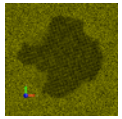
SLACS CNR-INFM

Sardinian Laboratory for Computational Materials Science

L. Colombo, A. Mattoni

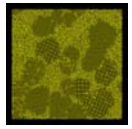
In collaboration with: L. Ferraro, L. Bagolini, G. Fugallo

TASK 1.1 Classical MD simulation of the nanostructure of nc-Si in one a-Si matrix



embedded nanograin*: morphology and growth*

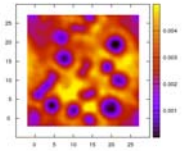
A. Mattoni et al. PRL 99 205501 (2007)



distribution of grains: crystallization kinetics

A. Mattoni et al. PRB 78 075408 (2008)

TASK1.2 Calculation of electronic properties of the nc-Si and a-Si matrix quantum confinement.

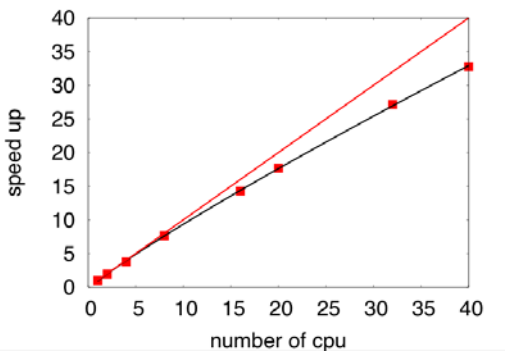


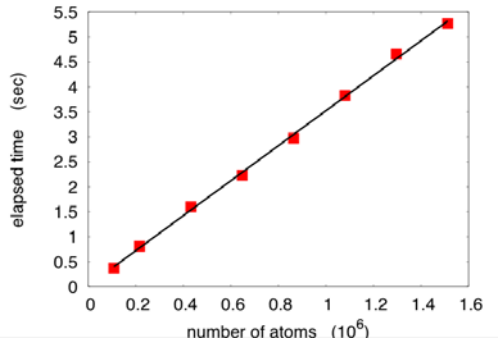
Optoelectronic properties of nc-Si vs. structure

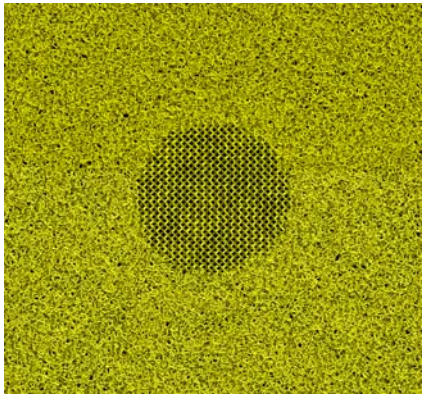
A.Mattoni et al. submitted (2008), L. Bagolini et al. submitted (2008), G. Fugallo et al. In preparation

Generation of atomistic models

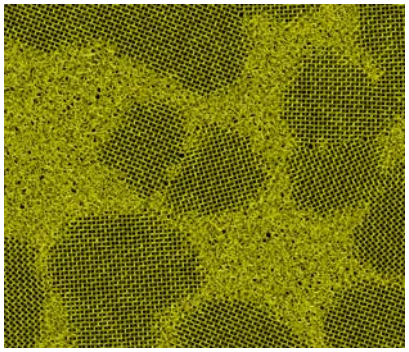
D1.1.1.1 Generation of **atomistic models** of nc-Si and nc-Si/a-Si interfaces by large-scale MD simulations







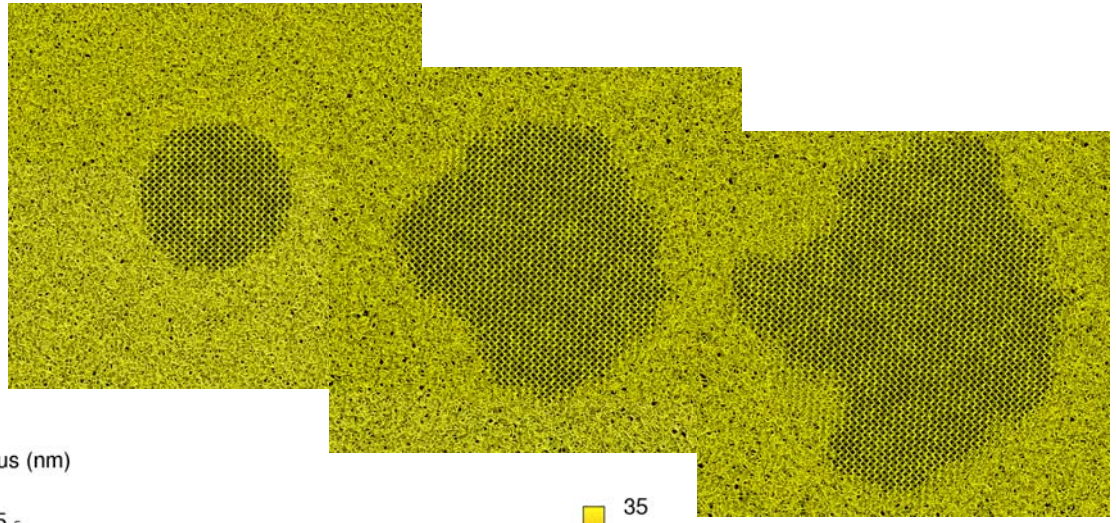
CMPTool: a set of higly efficient parallel numerical libraries for computational materials science developed in collaboration with Caspur (ROME)



Thermal induced crystallization: Crystalline fiber embedded into an amorphous phase acts as seed for recrystallization

Interface atomic mobility

D2.1.1.1 Structural characterization of nc-Si and nc-Si/a-Si (e.g. crystalline vs. amorphous ratio, stress effects due to lattice-mismatched substrates), Determination of **a/c interface atomic mobility** under arbitrary temperature/stress conditions; Modelling of microstructural evolution



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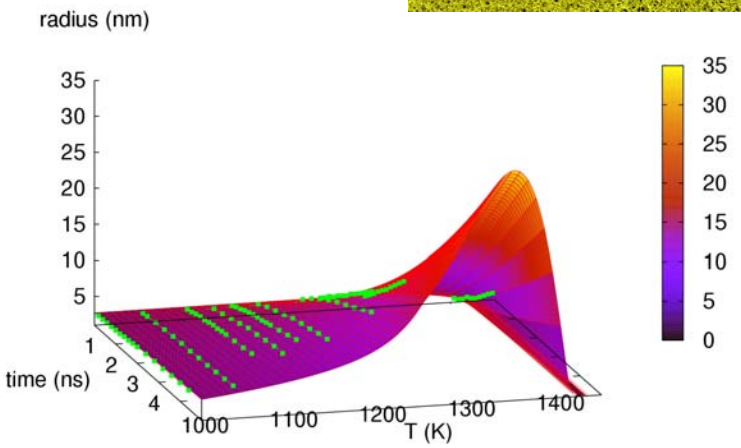
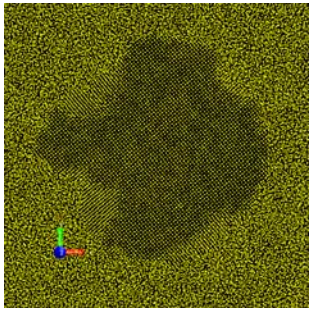
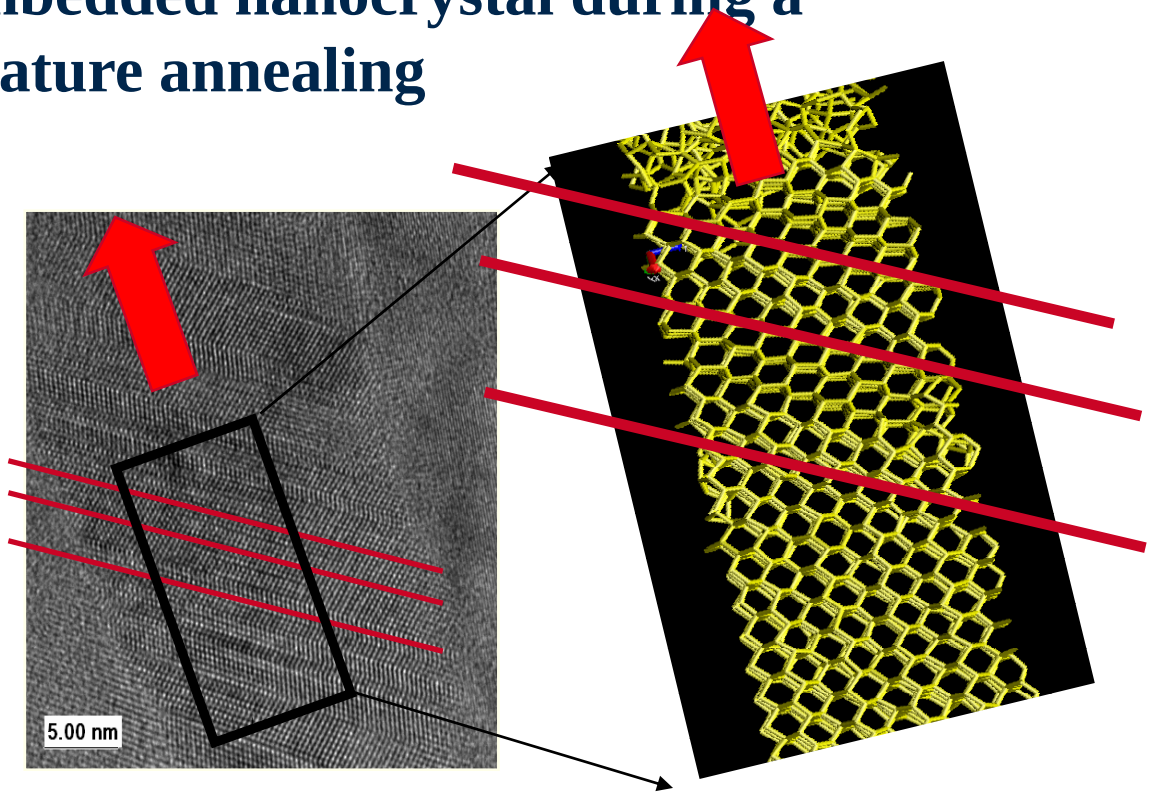


Isolated embedded grain



Growth of an embedded nanocrystal during a constant temperature annealing

RESULTS:



- the growth of embedded nanograins is described by a power law of time

- faceting phenomena are observed

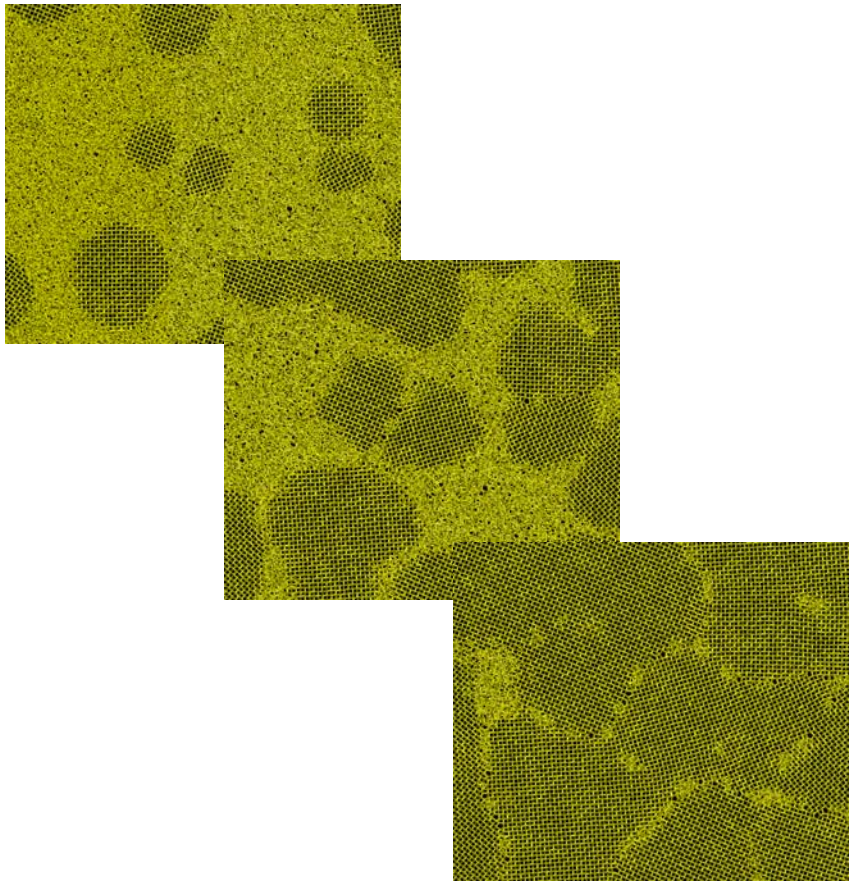
- spontaneous formation of twin boundaries

HRTEM

A. Mattoni et al. PRL 99 205501 (2007)

Distribution of grains

Kinetics of crystallization distribution of grains during a constant temperature annealing



RESULTS:

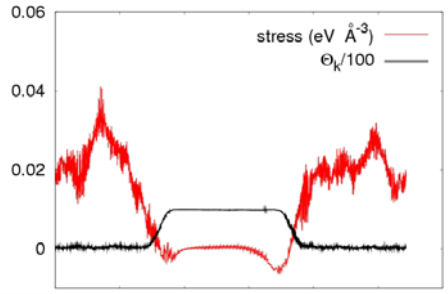
- crystallization is thermally activated

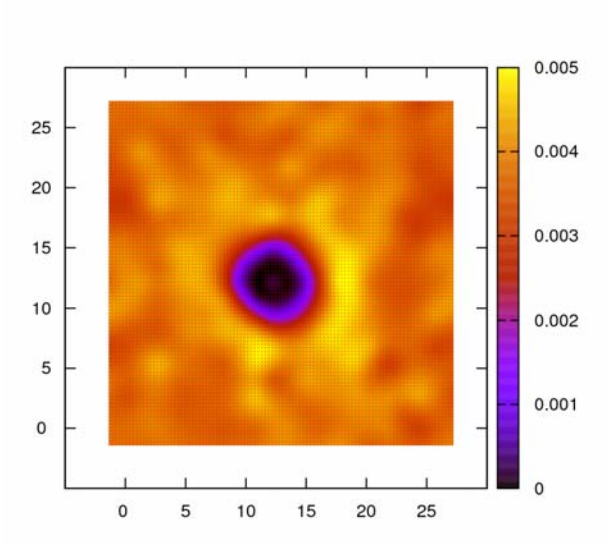
- the kinetics of growth deviates from the continuum theory of phase transformation because of atomic scale features (grain boundaries, local strain, etc.)

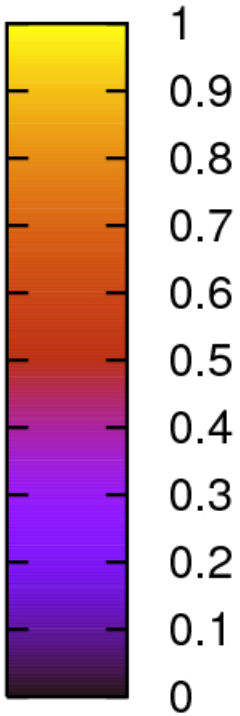
A. Mattoni et al. PRB 78 075408 (2008)

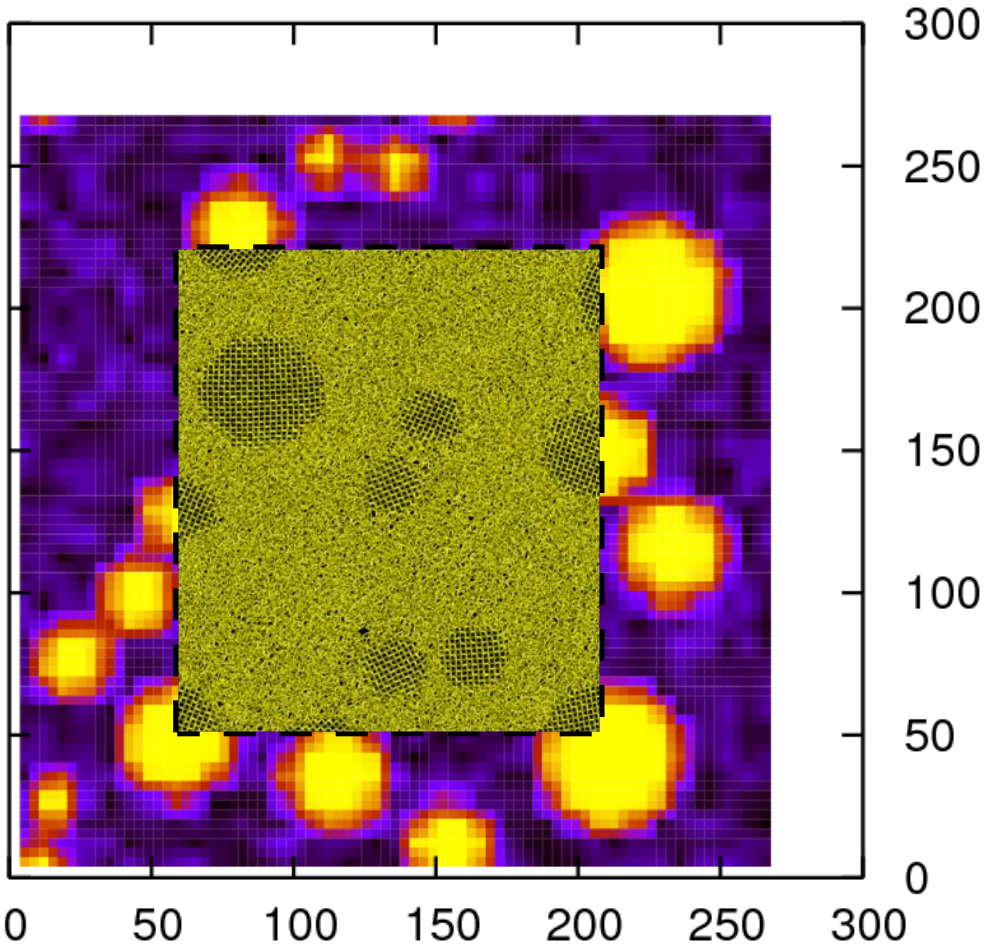
tools for characterization

D1.1.1.2. Development of **new computational tools (software) for structural characterization** of **stress/strain fields** in complex nanostructured and amorphous systems



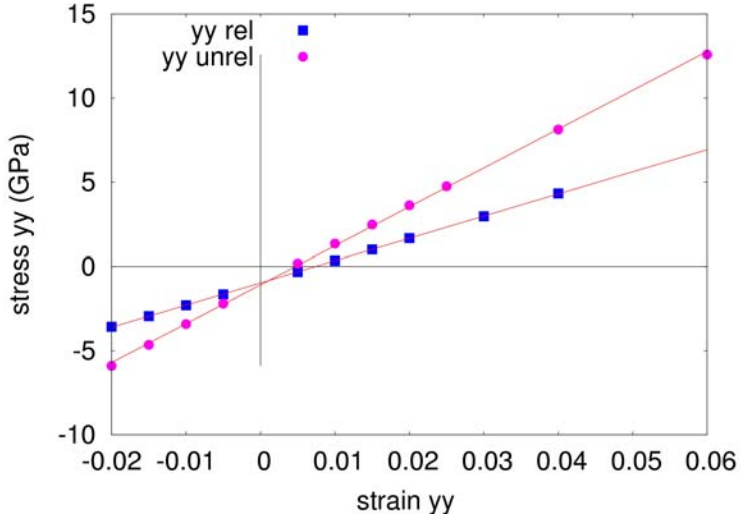


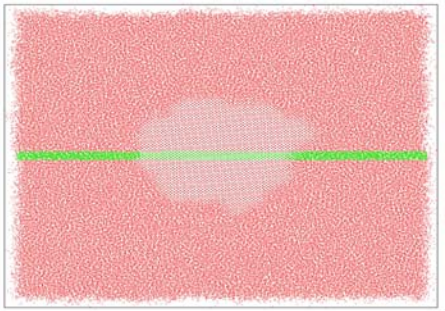


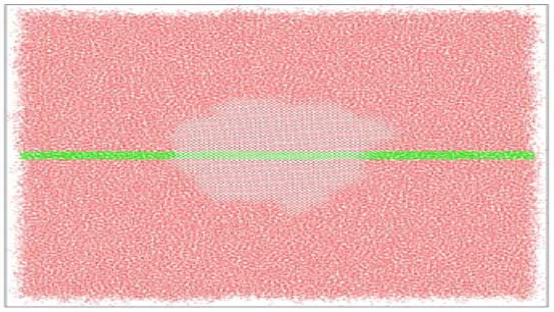


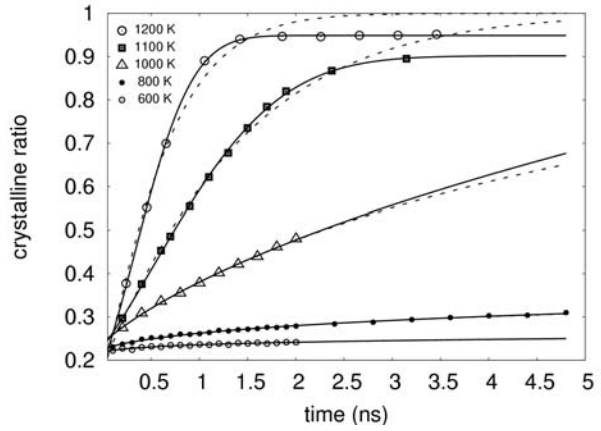
atomistic-continuum

D2.1.1.2 Report about the integration between **atomistic modelling of stress-strain relationship with continuum theory**







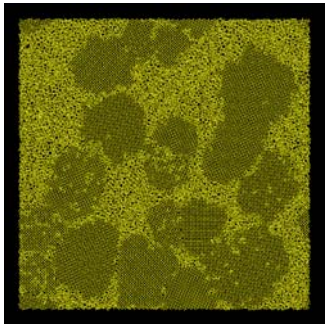


Optoelectronic properties of nc-Si

Task 1.2 Semiempirical calculation of electronic properties of the nc-Si and a-Si matrix quantum confinement. (SLACS CNR-INFM team)

Is it possible to calculate the absorption properties of such large Systems?

What is the relation between the optical absorbtion and the actual amount of crystalline and amorphous phase?



Nearsightedness (NEM)

D3.1.2.1 Development of a **new code (software) for electronic structure calculations of large systems**, as base on empirical methods, like tight-binding or pseudo-potential ones.

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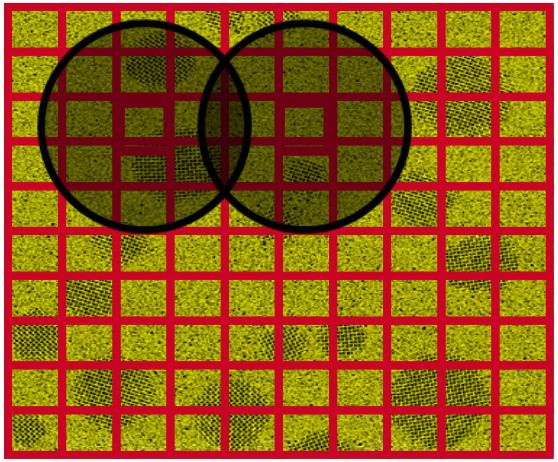
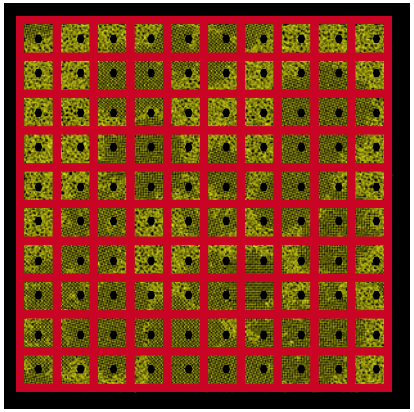
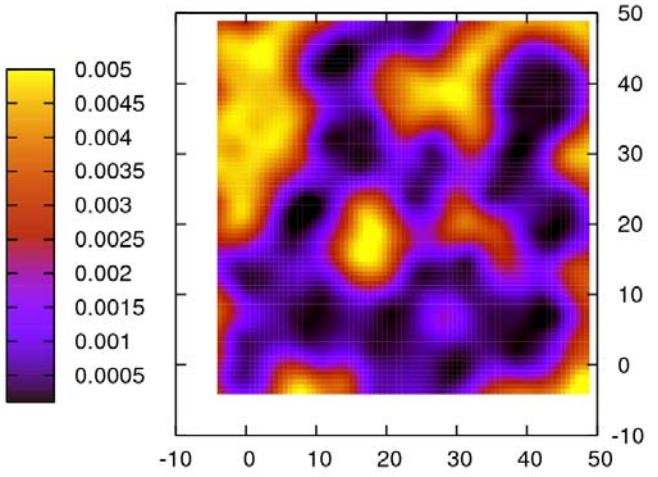
$$MEM \sim nat_{cell} N$$





Divide and conquer (DaC) approach for DFT
Yang et al. PRL 66, 1440 (1991)

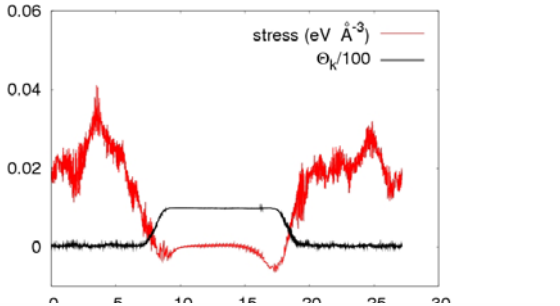


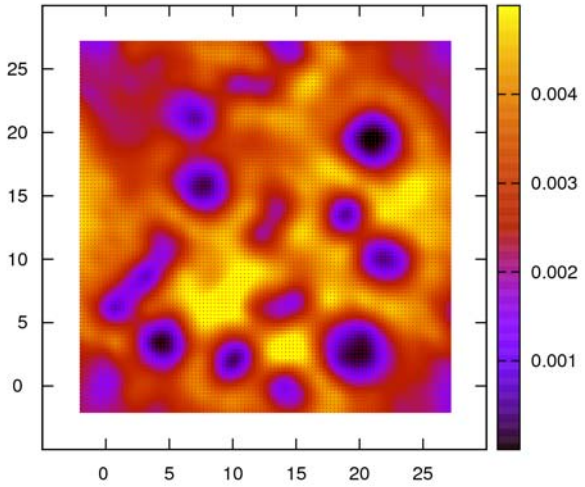
DaC based on Empirical Tight Binding sp^3s^* (TB model of Vogl, 1981)

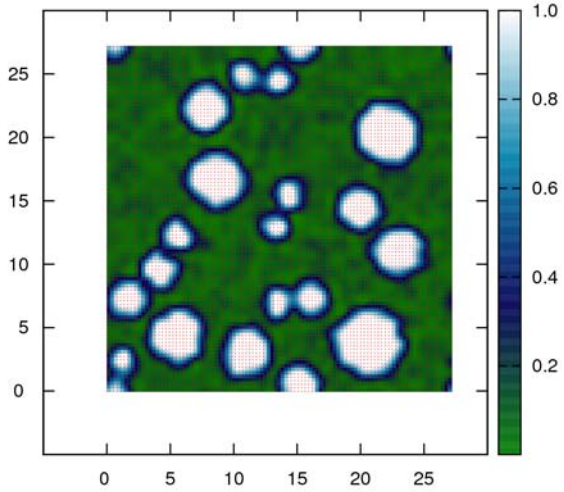
Structure vs. optoelectronics

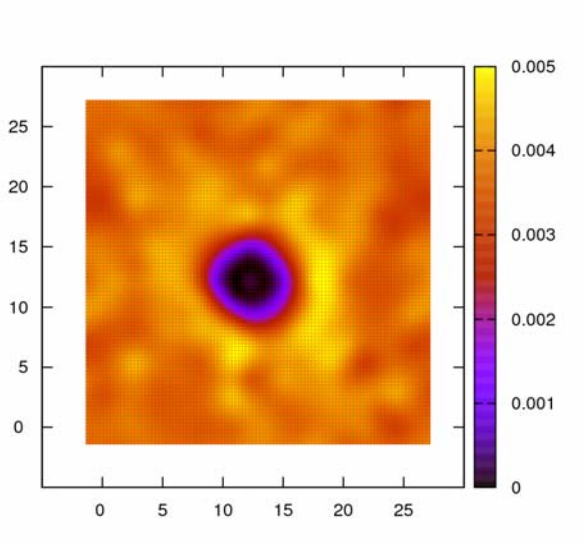
D4.1.2.1 Determination of the average valence band-offset at nc-Si/a-Si interfaces and mixed-phase silicon Determination and reporting about the **role of local strain conditions on the electronic structure**

Comparison with experimental data coming from nanostructural and optoelectronic characterization (WP3, tasks 3.1 and 3.2) and from quantum confinement studies (WP3, task 3.1)

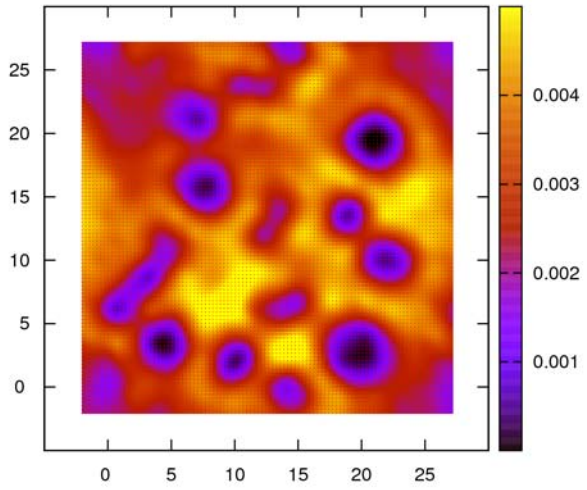








2D maps t=2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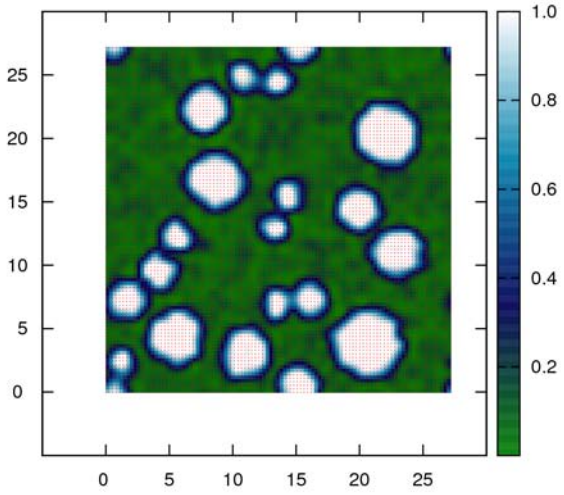
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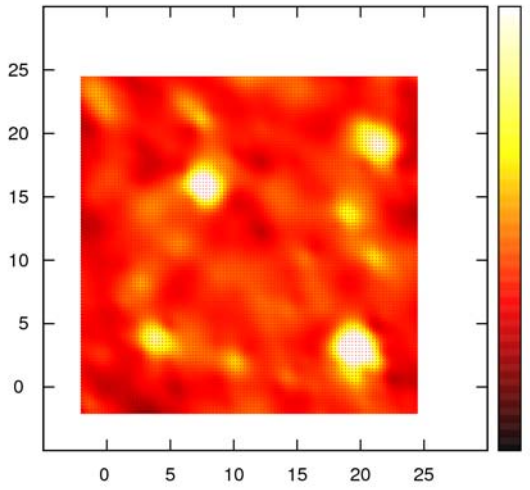
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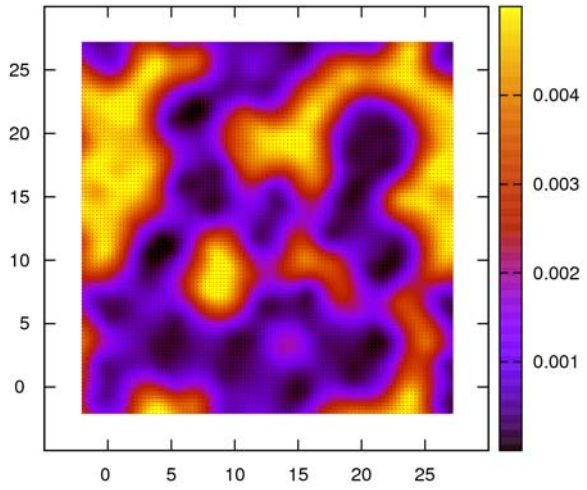
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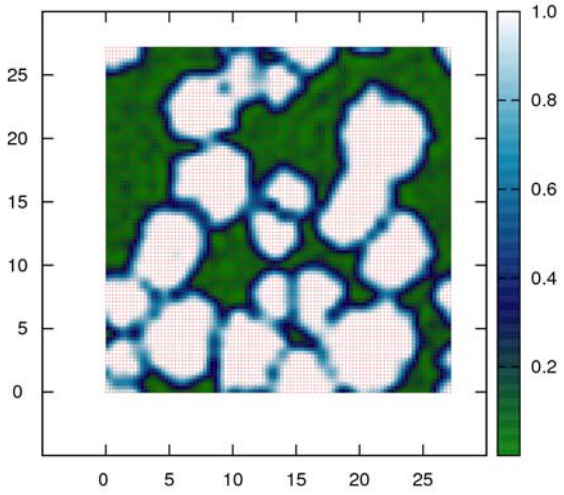
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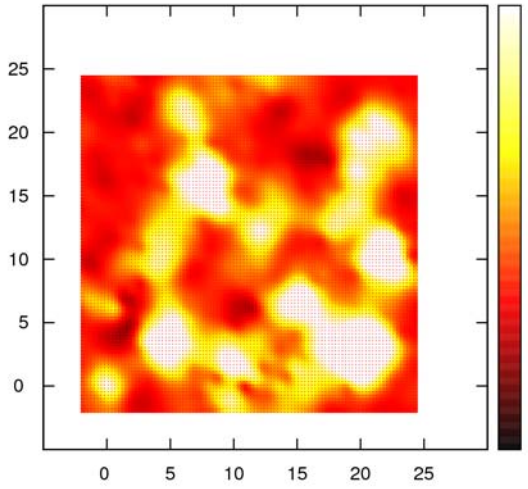
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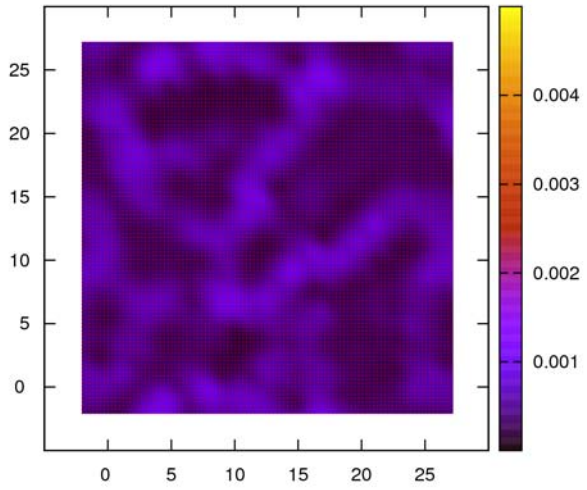
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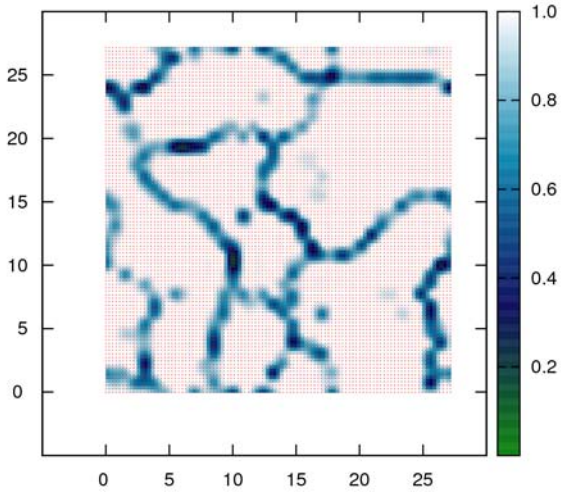
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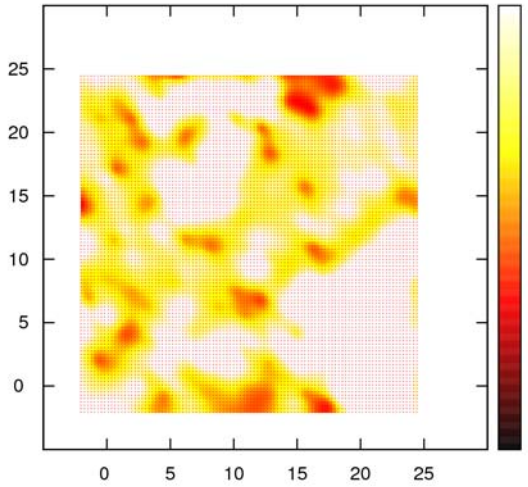
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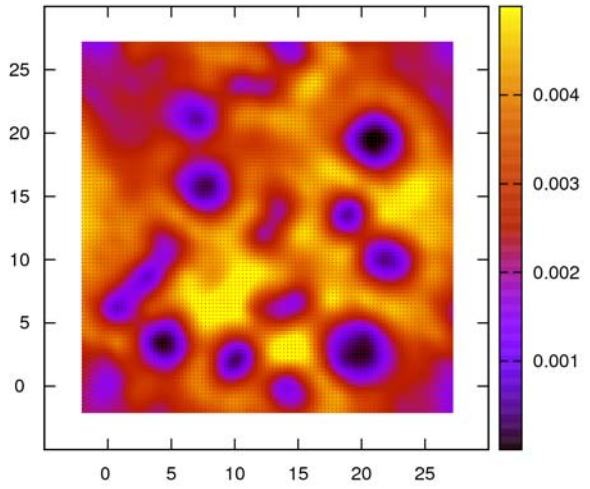
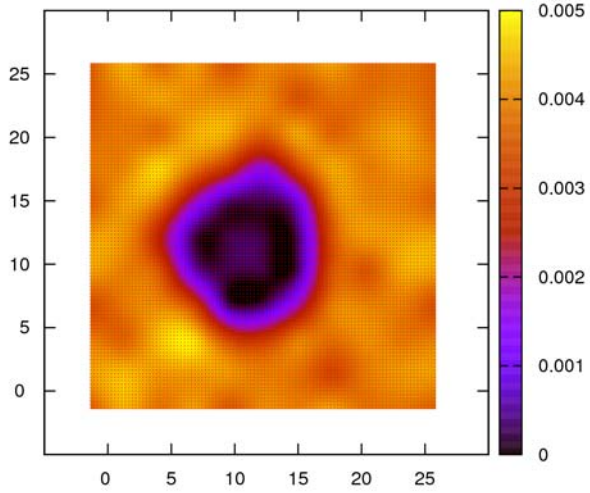
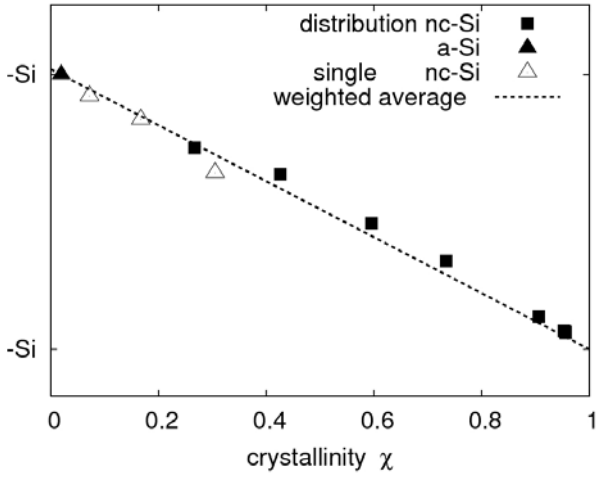
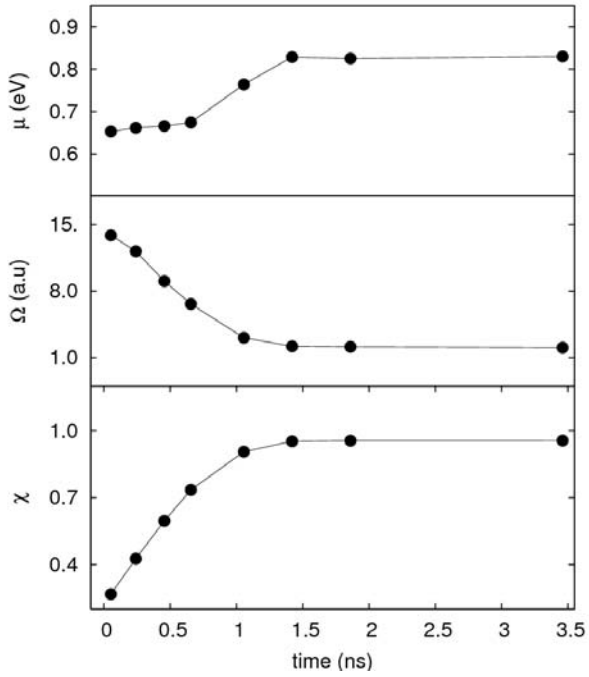
Structure vs. optoelectronics







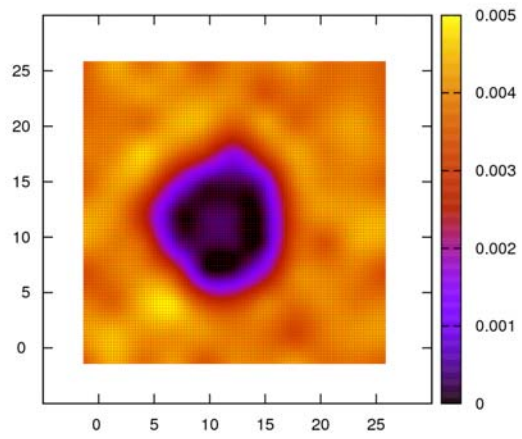
$$\Omega(\chi) = \Omega_a - (\Omega_a - \Omega_c)\chi$$



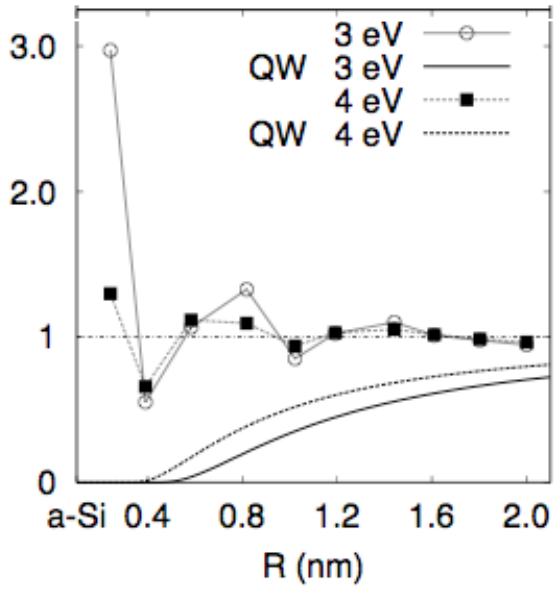
Confinement

D5.1.2.1. Investigation of **electron wave-function confinement** effects within the nanocrystalline phase

$$\Omega(\chi) = \Omega_a - (\Omega_a - \Omega_c)\chi$$



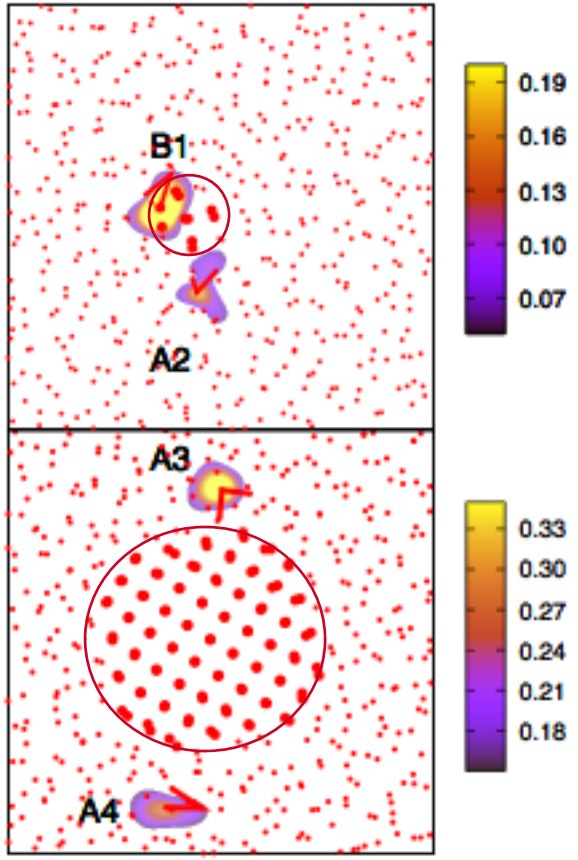
$$\Omega^{effective}(R)$$



Confinement vs. localization

D5.1.2.2. Determination of the role of **structural defects on electronic properties** Comparison with experimental data coming from both nanostructural and optoelectronic characterization (WP3, tasks 3.1 and 3.2) and from quantum confinement studies (WP3, task 3.1)

1. **Electronic localization is due to angular distortions and occurs mostly in the amorphous phase and sometimes at the a-c boundary**
2. **Electrons are localized in the crystal phase in case of subnanometric grains (paracrystalline phase)**



Role of hydrogen

D6.1.2.1. Determination of the effect of **dissolved hydrogen** on the underlying electronic
properties of the mixed-phase system.

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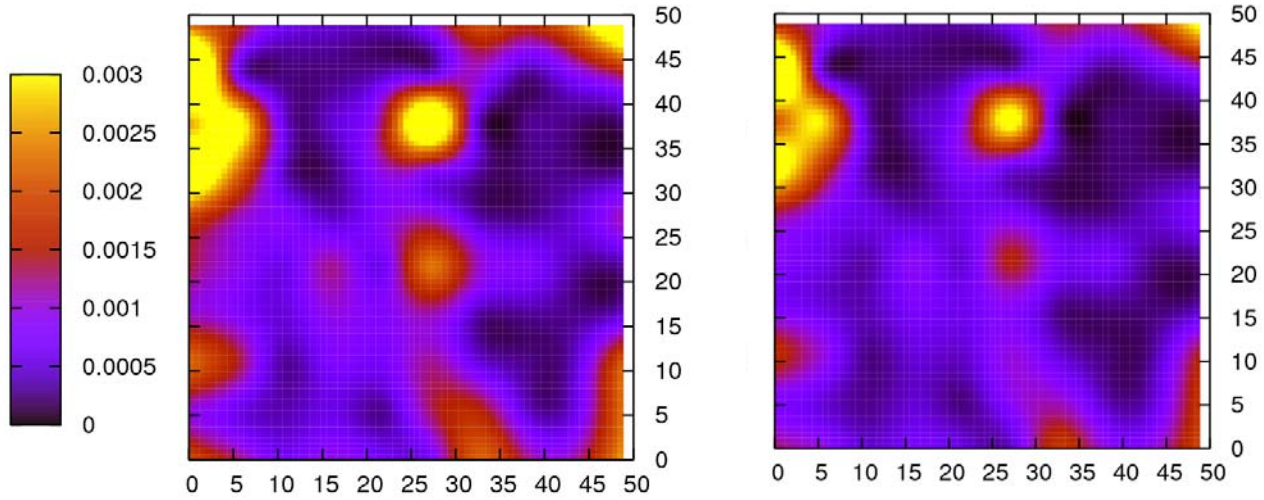
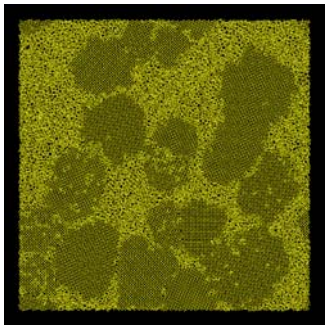


Conclusions



1. Understanding atomic scale structural features (twin boundaries, a-c interfaces, local strain)
2. The role of temperature induced microstructure evolution (crystallization)
3. The sensitivity of the absorption properties of the amorphous phase
4. Confinement related to hydrogen
5. Localized states in subnanometric grain

List of publications

List of publications (inverse chronological order)

[1] Ò*Role of hydrogen on the structural and optoelectronic properties of nanocrystalline silicon*Ó
G. Fugallo, A. Mattoni, and L. Colombo, in preparation (2008)

[2] Ò*Electronic localization in nanocrystalline silicon*Ó
L. Bagolini, A. Mattoni and L. Colombo, submitted for publication to Appl. Phys. Lett. (2008)

[3] Ò*Space-resolved calculation of the optoelectronic properties of nanostructured silicon*Ó
A. Mattoni, L. Ferraro and L. Colombo, submitted for publication to Phys. Rev. Lett. (2008)

[4] Ò*Crystallization kinetics of mixed amorphous-crystalline nanosystems*Ó
A Mattoni, L Colombo, Phys. Rev. B vol. **78**, 075408 (2008)

[5] Ò*Nonuniform growth of embedded silicon nanocrystals in an amorphous matrix*Ò
A. Mattoni, and L. Colombo, Phys. Rev. Lett. **99**, 205501 (2007)

[6] Ò*Nanocrystalline silicon films as multifunctional material for optoelectronic and photovoltaic applications*Ó
S. Pizzini, M. Acciarri, S. Binetti, D. Cavalcoli, A. Cavallini, D. Chrastina, L. Colombo, E. Grilli, G. Isella, M. Lancin, A. Le Donnne, A. Mattoni, K. Peter, B. Pichaud, E. Poliani, M. Rossi, S. Sanguinetti, M. Texier and H. von KŠnel
Mat. Sci. Eng. B **134**, 118 (2006)

Conference proceedings

[7] Ò*Temperature and Strain induced microstructural evolution of nanocrystalline silicon*Ó
A. Mattoni, and L. Colombo, Proceedings of the Ò3th International Conference Multiscale Materials and ModelingÓ p. 164, editor P. Gumbsch (September 18-22 Freiburg 2006) -- ISBN-13: 978-3-8167-7206-4

List of Invited talks

Invited talks (inverse chronological order)

[1] L. Colombo – "*Growth and optical properties of embedded silicon nanoparticles*"
Invited talk at the Symposium "Computational modeling of growth", 2009 APS March Meeting
March 16-20, 2009, Pittsburgh (USA)

[2] L. Colombo – "*Growth phenomena in nanocrystalline silicon*"
Invited lecture at the Donostia International Physics Center
October 1, 2008, San Sebastian (Spain)

[3] A. Mattoni - "*Growth phenomena and transformation kinetics of nanocrystalline silicon*"
Intived talk at the Fall E-MRS Meeting
September 14-19, 2008 Warsaw (Poland)

[4] L. Colombo – "*Atomistic simulation of microstructure evolution of nanocrystalline silicon*"
Intived talk at the 2nd Computational Chemistry Summer School @ Universidad de Barcelona
June 16-20, 2008, Barcelona (Spain)

[5] L. Colombo - "*Atomistic simulations of silicon nanocrystals growth*"
Intived talk at the International workshop on "Modeling and computational methods in fluid dynamics and material science: towards the challenge of the nanoscales"
December 19-22, 2007, Bressanone (Italy)

[6] A. Mattoni - "*Atomically informed models of microstructure evolution of nanocrystalline materials*",
Intived talk at the Workshop on "Mathematical models for dislocations"
December 13, 2007, Roma (Italy)

[7] A. Mattoni - "*Nanocrystalline silicon for photovoltaics: highlights in modelization*"
Intived talk at the Workshop "NANOFORUM"
September 17, 2007, Milano (Italy)

[8] A. Mattoni - "*Modeling and understanding the interface kinetics of amorphous-crystalline systems*"
Intived talk at the Workshop "LASERION 2007"
July 1-5, 2007 Schloss-Ringberg (Germany)

[9] A. Mattoni - "*Microstructural evolution of nanocrystalline silicon systems*"
Invited lecture at IEMN, Institut d'Electronique et de Microelectronique et de Nano-technologie"
May 14, 2007, Lille (France)