwald ripening of defects

Nucleation of extended defects – reduction of the system energy

Growth of the nuclei by absorption of the residual interstitials

 \rightarrow pure growth

• Ostwald ripening (dynamical equilibrium) extended defects ↔interstitial supersaturation



TED and Dislocation Loops (DL)

JOURNAL OF APPLIED PHYSICS

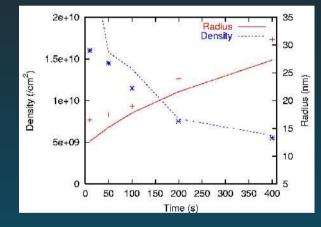
VOLUME 85, NUMBER 12

15 JUNE 1999

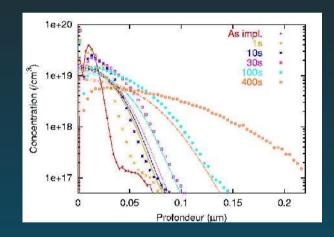
Modeling of the transient enhanced diffusion of boron implanted into preamorphized silicon

E. Lampin^{a)} and V. Senez IEMN-Dpt. ISEN, UMR CNRS 9929, BP 69, 59652 Villeneuve d'Ascq Cédex, France

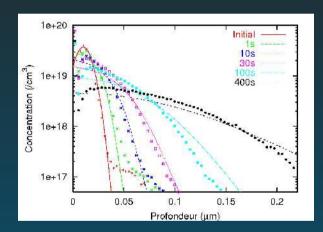
A. Claverie CEMES-CNRS, BP 4347, 31055 Toulouse Cédex, France



Evolution of density and size of Dislocations loops (DL)



Final TED diffusion effects underestimated if DL not considered



Good predictivity of TED effects with the incorparation of DL and Si interstitials evolution















Atom-by-atom model of defects evolution

Appl. Phys. A 76, 1025-1033 (2003)

Applied Physics A

 $\circ \circ$

10

105

 10^{3}

10

10

0

10

DOI: 10.1007/s00339-002-1944-0

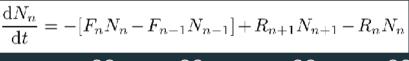
Materials Science & Processing

A. CLAVERIE B. COLOMBEAU B. DE MAUDUIT¹ C. BONAFOS¹ X. HEBRAS^{1,2}

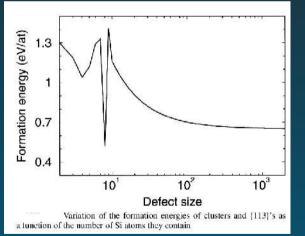
G. BEN ASSAYAG F. CRISTIANO²

Extended defects in shallow implants

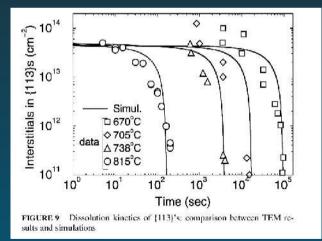
1 Ion Implantation Group CNRS Toulouse, CEMES/CNRS, BP 4347, 31055 Toulouse Cedex, France ² Ion Implantation Group CNRS Toulouse, LAAS/CNRS, 7 Ave, Colonel Roche, 31055 Toulouse Cedex, France







Formation energies for clusters, {113} Cowern et al.



Dissolution of {113}'s

A. Claverie et al., Appl. Phys. A, Vol. 76, 2003 (Frendtech results)











10



600°C

-- 700°C ----- 800°C

10⁵

000

101

Time (sec)

Coupling atom-by-atom model & diffusion

JOURNAL OF APPLIED PHYSICS

VOLUME 94, NUMBER 12

15 DECEMBER 2003

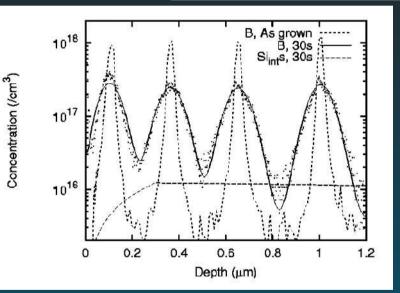
Prediction of boron transient enhanced diffusion through the atom-by-atom modeling of extended defects

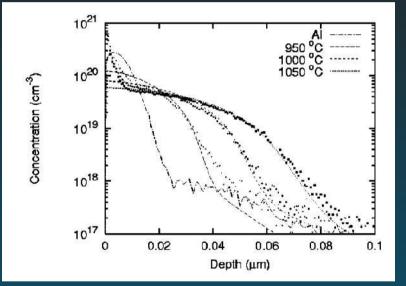
E. Lampin^{a)}

IEMN/ISEN, UMR CNRS 8520, 59652 Villeneuve d'Ascq, Cedex, France

F. Cristiano, Y. Lamrani, and A. Claverie Ion Implantation Group, CEMES/LAAS-CNRS, 31055 Toulouse, France

B. Colombeau and N. E. B. Cowern Advanced Technology Institute, University of Surrey, Guildford, GU2 7XH Surrey, United Kingdom





Nice simulation of TED effects for marked layers experiments Nice simulation of TED for ultra-low Energy B+ implant

However, simplified model for Sprocess needed

E. Lampin et al., J. App. Phys., Vol 94, n°12, 2003 (Frendtech results)













Advanced annealing schemes

On a Computationally Efficient Approach to Boron-Interstitial Clustering

Johann Schermer and Peter Pichler Fraunhofer-Institute of Integrated Systems and Device Technology, Erlangen, Germany Christoph Zechner Synopsys Switzerland LLC Zurich, Switzerland Wilfried Lerch and Silke Paul Mattson Thermal Products GmbH Dornstadt, Germany

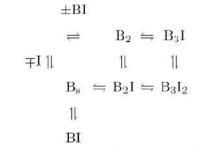
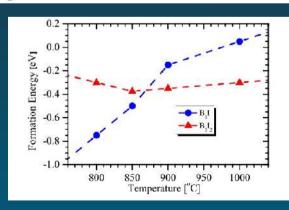
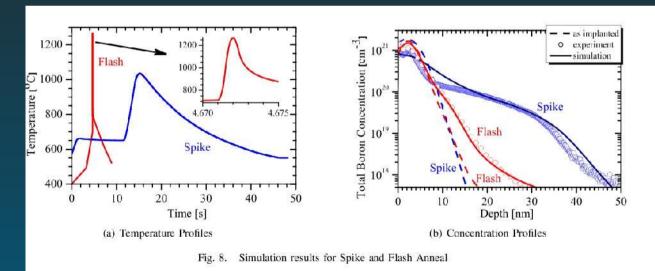


Figure 1: Scheme of reactions for the BICs model







J. Shermer et al., ESSDERC 2007 (PULLNANO results)









Boron diffusion modeling & Device simulation

Process Models for Advanced Annealing Schemes and their Use in Device Simulation

P. Pichler^{1,2,*}, A. Martinez-Limia¹, C. Kampen¹, A. Burenkov¹, J. Schermer¹, S. Paul³, W. Lerch³, J. Gelpey⁴, S. McCoy⁴, H. Kheyrandish⁵, A. Pakfar⁶, C. Tavernier⁶, D. Bolze⁷

1E21

1E20

1E18

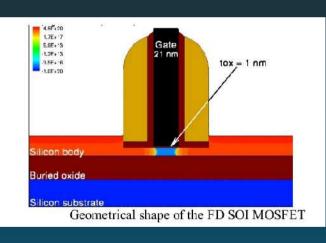
1E17

-0.10

-0.05

 $N_{B} (cm^{-3})$

¹Fraunhofer-Institute of Integrated Systems and Device Technology (IISB), Schottkystrasse 10, 91058 Erlangen, Germany



FD nanometric SOI device

Impact of the diffusion modeling on the boron profile

0.00

Lateral direction (um)

nealed

Lateral boron doping concentration flash an-

Large impact on the PMOS electrical characteristic predicted

P. Pichler et al., International Workshop on junction Technology (2008), ATOMICS & PULLNANO Results











conv. model

0.10

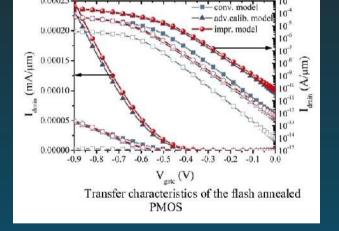
adv.calib. model

- impr. model

0.05









- Large progress have been done in junction processing modeling in the framework of several european projects (Rapid, Frendtech, Pullnano, Atomics) with the collaboration of Synopsys (Zurich)
- Some of the models presented (simplified form) in Sentaurus Process or script transfered to semiconductor compagnies
- But still a lot of work:
 - Influence of stress effects
 - New Material (SiGe S/D, Ge....)
 - Advanced annealing scheme (laser annealing, solid phase epitaxy)
- More information :



















Atomistic TCAD : towards some computer experiment ?







isen











Complexity & Limits of a full experimental optimisation (1)?

Complex integration in nanodevices

APPLIED PHYSICS LETTERS 90, 241912 (2007)

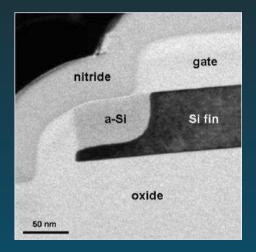
Solid phase epitaxy versus random nucleation and growth in sub-20 nm wide fin field-effect transistors

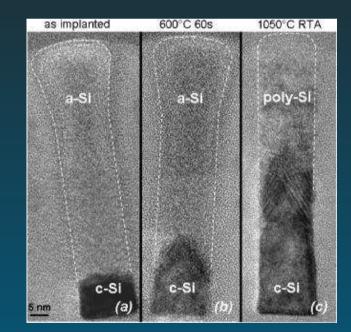
R. Duffy,^{a)} M. J. H. Van Dal, and B. J. Pawlak NXP Semiconductors, Kapeldreef 75, 3001 Leuven, Relgium

M. Kaiser and R. G. R. Weemaes Philips Research Laboratories Eindhoven, High Tech Campus 11, 5656 AE Eindhoven, The Netherlands

B. Degroote, E. Kunnen, and E. Altamirano IMEC, Kapeldreef 75, 3001 Leuven, Belgium

(Received 26 March 2007; accepted 22 May 2007; published online 13 June 2007)





(PULLNANO results)















Complexity & Limits of a full experimental optimisation (2) ?

How to characterised diffusion mechanism during a solid phase epitaxy when Time/Temperature window available reduced by recrystallisation ?



 \rightarrow A solution proposed by Venezia et al.: Diffusion in completely amorphised silicon layer (but the influence of recrystallisation is not taken into account)

→Computer experiment (Atomistic TCAD) needed but it will not replace standard TCAD !















Which method for computer experiment?

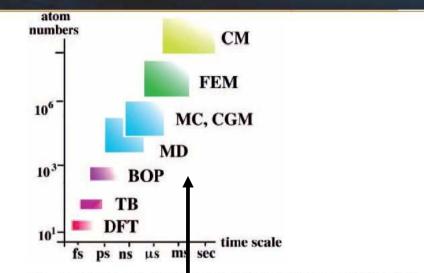


Fig. 1. Length and timescales in various modeling methods: DFT = density-functional theory, TB = tight-binding approximations, BOP = bond-order potentials, MD = empirical molecular dynamics, MC, CGM = Monte-Carlo/conjugate-gradient techniques, FEM = finite element methods, CM = continuum mechanics

[Scheerschmidt07] http://www.mpi-halle.de/mpi/publi/pdf/6735_06.pdf

Development of atomistic approach based on molecular dynamics (MD)















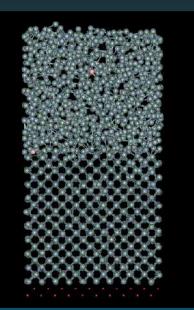
Molecular Dynamics of LPE, SPE regrowth

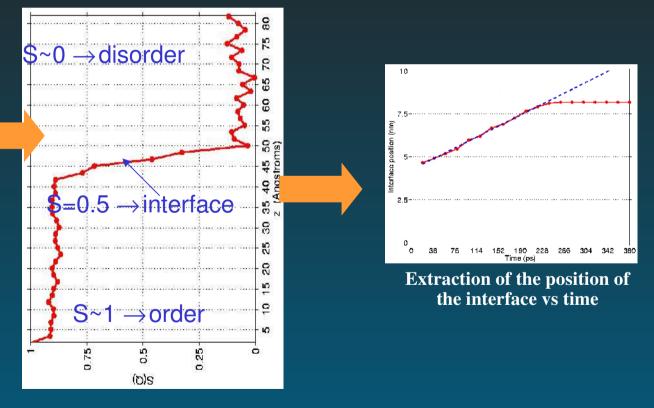
Simulation of the annealing and exploitation

Example of annealing, Stillinger-Weber, 1200 K

Extraction interface from 1D structure factor

Procedure repeated to extract the recrystallization velocity















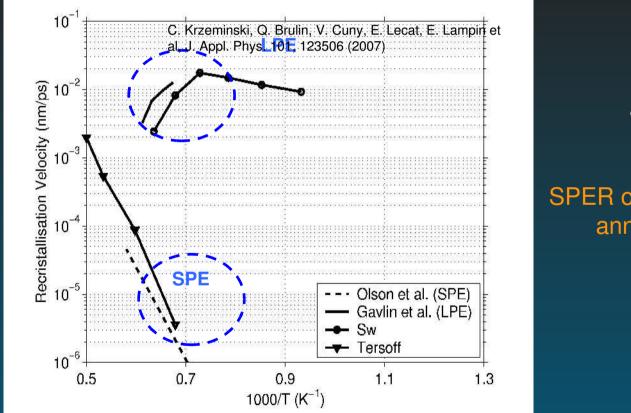


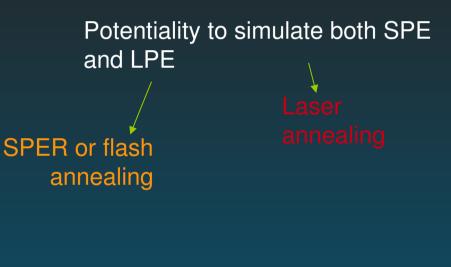


Molecular dynamics of SPE, LPE regrowth (2)

Conclusion :

Analysis of the velocities of recrystallization and of the structure of disordered part :





(PULLNANO results)











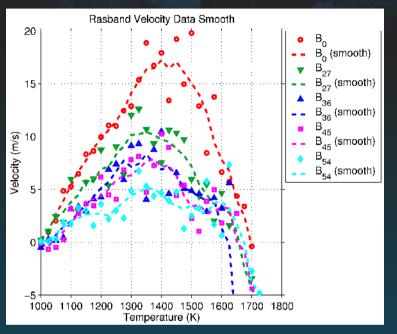




Boron doped LPE regrowth

Reduction of the velocity for large B concentration

Interface roughening & amorphous pockets

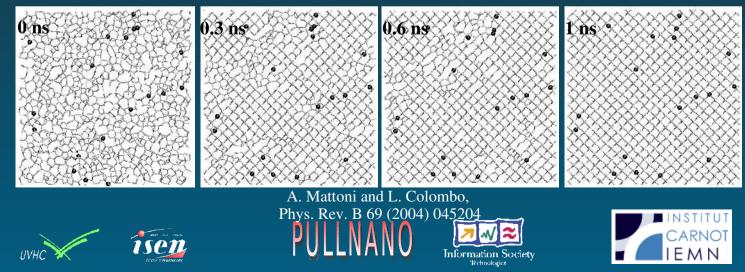






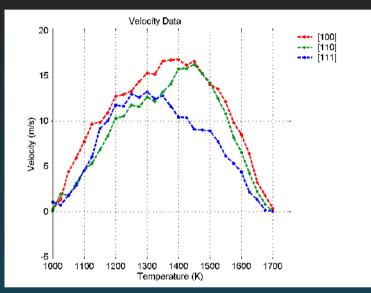
(PULLNANO unpublished results)

Incorporation of boron atoms in c-Si

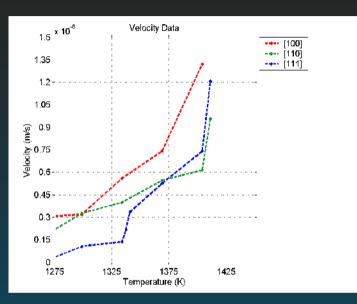




LPE or SPE: influence orientation effects



Orientation influence for LPE [100]>[110]>[111]



Orientation influence for SPE [100]>[110]>[111]

(PULLNANO unpublished results)











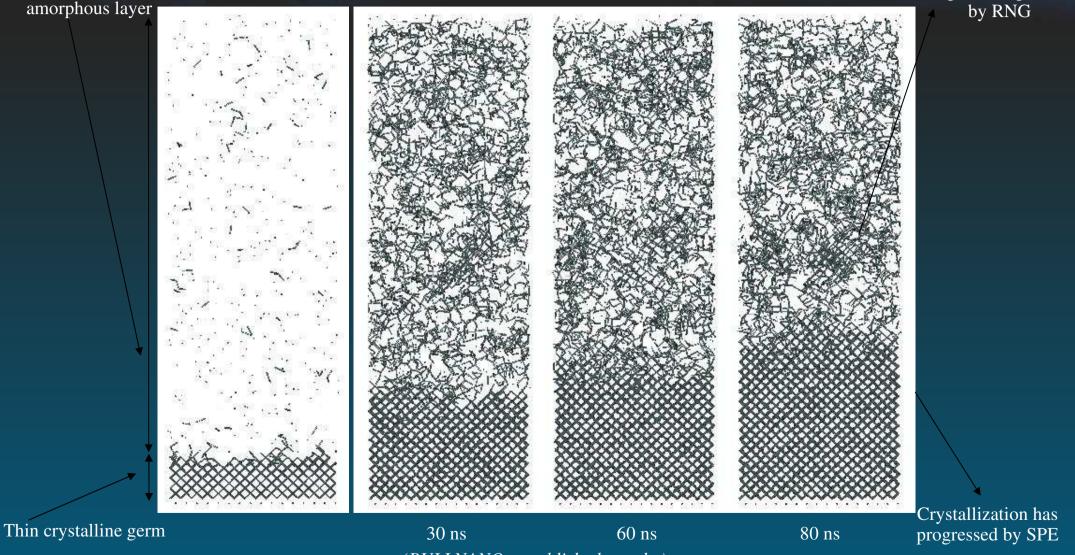






Competition SPE/RNG

Thick amorphous layer







(PULLNANO unpublished results)









Some grains begin to form

NRS 8520 Formation Transfert 53