An atomic level`s simulation approach to materials

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www.gnm.cl

Ju Li`s group, Jan. 23th, 2014
Nuclear Science Engineering Dept., MIT

Chile

Mixture of (mainly) native people +european+african+asian

- 17 million: Antofagasta (400.000); Santiago (4 mill); Valparaíso (1 mill); Concepcion (1 mill); Temuco (500.000)
- Economy: GPD/pp: U$15.363; Growth: 5,6% py, **BUT** great inequality (worse than 20/80)
- Education: 60 univ, 1/3 state univ; only 8 research universities
- Research: 300 phyicisists (with PhD, 1 paper/y); 150 cond mat; but only 50 out 300 experimentalists

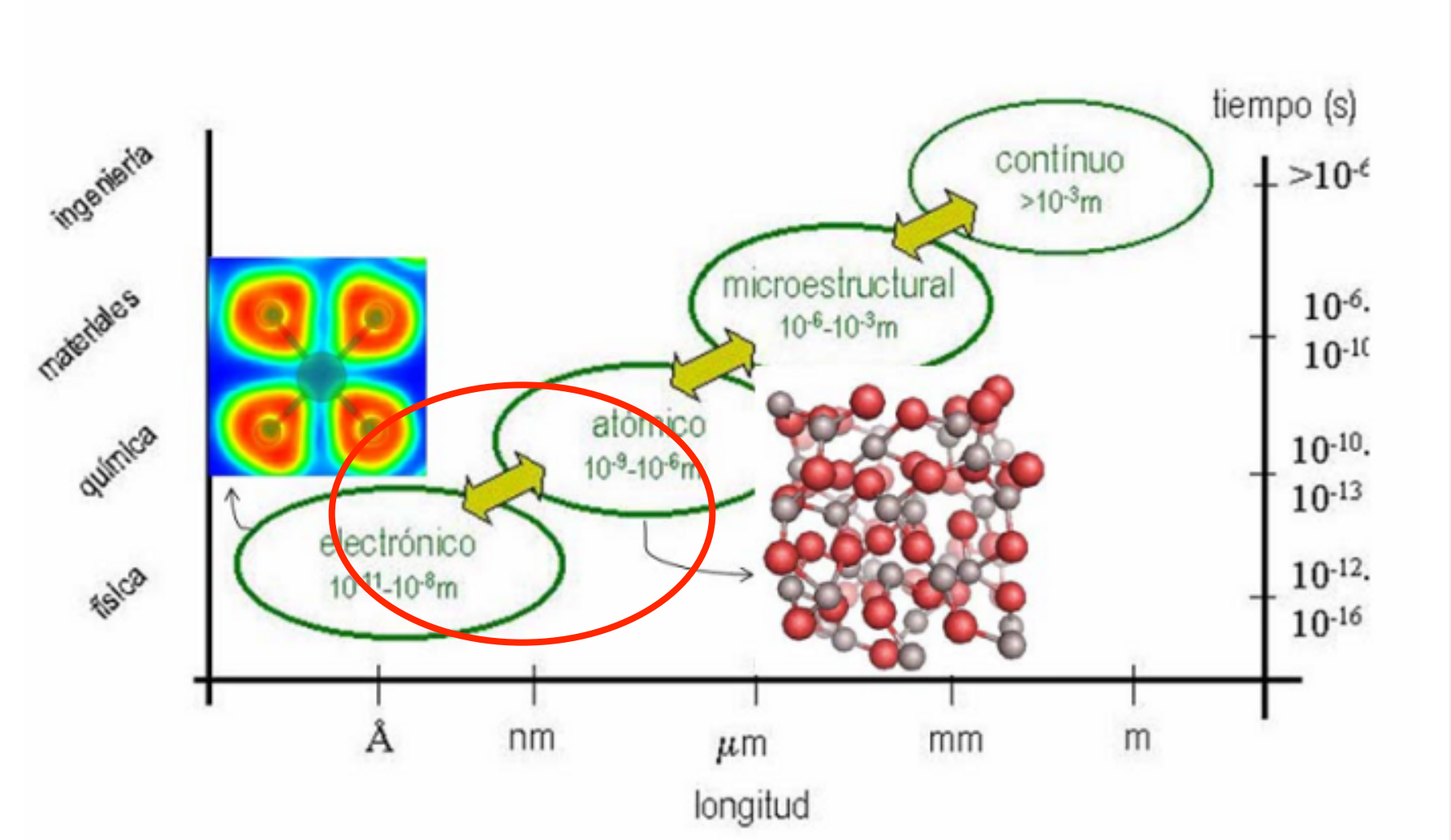
Computer simulation of materials: 40 (?)

Grupo de NanoMateriales,
www.gnm.cl
Universidad de Chile, Santiago

- Profs: Eduardo Menéndez, Sergio Davis, Gonzalo Gutiérrez
- Postdoc: Emilio Figueroa, Germán Miño
- Postgrad students: F. González, Y. Navarrete, N . Amigo, J. Wachter, M. Sepúlveda, D. González.
- Several undergrad per year
- Collaborators in Chile and abroad: E. Bringa (Arg), K. Rajan(IU), CACS (USC), Uppsala U.

Computer simulation at atomic level

Classical and ab-initio MD; MC;



GNM: Research areas (www.gnm.cl)

1. Foundations of statistical mechanics:
a) melting theory
b) information theory and bayesian probability
c) non-extensive statistics

2. Material science
a) solar cell materials: electronic and optical properties (ab-initio)
b) nano-structured materials: carbon nanotubes
c) glasses: structures, dynamical and mechanical properties
d) materials under extreme conditions: melting curve, structure & dynamics
e) mechanical properties of metals
f) nuclear materials: radiation damage
e) biological systems: protein molecular simulation

3. Computer simulation techniques
a) Computer programming: Las Palmeras Molecular Dynamics, www.lpmd.cl (Computer Physics Communications, 181(12):2126 – 2139, 2010)
b) Free energy and entropy; melting curve
c) Algorithms for MD and MC: mpi, CUDA

Past projects

Al_2O_3 : Crystalline, amorphous and liquid

GeO_2 : amorphous and liquid

MAX phases: TiSiC, TiGaN

Current projects

- *Mechanical properties of metals: influence of impurities in Cu*
- *Mechanical properties of BMG: shear bands in* Cu-Zr-Ag
- *Radiation damage:* stacking fault tetrahedron in Au nanowires under irradiation; softening and hardenning; W

Statistical mechanics

- *Estimation of Tsallis' q-index in non-extensive systems*,
  Sergio Davis and Gonzalo Gutiérrez.
  AIP Conference Proceedings **1578**, 1779 (2013).

- *Newtonian dynamics from the principle of maximun caliber*

D. González, S. Davis, G. Gutiérrez, ArXiv:1310.1382 (2013).

- *Conjugate variables in continuous maximum-entropy inference*,
  S. Davis and G. Gutiérrez..
  Physical Review E 86, 051136 (2012).

Materials

- *Bayesian inference as a tool for analysis of first-principles calculations of complex materials: an application to the melting point of Ti_2GaN*,
  Sergio Davis and Gonzalo Gutiérrez.
  Modelling and Sim. in Mat. Sc. and Eng. **21**, 683-690 (2013)

- *Hypervelocity impact of copper nano-projectiles on copper*,
  N. Amigo, C. Loyola, S. Davis and G. Gutiérrez.
  Computational Materials Science 68, 245 (2013)

- *Ultrathin Carbon Nanotube With Single, Double, and Triple Bonds*,
  E. Menéndez-Proupin, A.L. Montero-Alejo, and J.M. García de la Vega.
  Physical Review Letters 109, 2 (2012).

Computer simulation techniques

- *Maximum entropy reconstruction of the configurational density of states from microcanonical simulations*,
  Sergio Davis.
  Journal of Physics: Conference Series 410, 012161 (2013)

- *Calculation of microcanonical entropy differences from configurational averages*,
  S. Davis.
  Physical Review E 84, 050101(R) (2011)

- *SearchFill: A stochastic optimization code for detecting atomic vacancies in crystalline and non-crystalline systems*,
  S. Davis, Anatoly B. Belonoshko and Börje Johansson.
  Physical Review B 84, 064102 (2011).

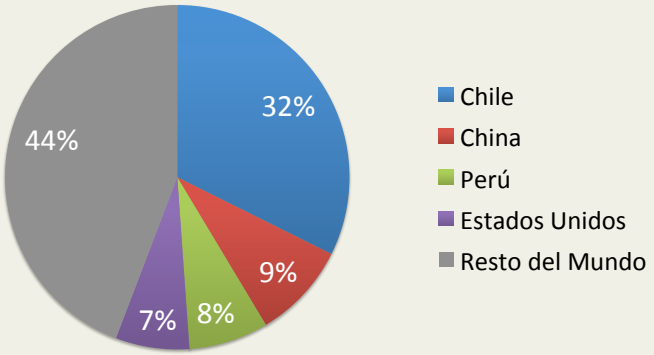
Atomistic simulation of single crystal copper nanowires under tensile stress: effect of silver impurities on the yield point

N. Amigo, G Gutiérrez, M. Ignat

- Motivation: qualification of copper products
- Effects of impurities in copper
- Silver impurities in nanowires
  - mono-crystal
  - poli-crystal
- Conclusion

Context

Codelco



Anodes
99.5%

Cathodes
99.99%

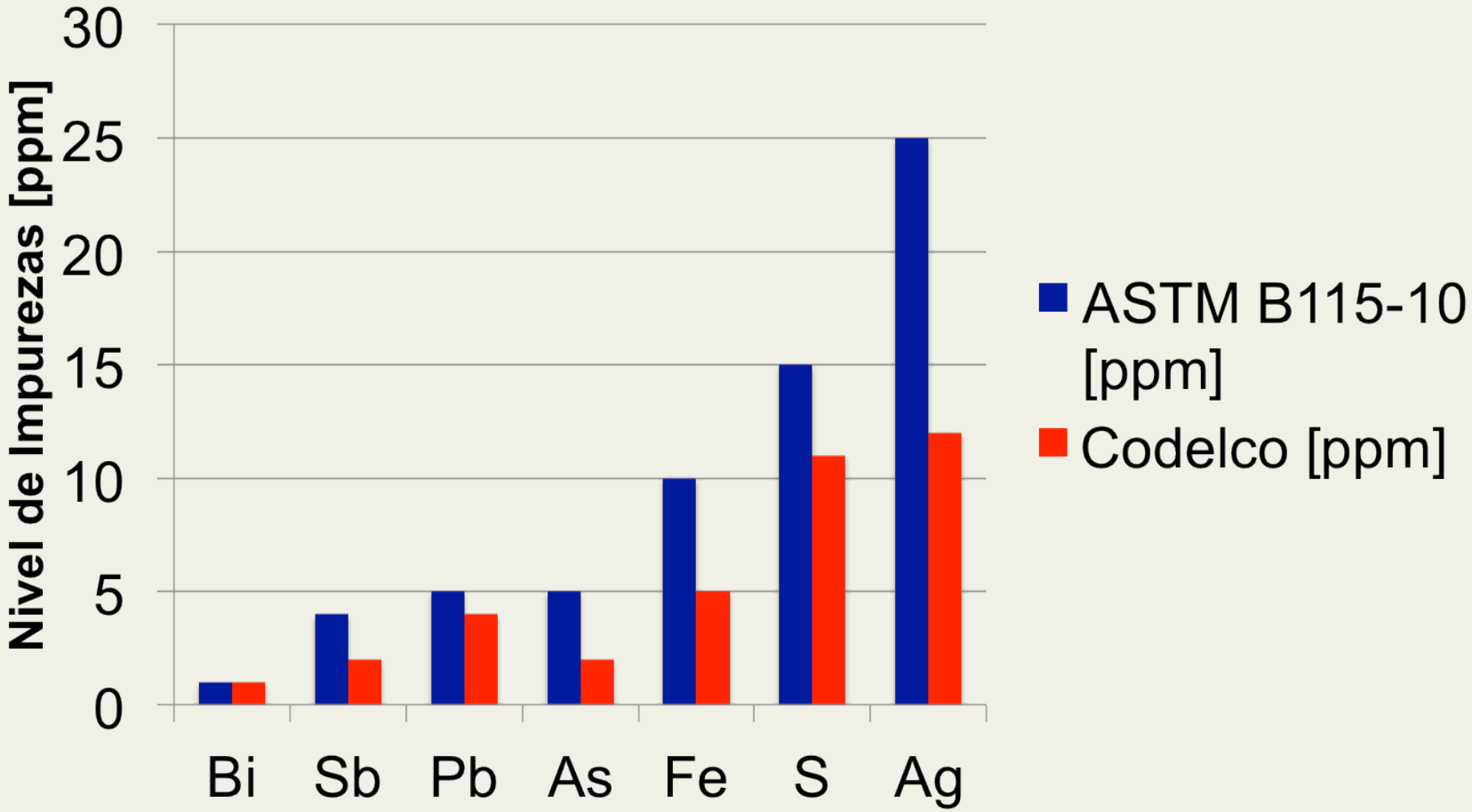
wires

Chemical analysis
Visual qualification

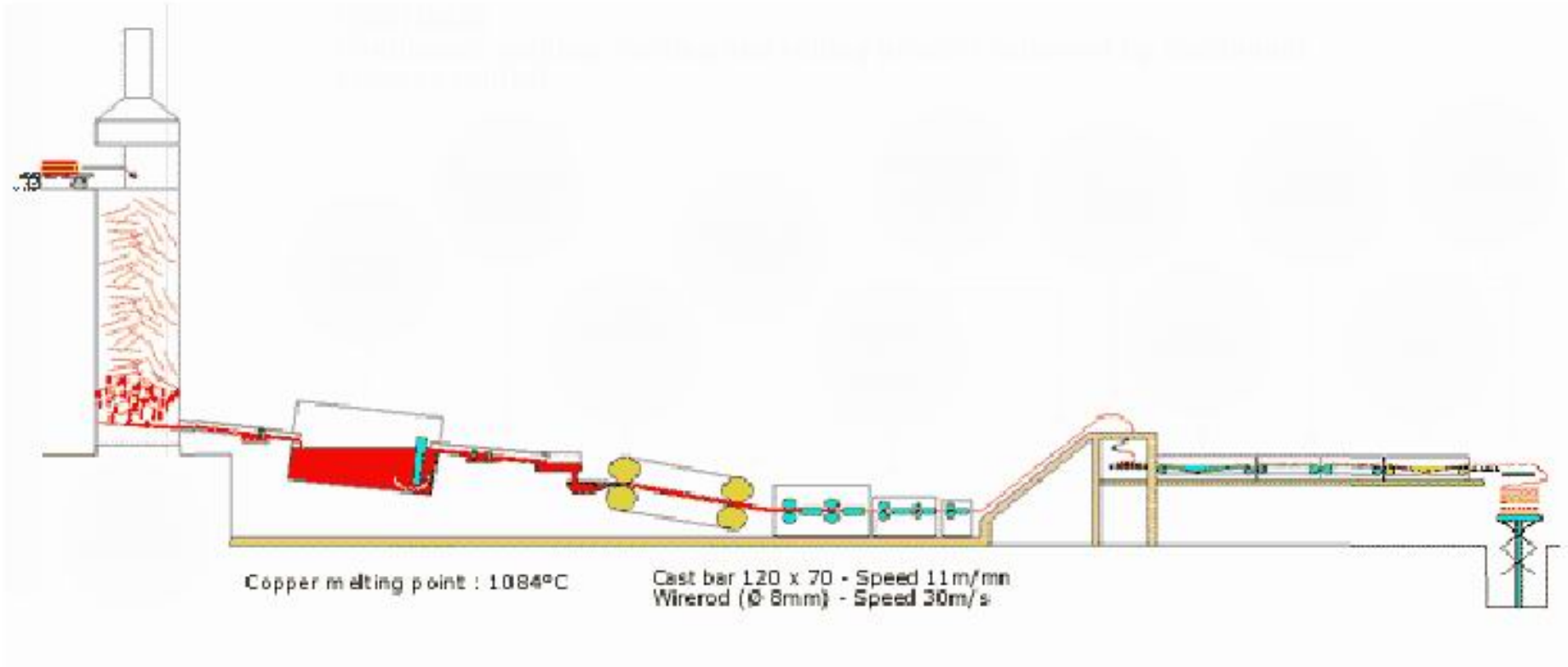
Chemical analysis
Mechanical test

(taken from Jil & Moya)

Chemical qualification: Cathode Grade A standard



From cathodes to wires



…qualification of the Cathodes (from Chile) is done form mechanical test performed on wire...(abroad)

Determinación de Propiedades Mecánicas de Productos de Cobre

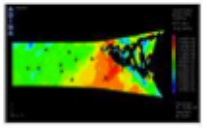
CODELCO
Orgullo de Todos

Proyecto CODELCO-IM2 36-11
Responsable de Proyecto: M.Ignat

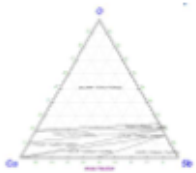
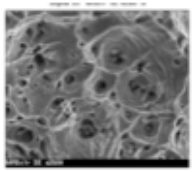
Marzo 2012

- Miguel Ignat: Análisis propiedades mecánicas
  - Docteur Ingenieur (1977), Docteur en-Sciences (1983)

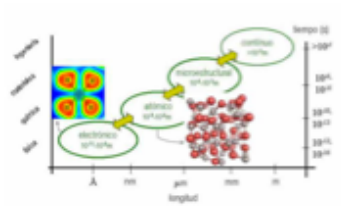
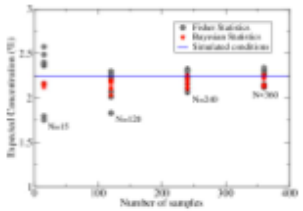




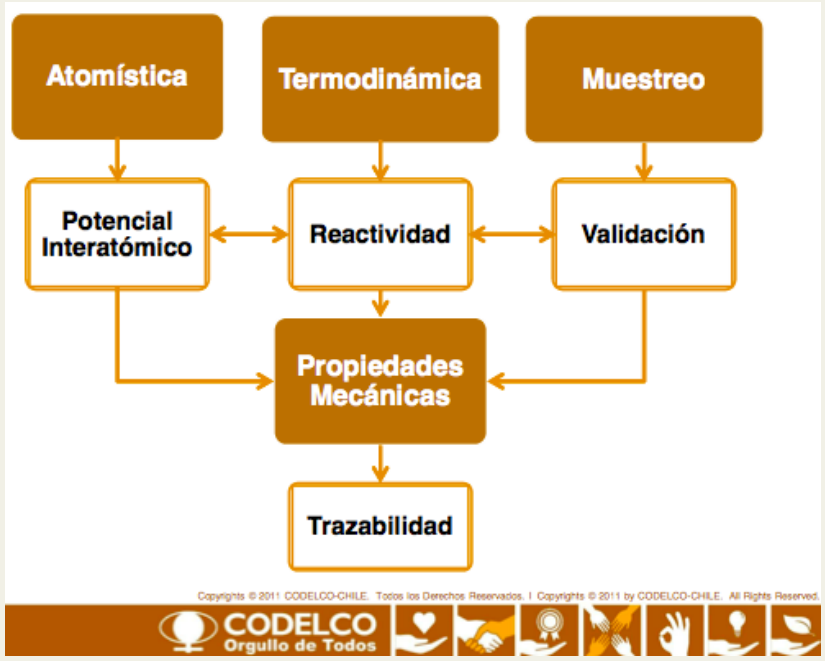

- Álvaro Valencia: Análisis Termodinámico
  - Dr-Ing. Ruhr-Universität Bochum, Alemania, 1993.


- Gonzalo Gutiérrez: Modelización Atómica
  - Doctor en Ciencias con Mención en Física, P. Universidad Católica de Chile, 1997

- Sergio Davis: Estadística de Muestreo
  - Ph.D in Applied Material Physics, Royal Institute of Technology (KTH), Estocolmo, Suecia (Septiembre 2009)



CODELCO Orgullo de Todos

Goals

- To study the chemical and mechanical properties from anode-cathode-wire: complete traceability.
- To determine the effect of impurities on the mechanical properties ant the recristalization process
- To demonstrate the microestructural, chemical and mechanical discontinuity between cathodes and wires

To propose a mechanical qualification protocol for chilean copper products

Theory and simulation can contribute to give insight on the problem

ARTICLES

Bismuth-induced embrittlement of copper grain boundaries

GERD DUSCHER[1,2], MATTHEW F. CHISHOLM[1]*, UWE ALBER[3] AND MANFRED RÜHLE[3]

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[2]North Carolina State University, Materials Science & Engineering Department, Raleigh, North Carolina 27692, USA
[3]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart, Germany
*e-mail: chisholmmf@ornl.gov

"We find that the copper atoms that surround the segregated bismuth in the grain boundary become embrittled by taking on a more zinc- like electronic structure".

Nature Materials, Sep.2004

Bismuth embrittlement of copper is an atomic size effect

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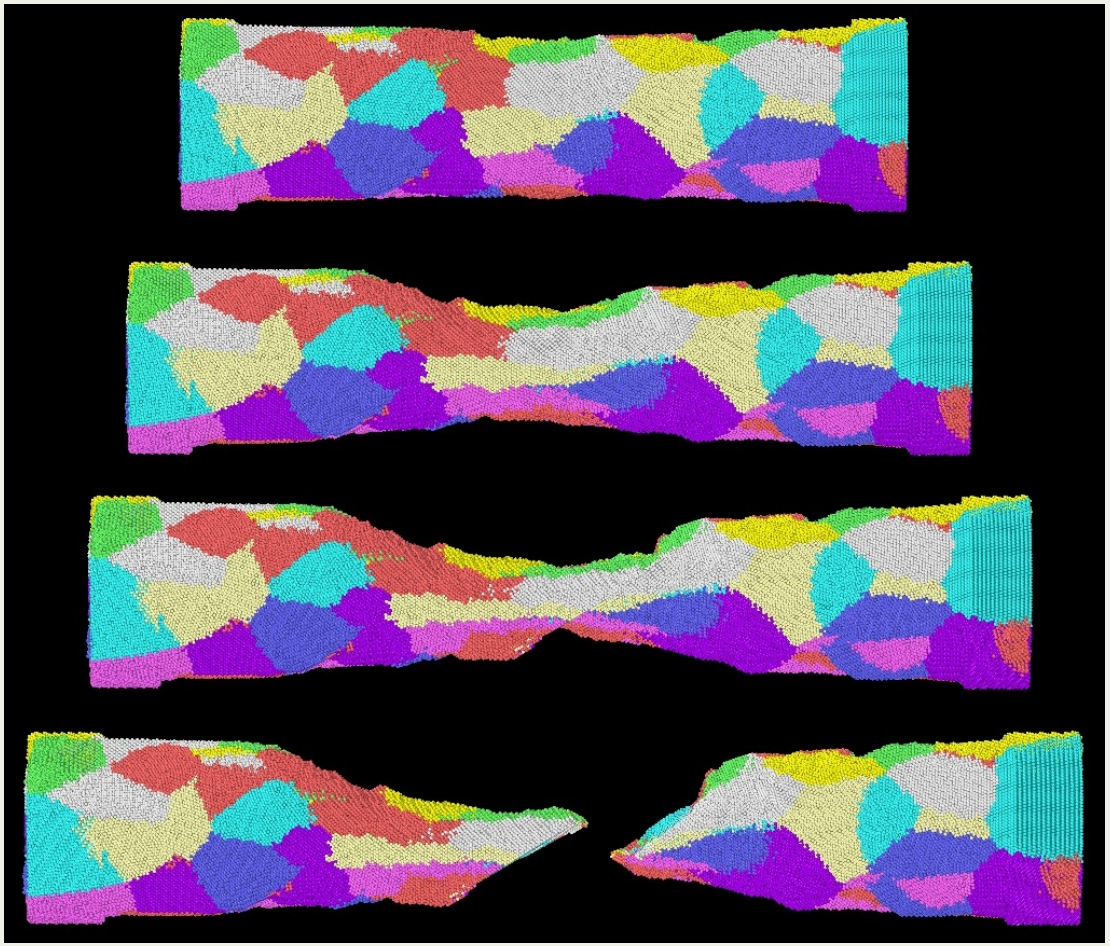
* Present address: Science+Computing ag, Hagellocher Weg 71–5, 72070 Tübingen, Germany

Embrittlement by the segregation of impurity elements to grain boundaries is one of a small number of phenomena that can lead to metallurgical failure by fast fracture[1]. Here we settle a question that has been debated for over a hundred years[2]: how can minute traces of bismuth in copper cause this ductile metal to fail in a brittle manner? Three hypotheses for Bi embrittlement of Cu exist: two assign an electronic effect to either a strengthening[3] or weakening[4] of bonds, the third postulates a simple atomic size effect[5]. Here we report first principles quantum mechanical calculations that allow us to reject the electronic hypotheses, while supporting a size effect. We show that upon segregation to the grain boundary, the large Bi atoms weaken the interatomic bonding by pushing apart the Cu atoms at the interface. The resolution of the mechanism underlying grain boundary weakening should be relevant for all cases of embrittlement by oversize impurities.

As A. H. Cottrell has put it "when a large force is applied to a crystal two things may happen: the atoms in the crystal may slide past one another; and they may pull apart." In the former case, a metal will fail gracefully with absorption of energy by dislocation generation and plastic deformation: the metal is said to be tough. Otherwise (in the latter case) the metal will fail by fracture. The applied force to cause failure is governed by the energy release rate, G, which is the energy that may be derived from the crystal plus loading train per unit area of crack advance[6]. In defining G one

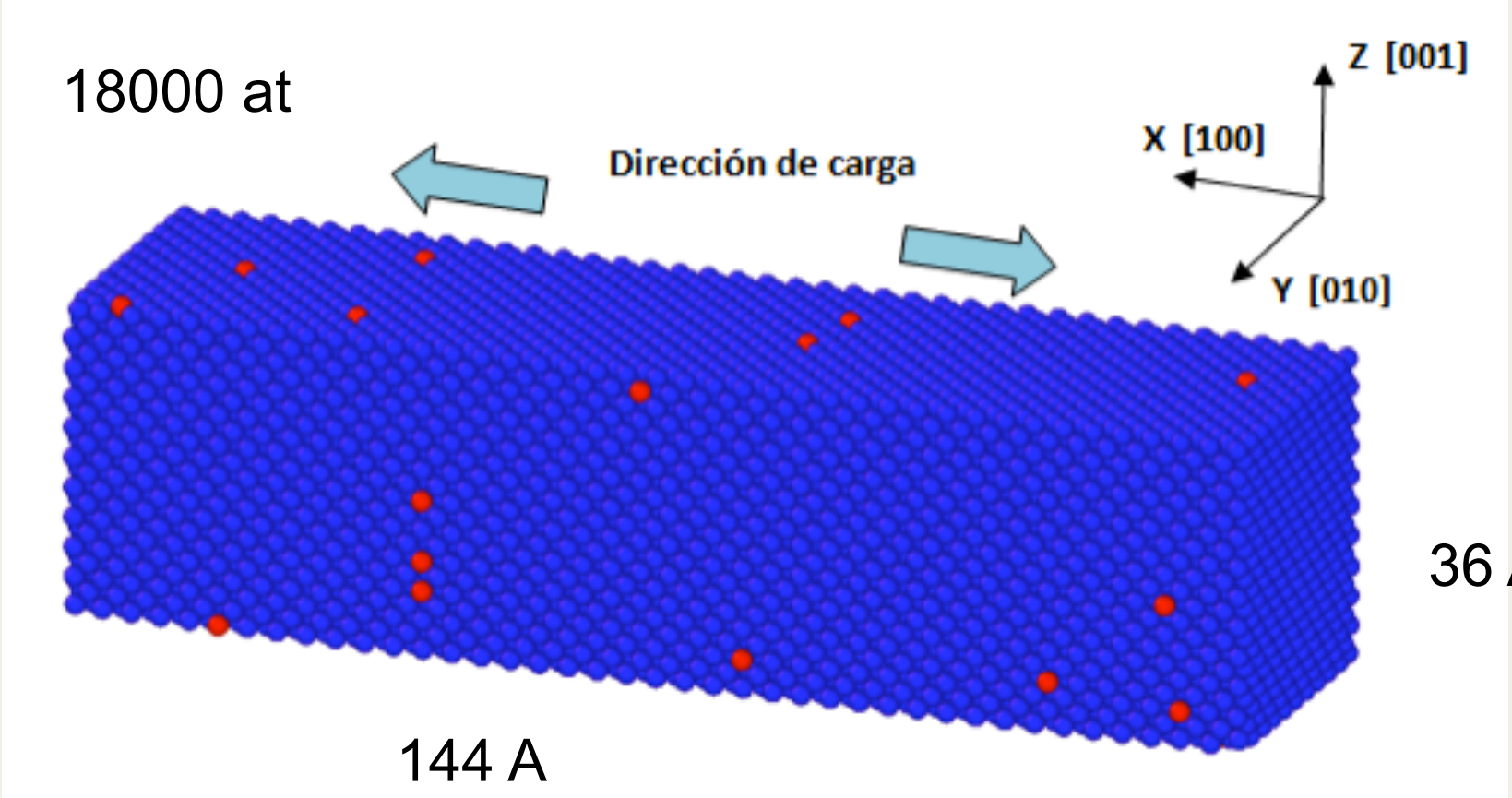
Mechanical properties by computer simulation: tensile test



Dpto. Física, Fac. Ciencias, U. Chile/Gonzalo Gutiérrez

Monocrystal copper nanowires with silver impurities

with **Nicolás Amigo**



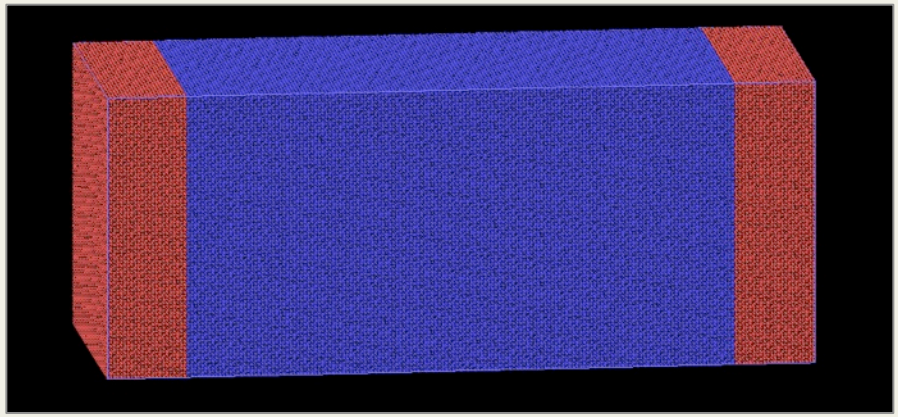
Technical details

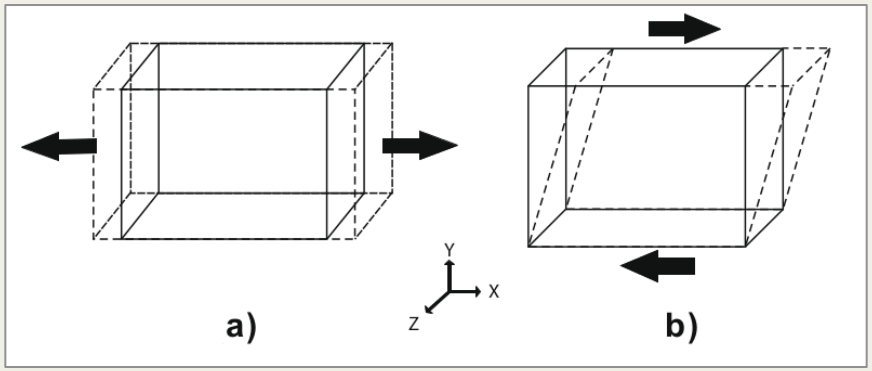
- Molecular dynamics simulation
- Embedded atom interatomic potential, Williams y Mishin (2006).
- T=0.1 K, NVT
- Deformation rate: 10^8 s^{-1}
- Surface impurities: 0.1% a 0.5%

Testing the potential with the elastic constants

$$c_{ijkl} = \frac{\partial \sigma_{ij}}{\partial \varepsilon_{kl}}, \quad (i,j,k,l = x,y,z)$$

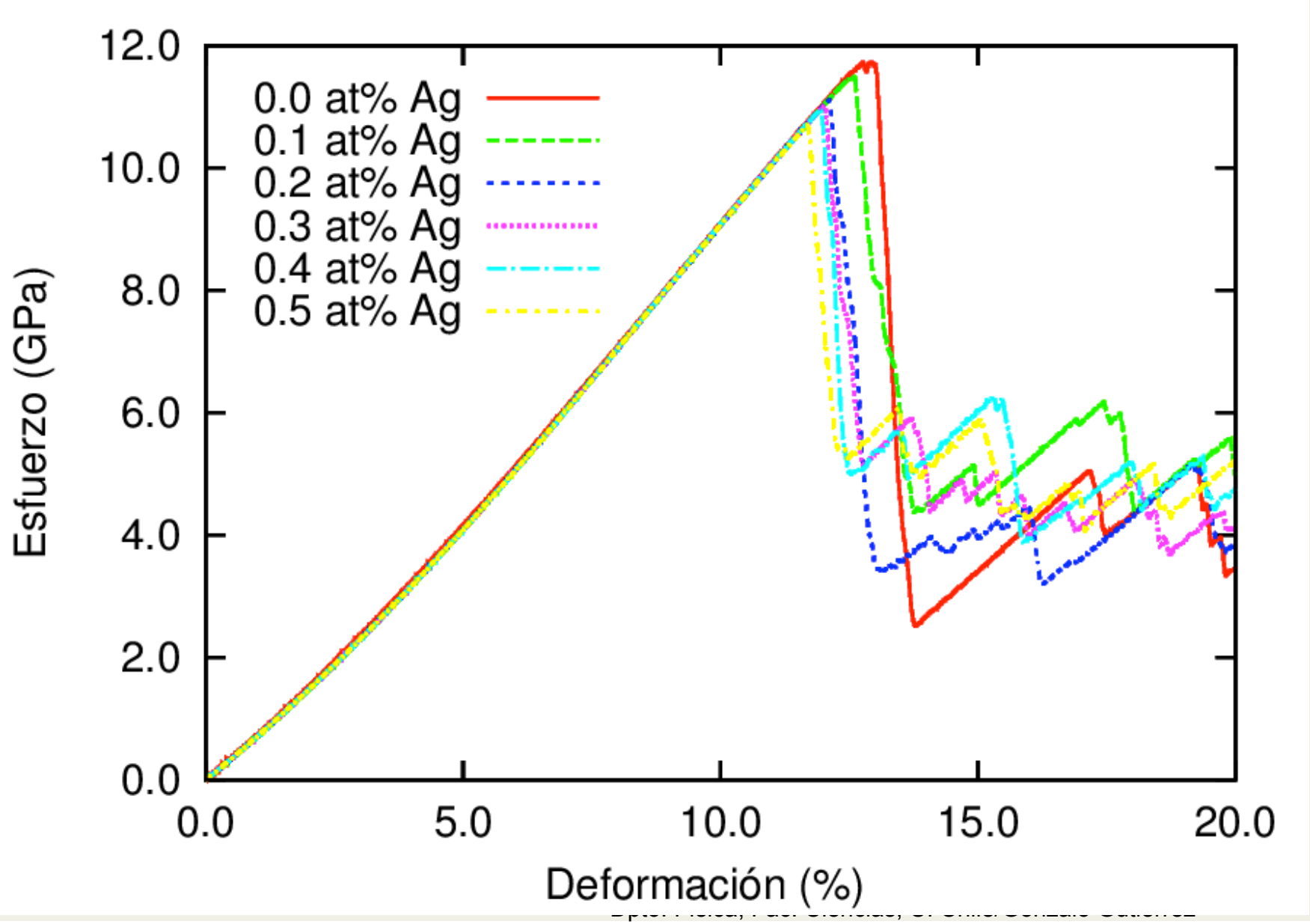
(Elastic properties of the bcc structure of Bismuth at high pressure,, G. Gutiérrez, E. Menéndez-Proupin, and A. K. Singh, Journal of Applied Physics 99, 103504 (2006))



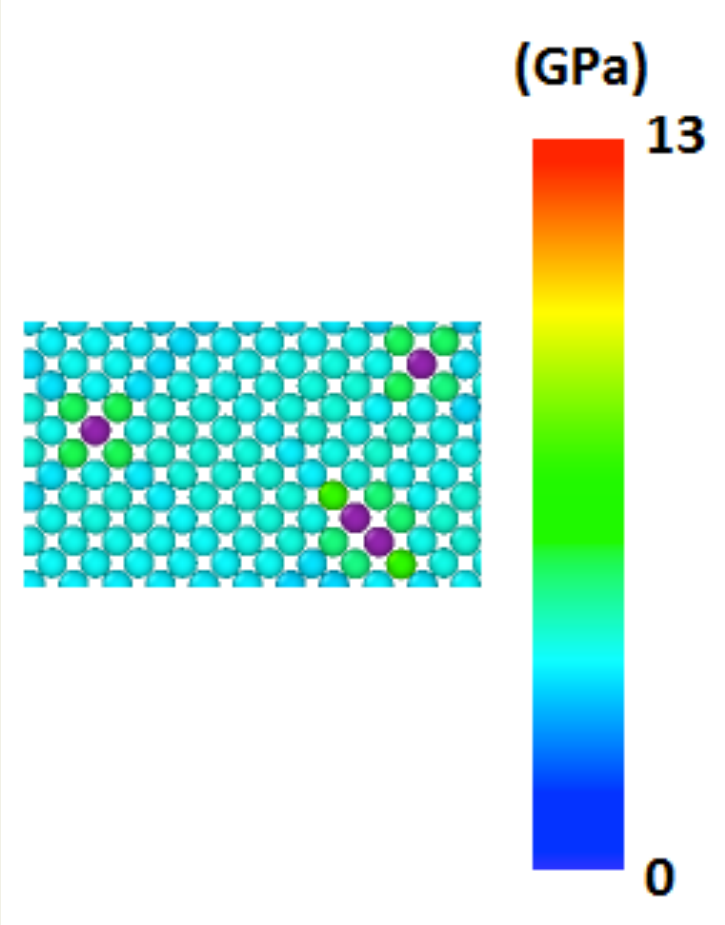


Constants	Literature [Gpa]	Simulation[Gpa]
C_{11}	176.2	171.0
C_{12}	125.0	126.3
C_{44}	82.0	79.9

Stress-strain curve



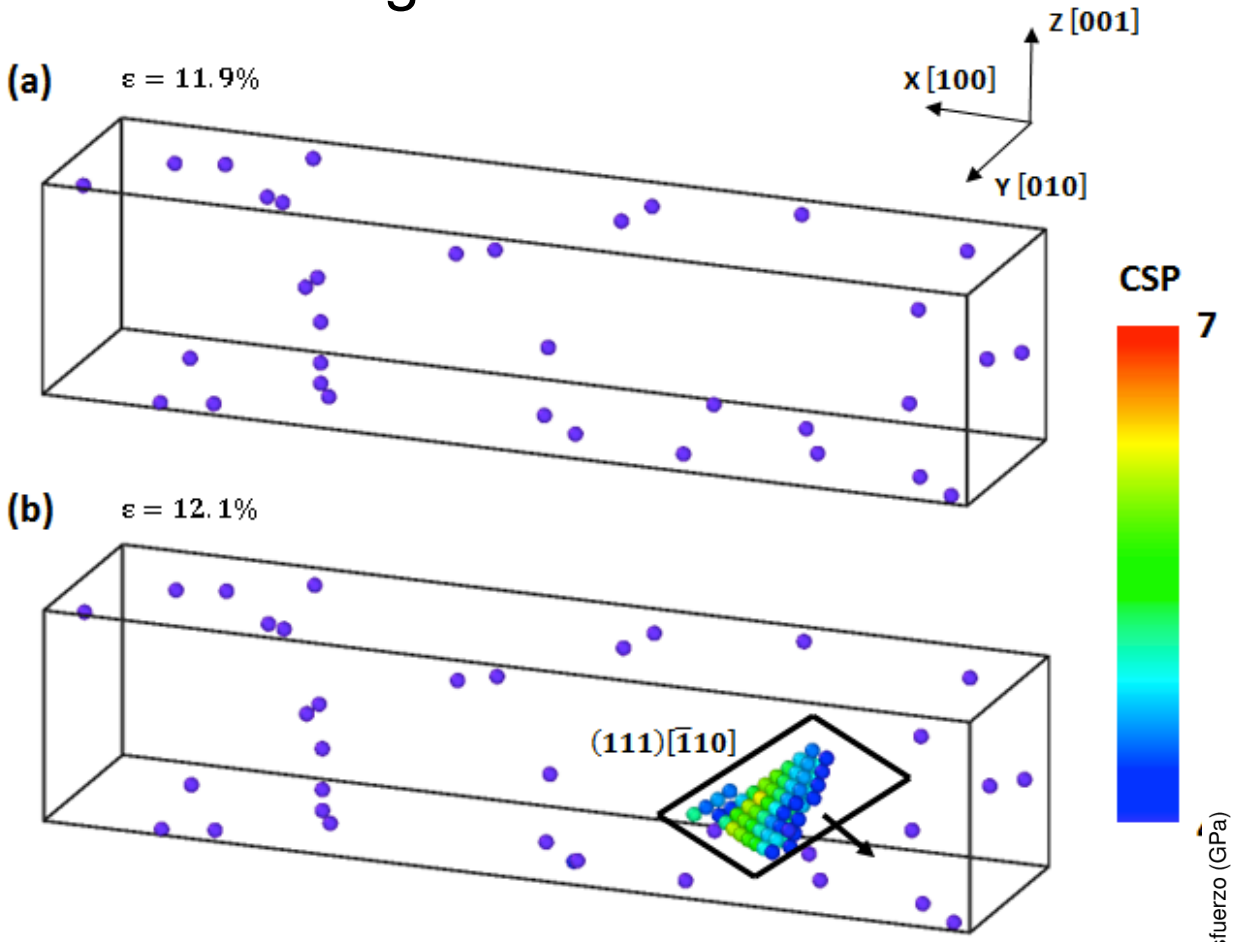
Dislocations begin at the surface

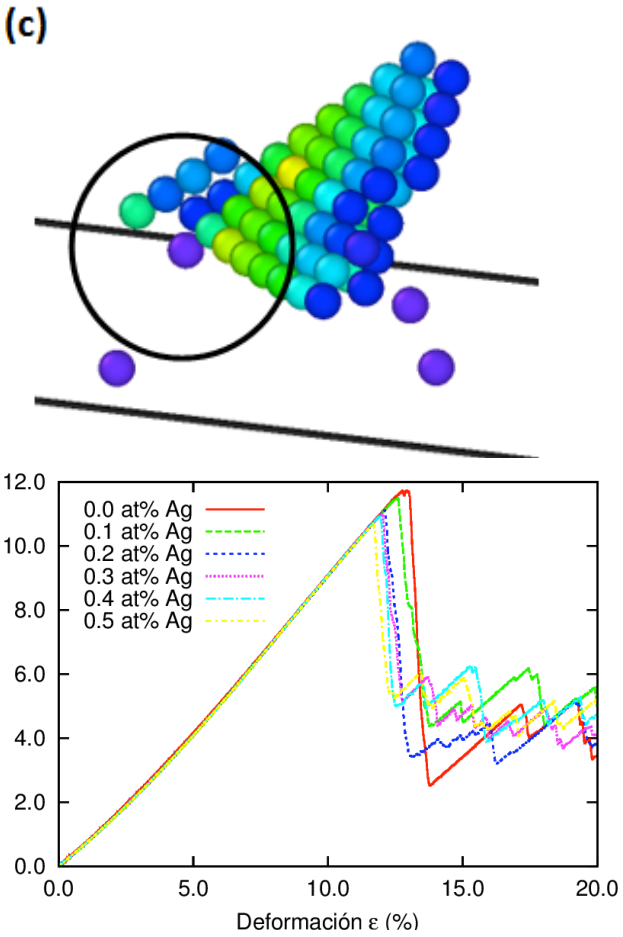


Surface stress because impurities

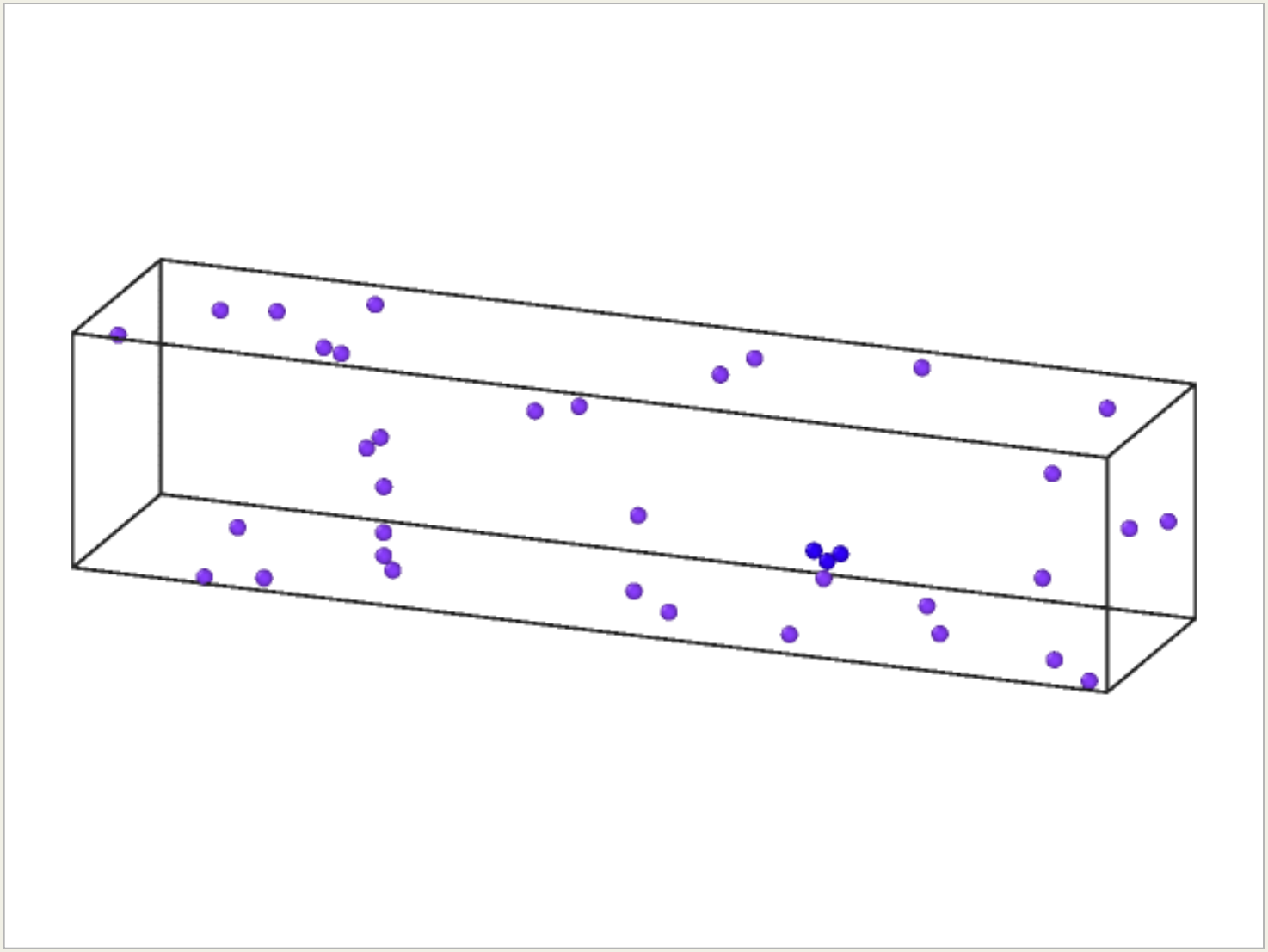
Emission of dislocations

0.2 %Ag

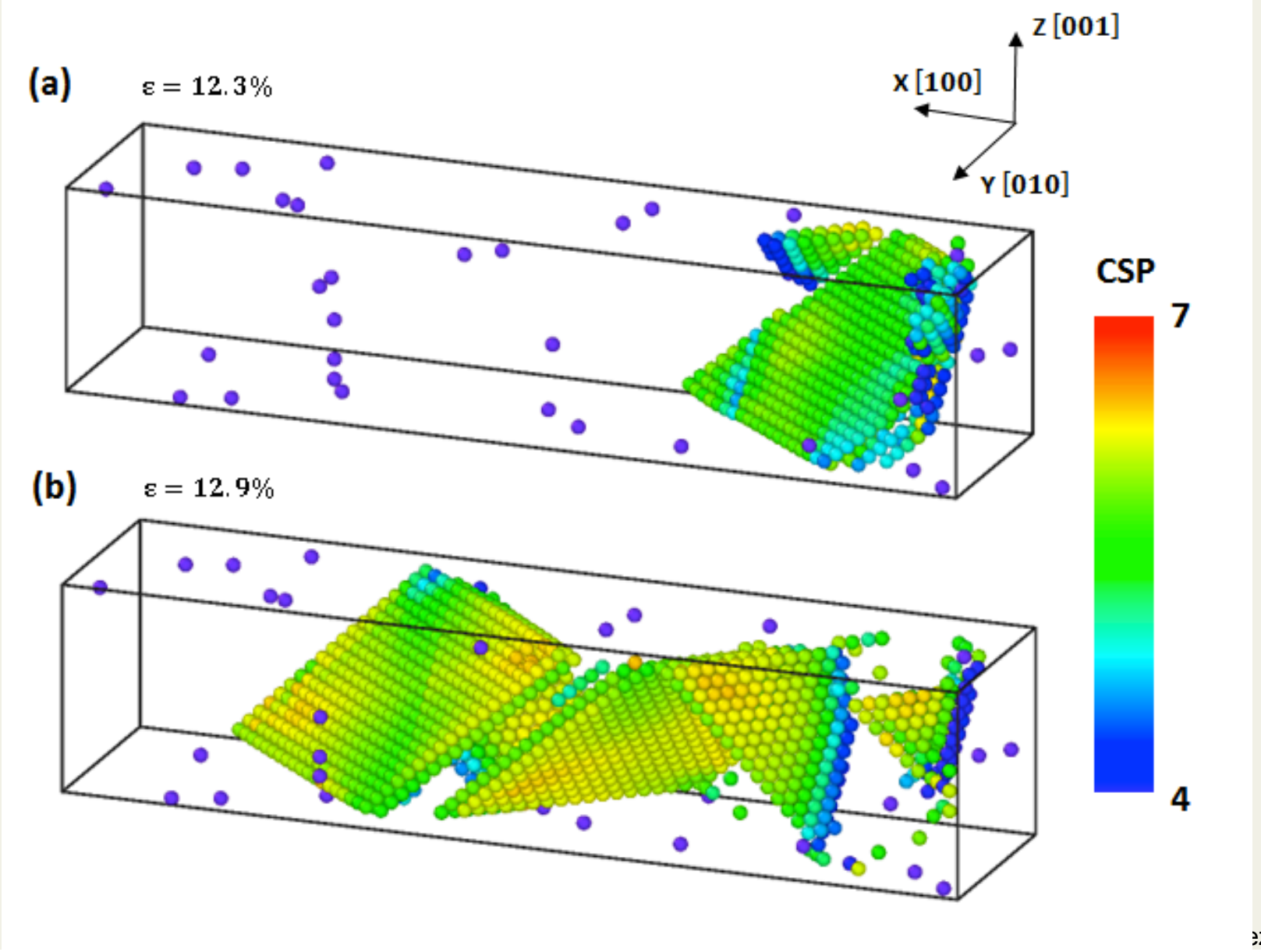




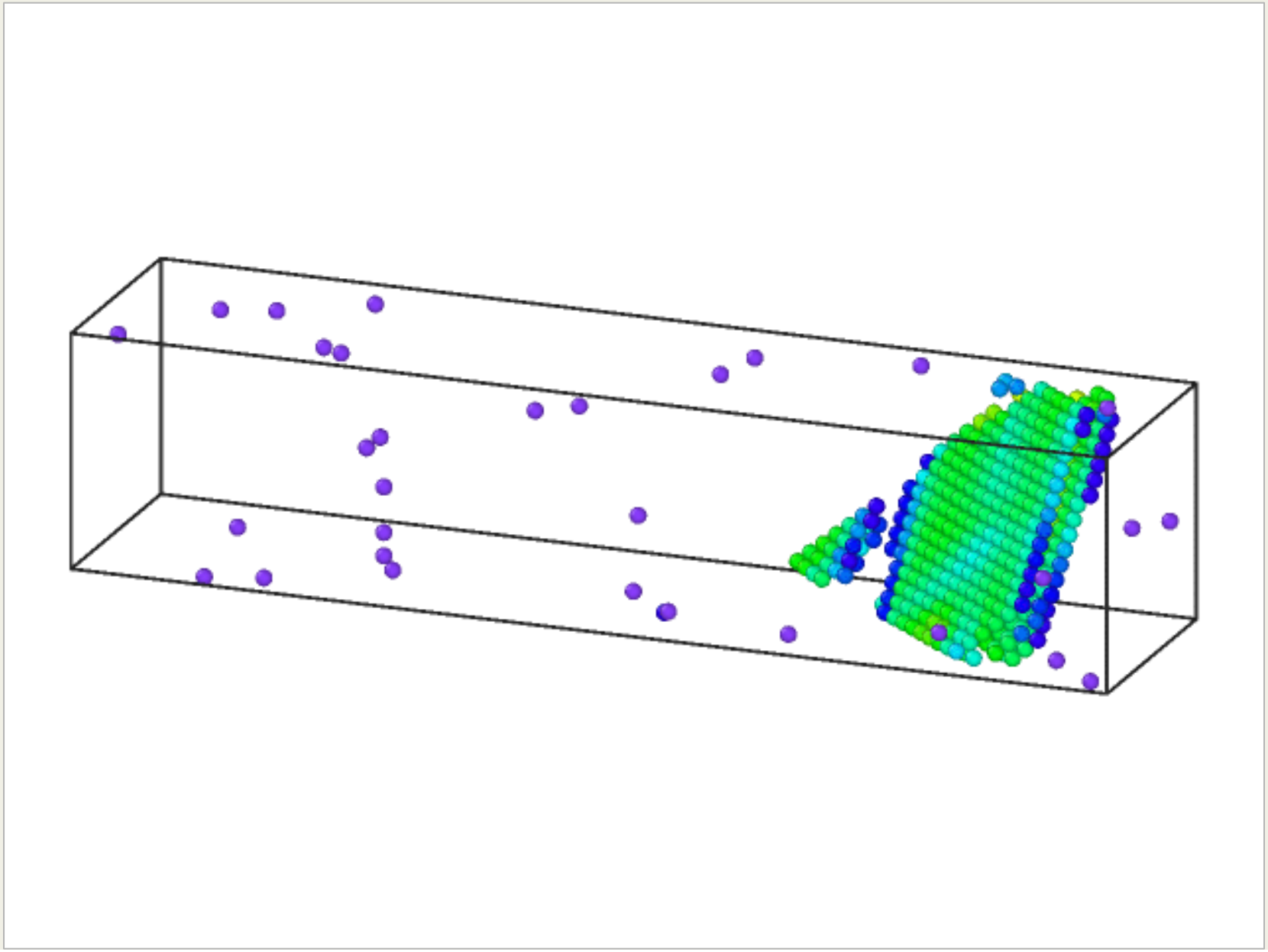
Onset of plasticity



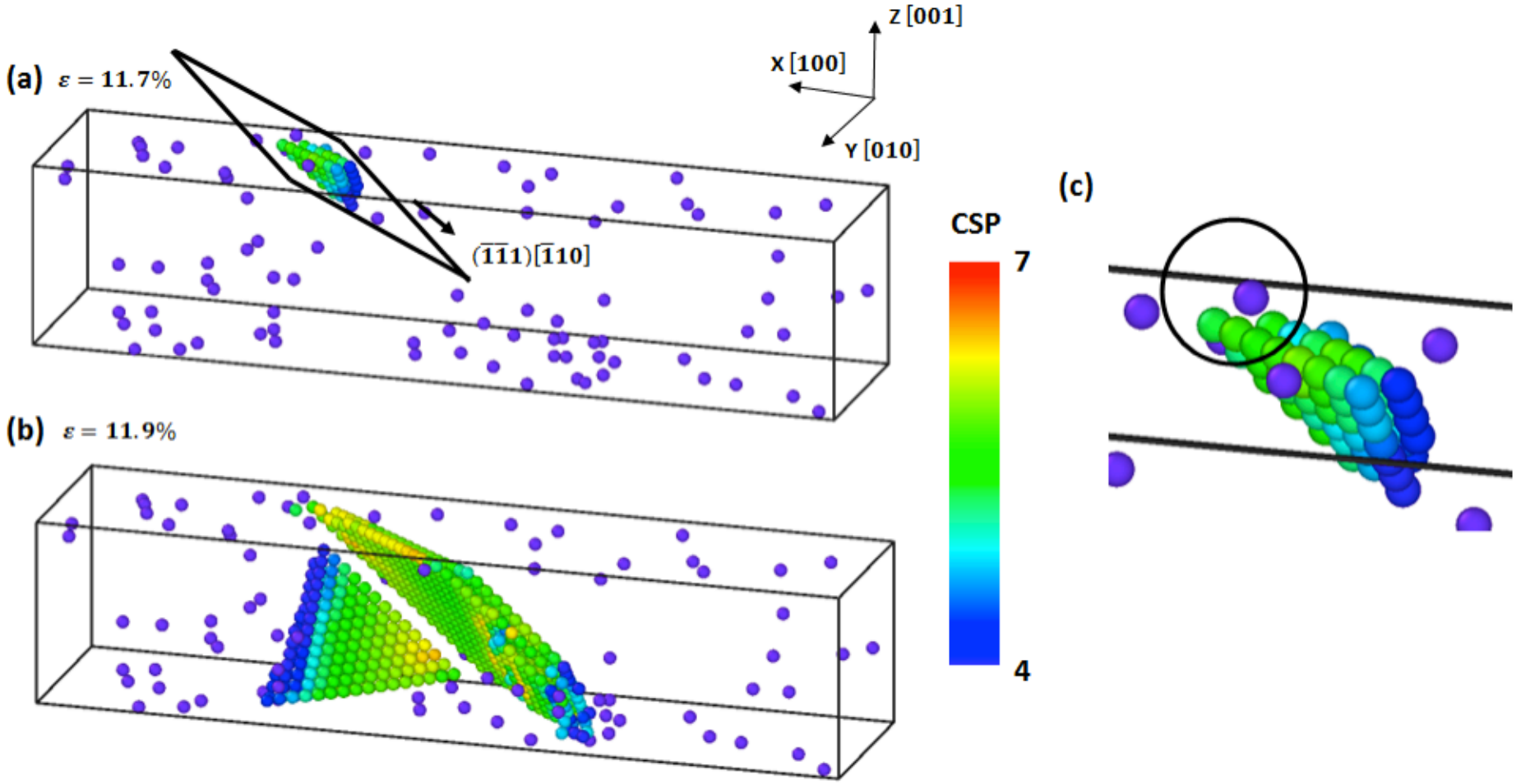
Next dislocation



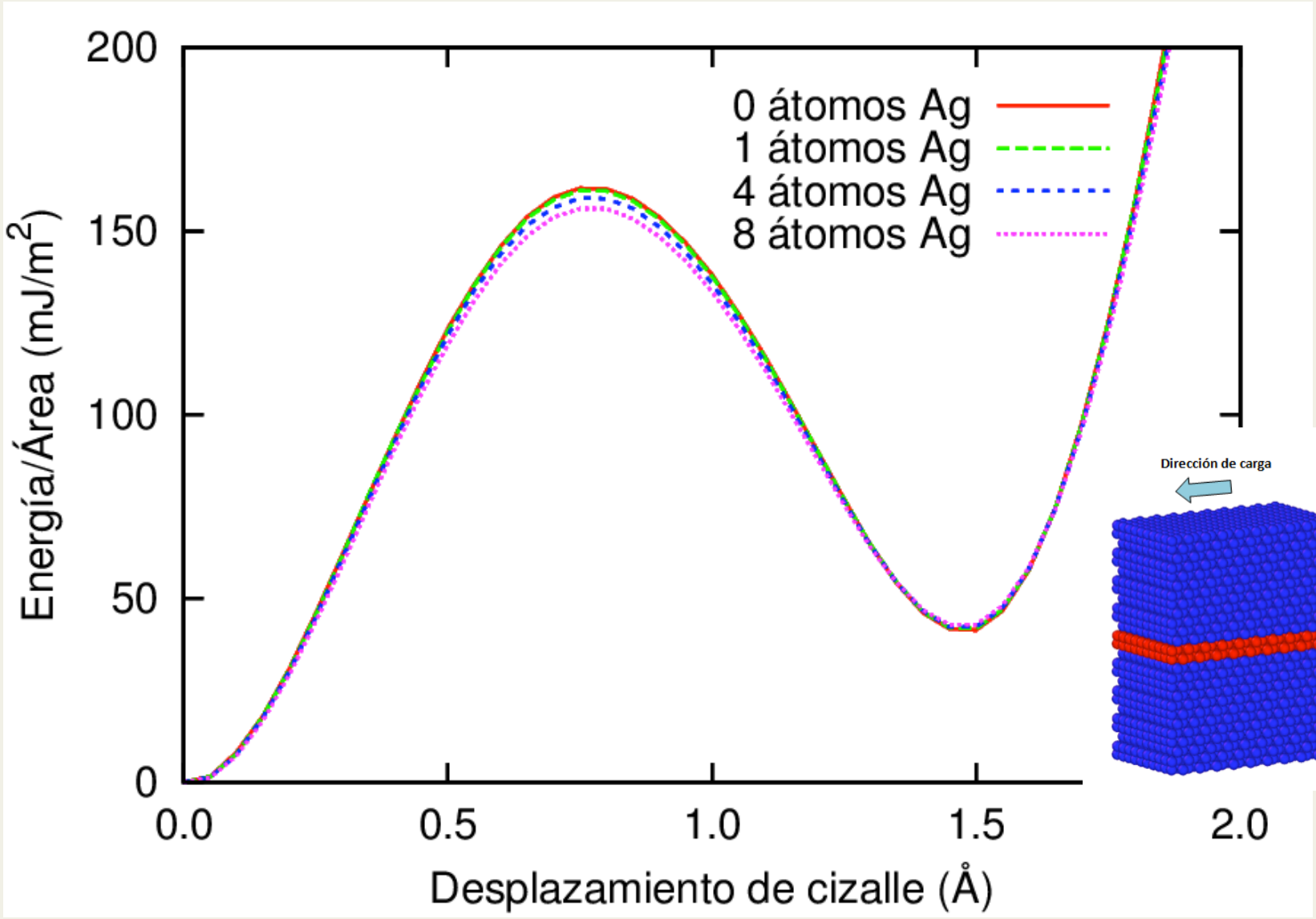
Generation and elimination of a stacking fault

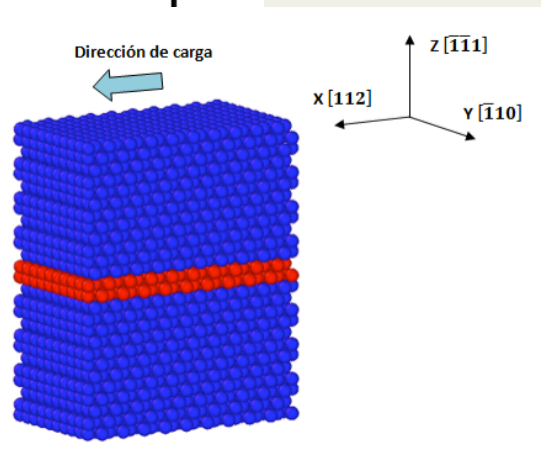


0.5%Ag case


(a) $\varepsilon = 11.7\%$
Z [001]
X [100]
Y [010]
$(\bar{1}11)[\bar{1}10]$
(b) $\varepsilon = 11.9\%$
CSP
7
4
(c)

Stacking fault energy





Unstable and stable staking fault energy in direction <112>

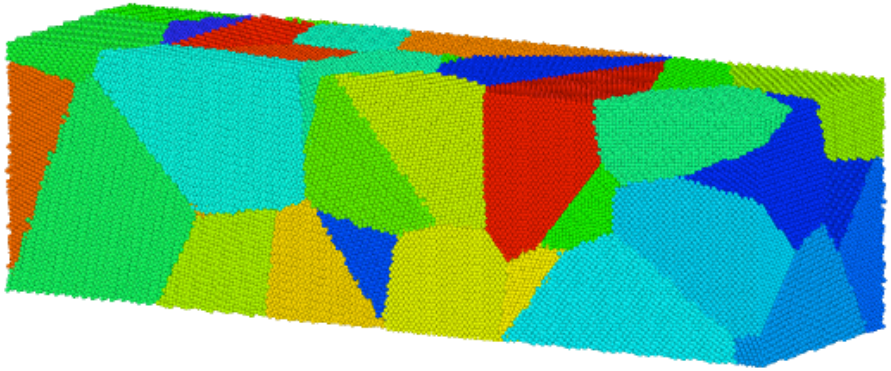
Contenido Ag (número de átomos)	γ_{usf} (mJ/m^2)	γ_{sf} (mJ/m^2)
0	161.7	41.4
1	161.2	41.8
4	159.0	42.2
8	156.2	42.8

Conclusions I

- Impurities:
  - no changes in the elastic regime
  - yield point decreases
  - promotion of dislocation emissions

Stacking faults energy calculations support this picture

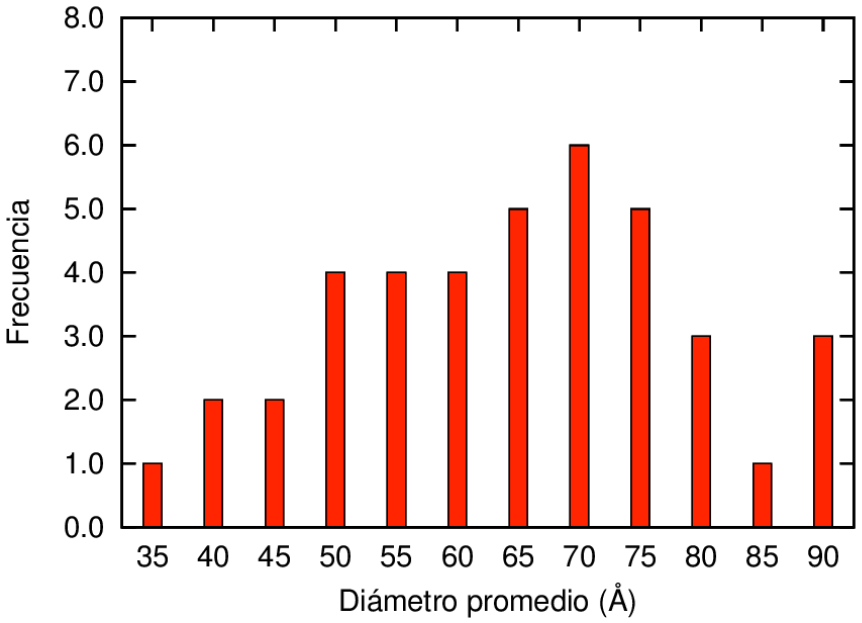
Impurities in poly-cristalline copper



126 A

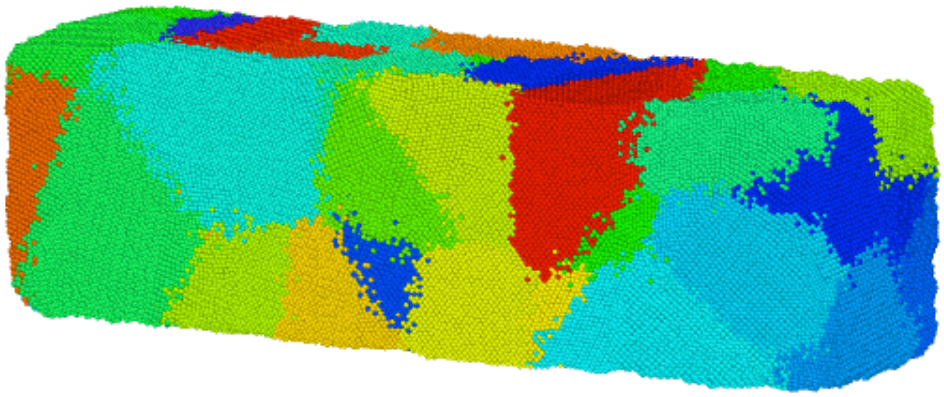
430 A

Diameter grains distribution



600 thousands atoms
40 grains

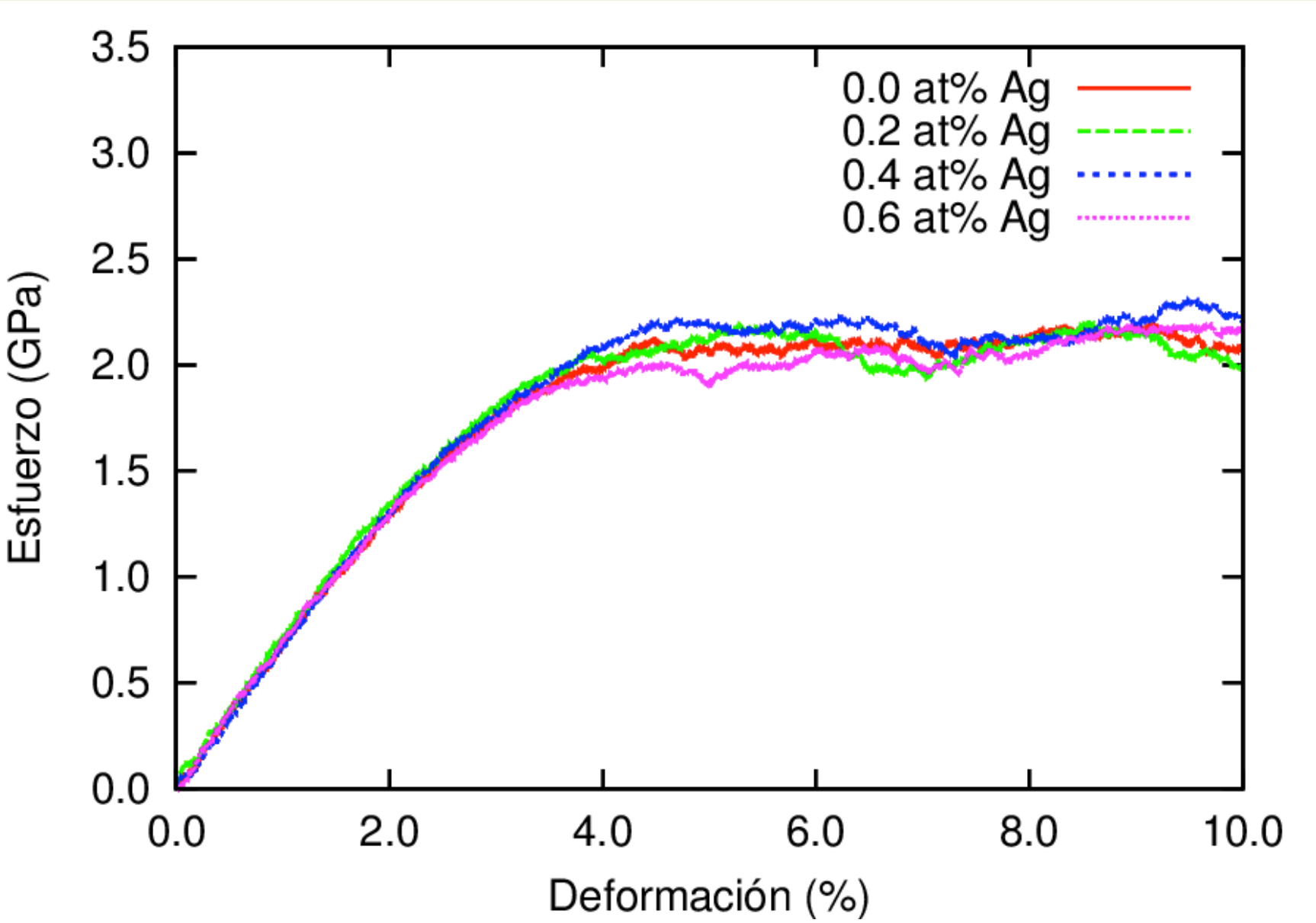
Technical details



-Ag: substitutional at Grains boundaries
-thermalization:
Langevin at 1000 K, 10 ps;
NVT 1000K, 100 ps;
Langevin at 300K, 10 ps;
NVT at 300 K 200 ps;
- During this process, several Stacking faults are generated.

Deformation rate: $5 \times 10^{8}\ s^{-1}$

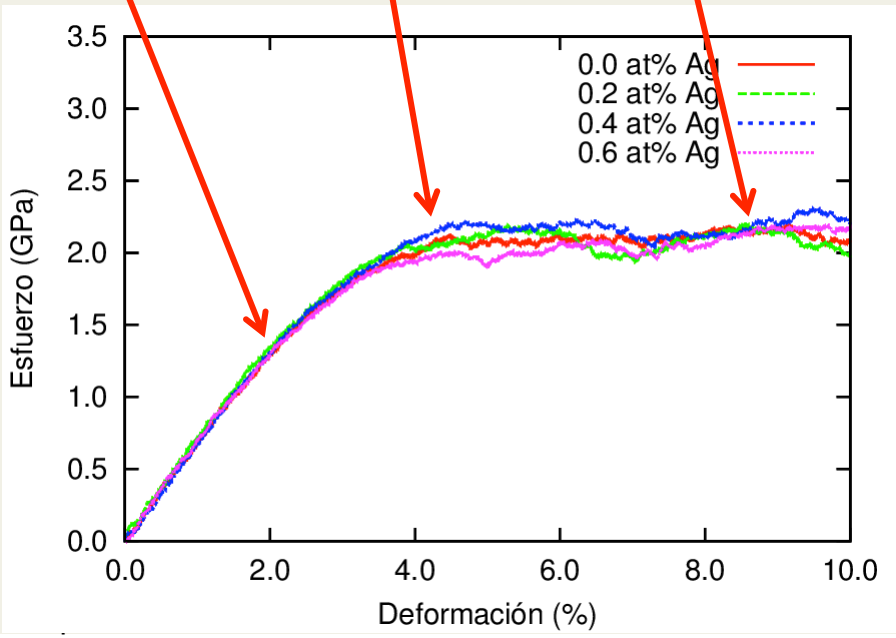
Stress-strain curve



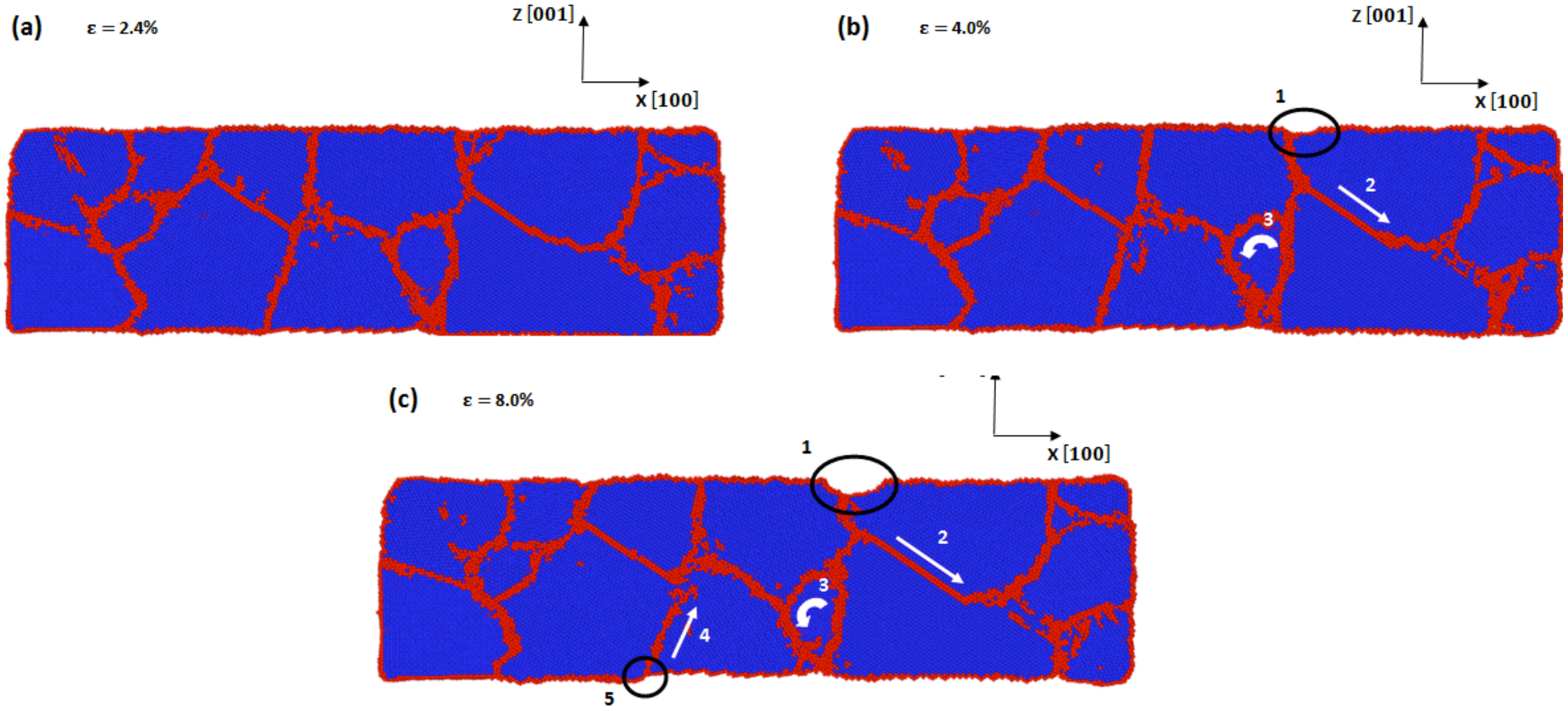
Young modules and other value

Sistema	E [GPa]	σ_f [GPa]	σ_{max} [GPa]	σ_p [GPa]
0.0 at % Ag	68.84	1.45	2.12	2.14
0.2 at % Ag	68.86	1.56	2.19	2.09
0.4 at % Ag	68.33	1.58	2.22	2.17
0.6 at % Ag	70.96	1.38	2.01	2.10

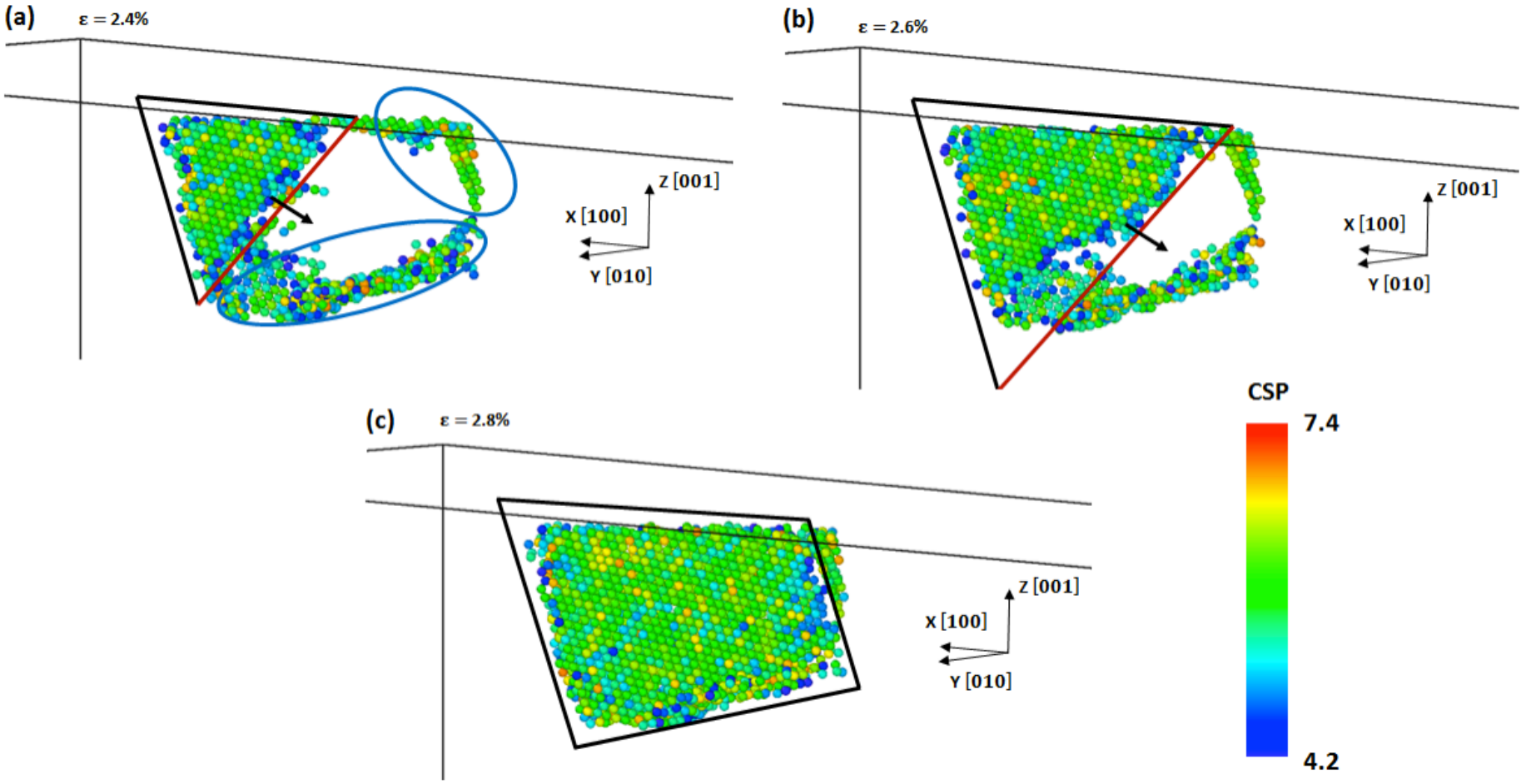
No significant changes!



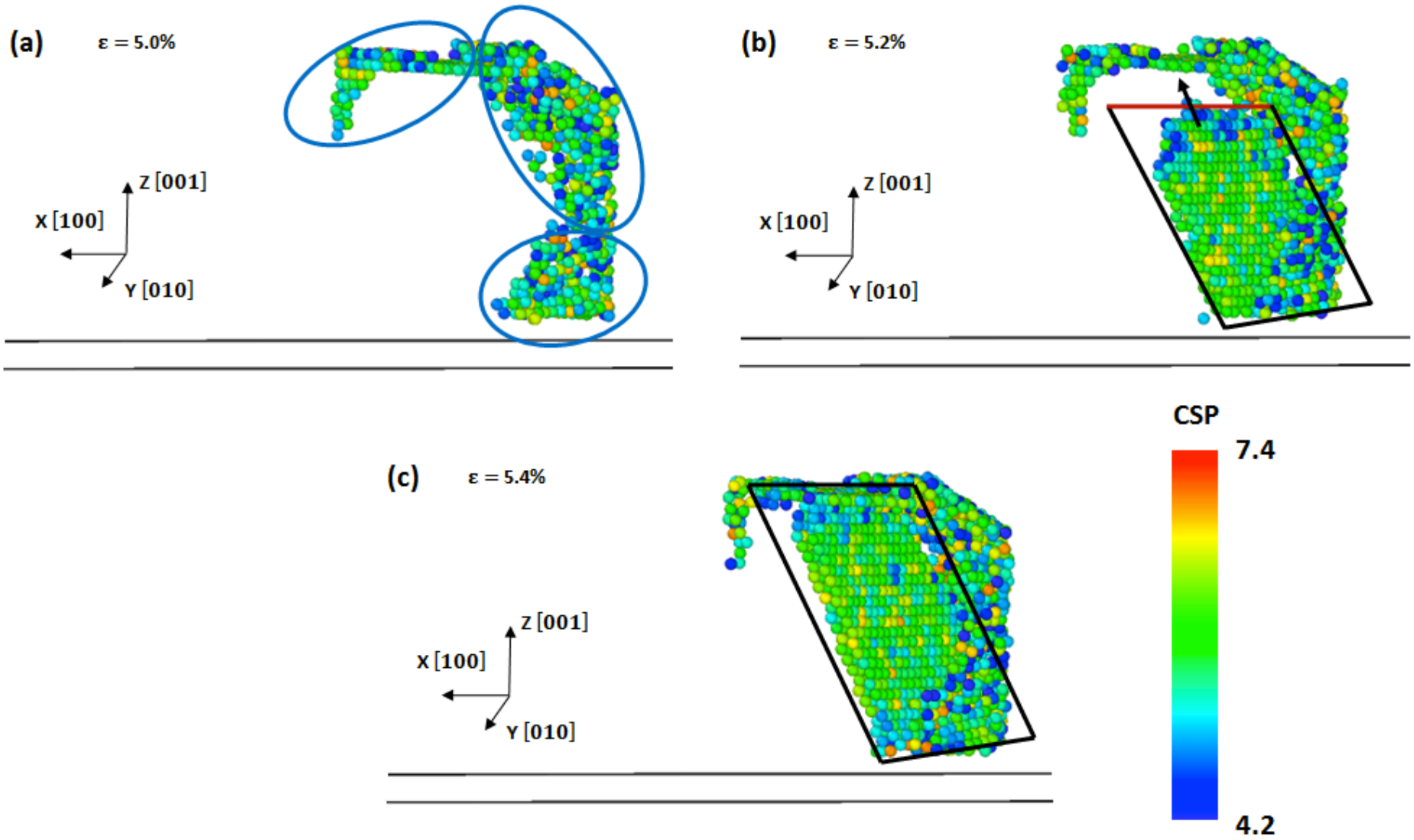
Mechanism of plasticity: rotation and sliding of grains



Dislocations at grains I



Dislocations at grains II



Conclusions II

- Impurities do not provoke significant changes for elastic nor plastic regime
- Plasticity is governed by grains rotation and sliding as well as by dislocations
- More study is needed to clarify the role of texture and grain size
- Nevertheless, is clear that there is no great changes in the mechanical properties, in good agreement with experiments.

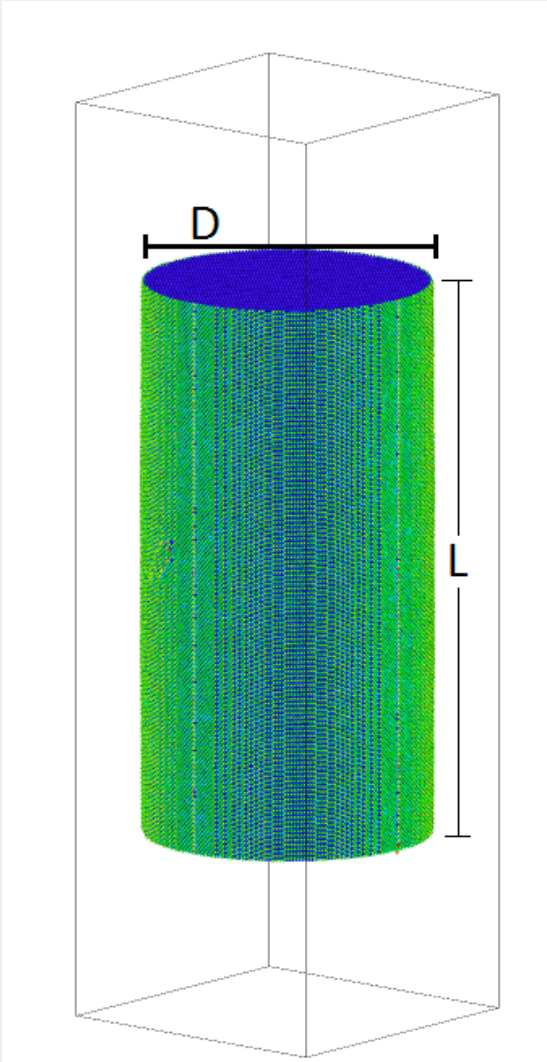
Radiation damage in Au nanowires

E. A. Figueroa
G. Gutierrez
Departamento de Física, Facultad de Ciencias,
Universidad de Chile
Chile

E. M. Bringa
D. Tramontina
Instituto de Ciencias Basicas,
Universidad Nacional de Cuyo, 5500 Mendoza,
Argentina

Nature of stacking fault tetrahedron in Au nanowires under irradiation.

PKA technique



L/D~2 D~25 nm
1.500.000 átomos
PKA 20 keV
r(t=0)=(0,0,0)
300 Kelvin
200 ps

↓

Cascade

↓

Thermal Spike
T=20.000 Kelvin (locally)

↓

SFTs + Voids +
vacancies + loops

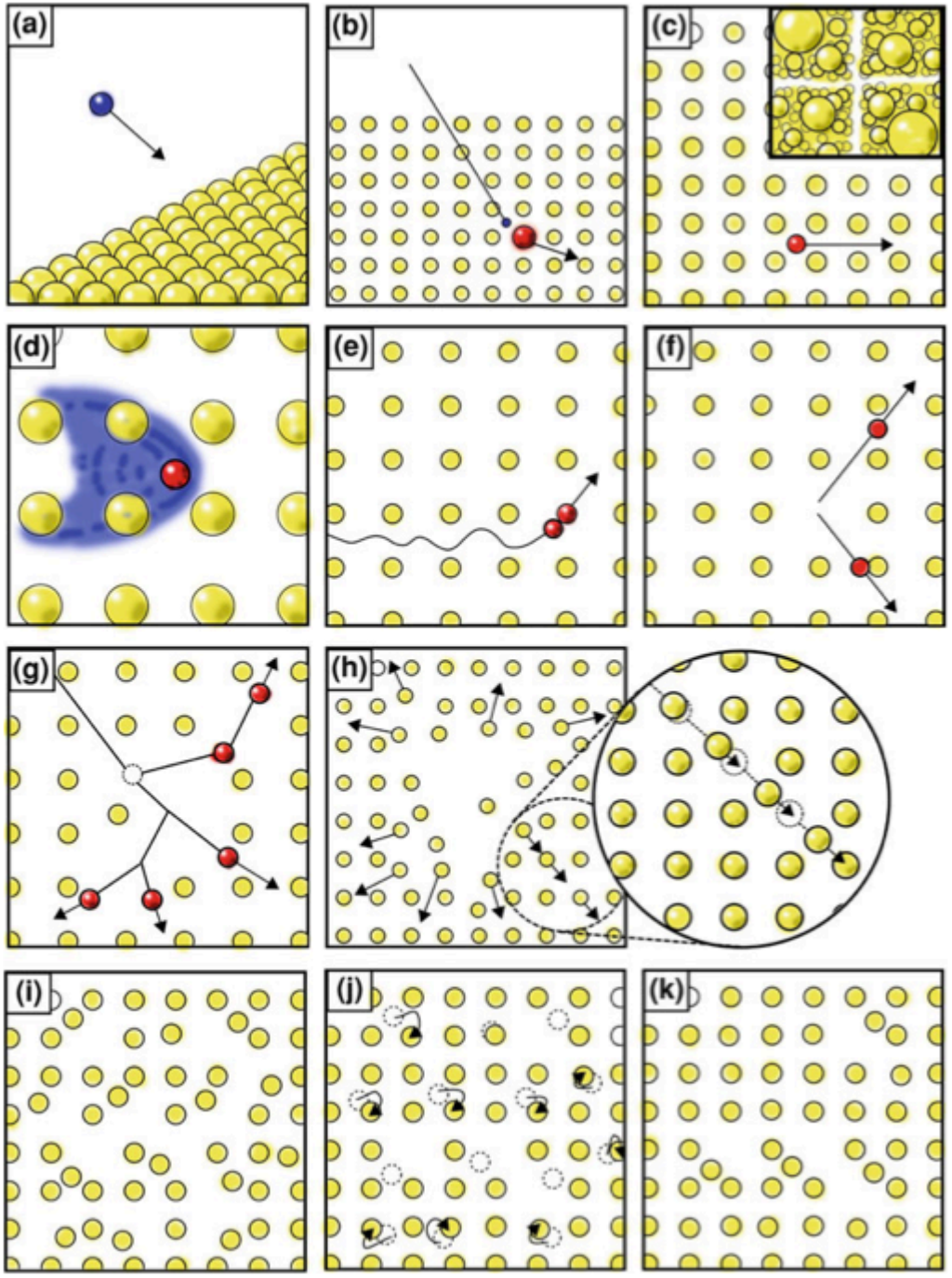


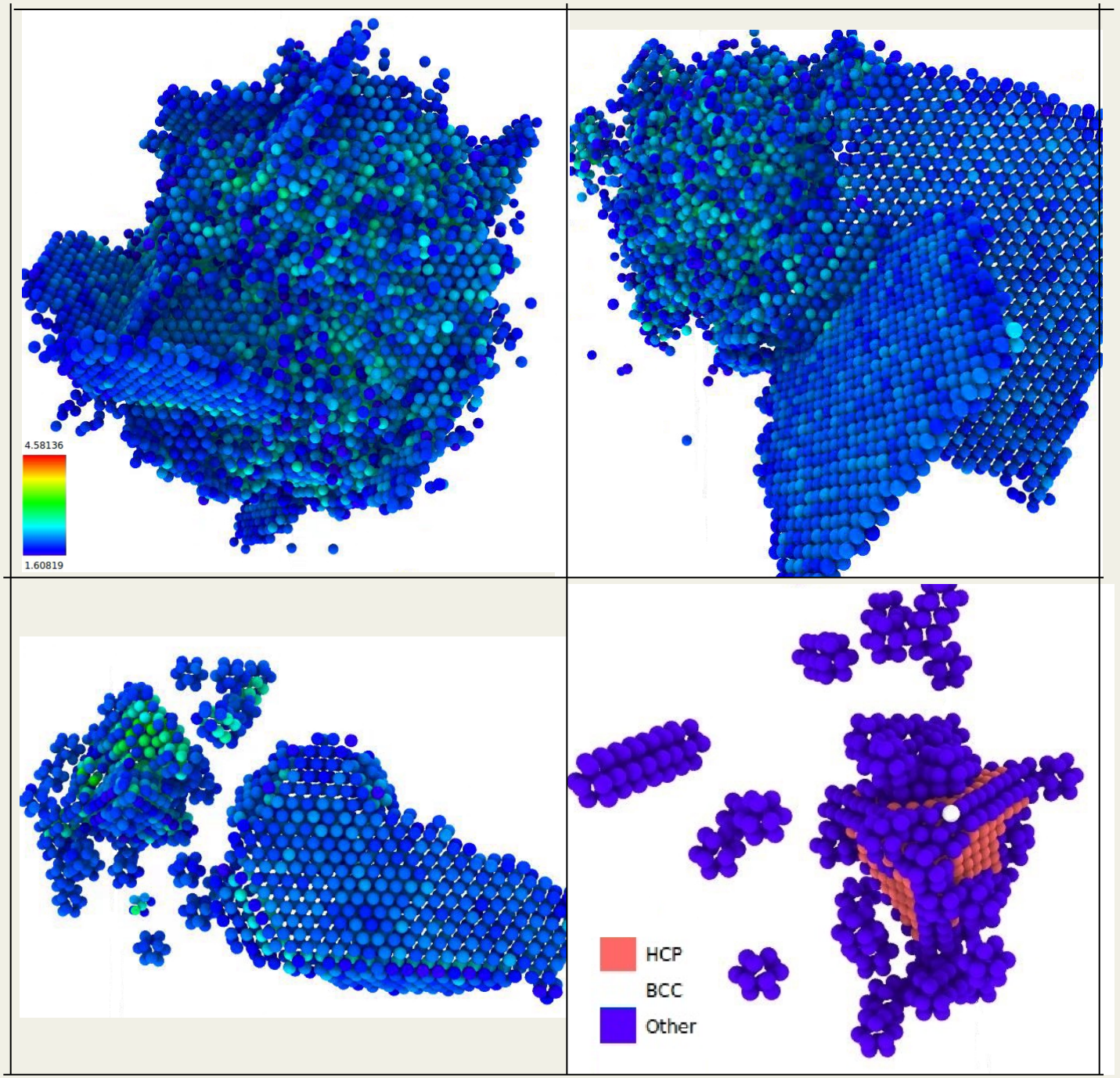
Fig. 2.1 Schematic representations of the stages of evolution of a collision cascade

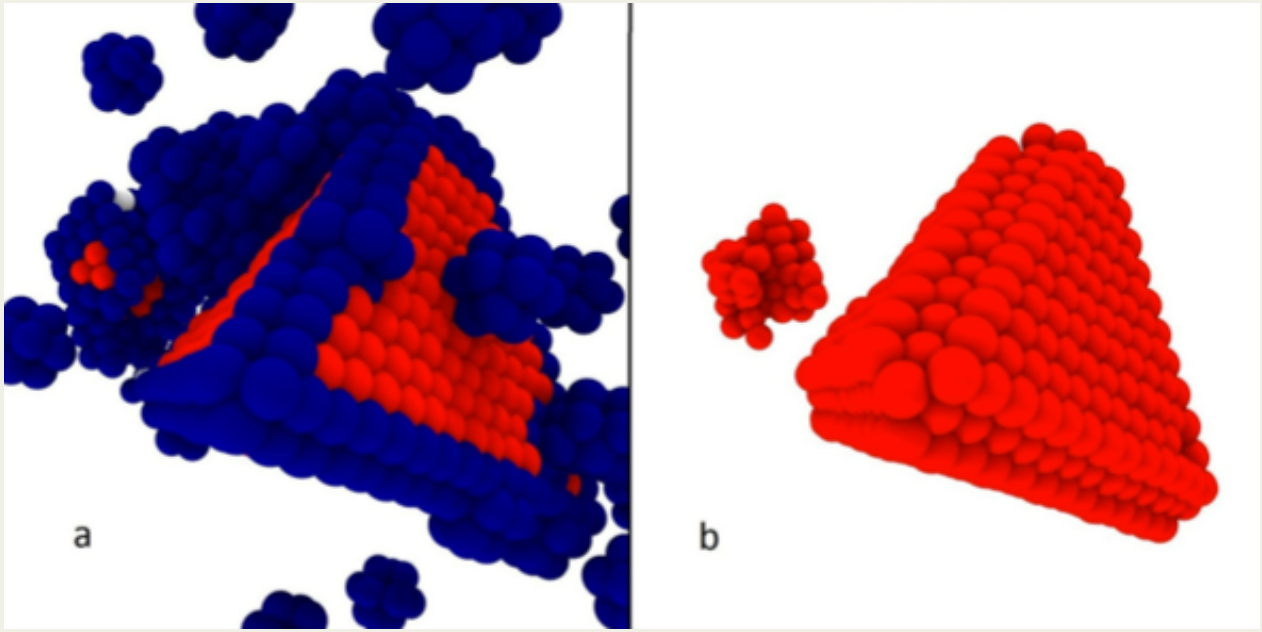
Colisión produce una cascada

From: C. Race, The modeling of Radiation Damage

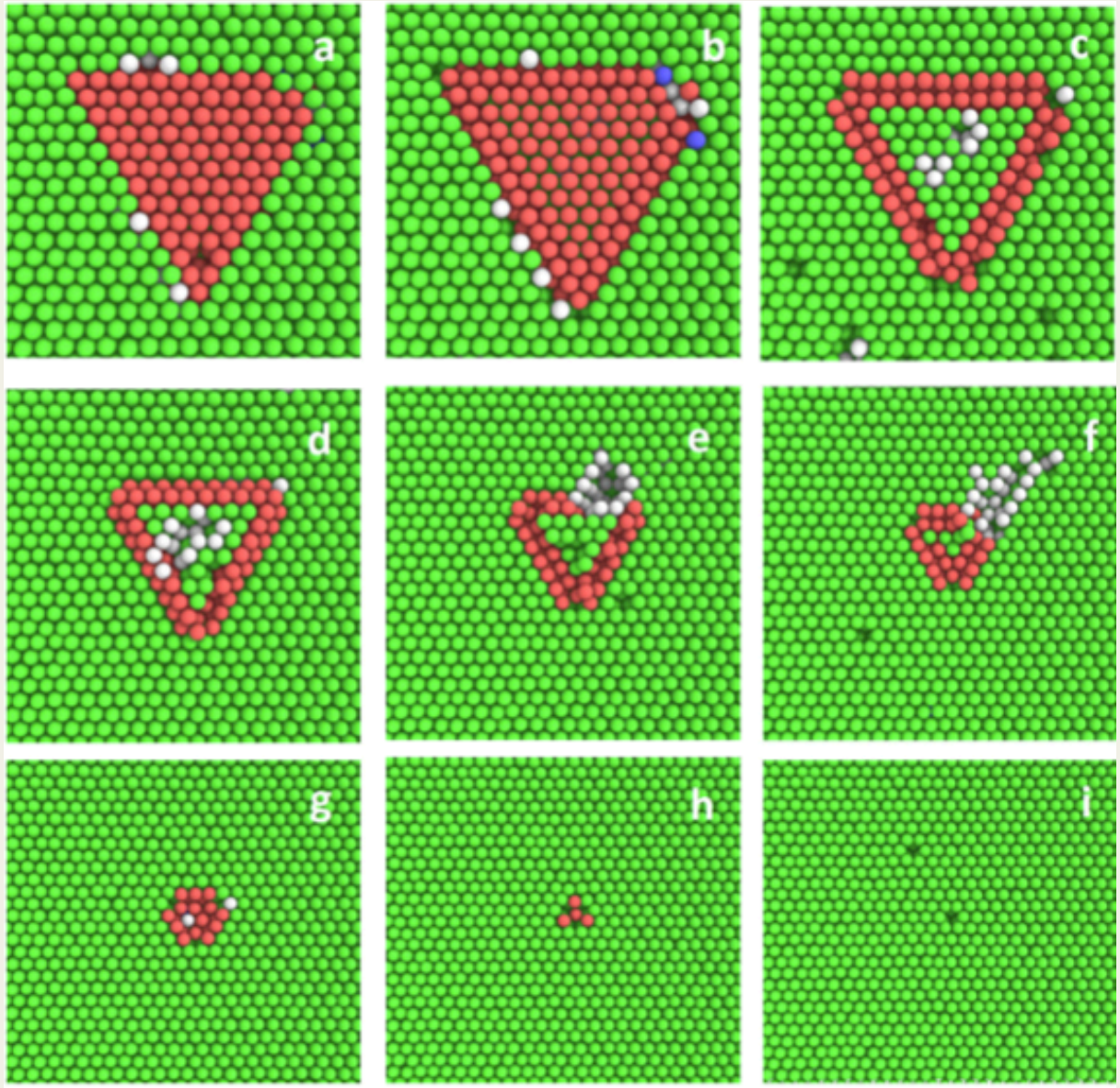
Stacking Fault Tetrahedron

SFT




a
b

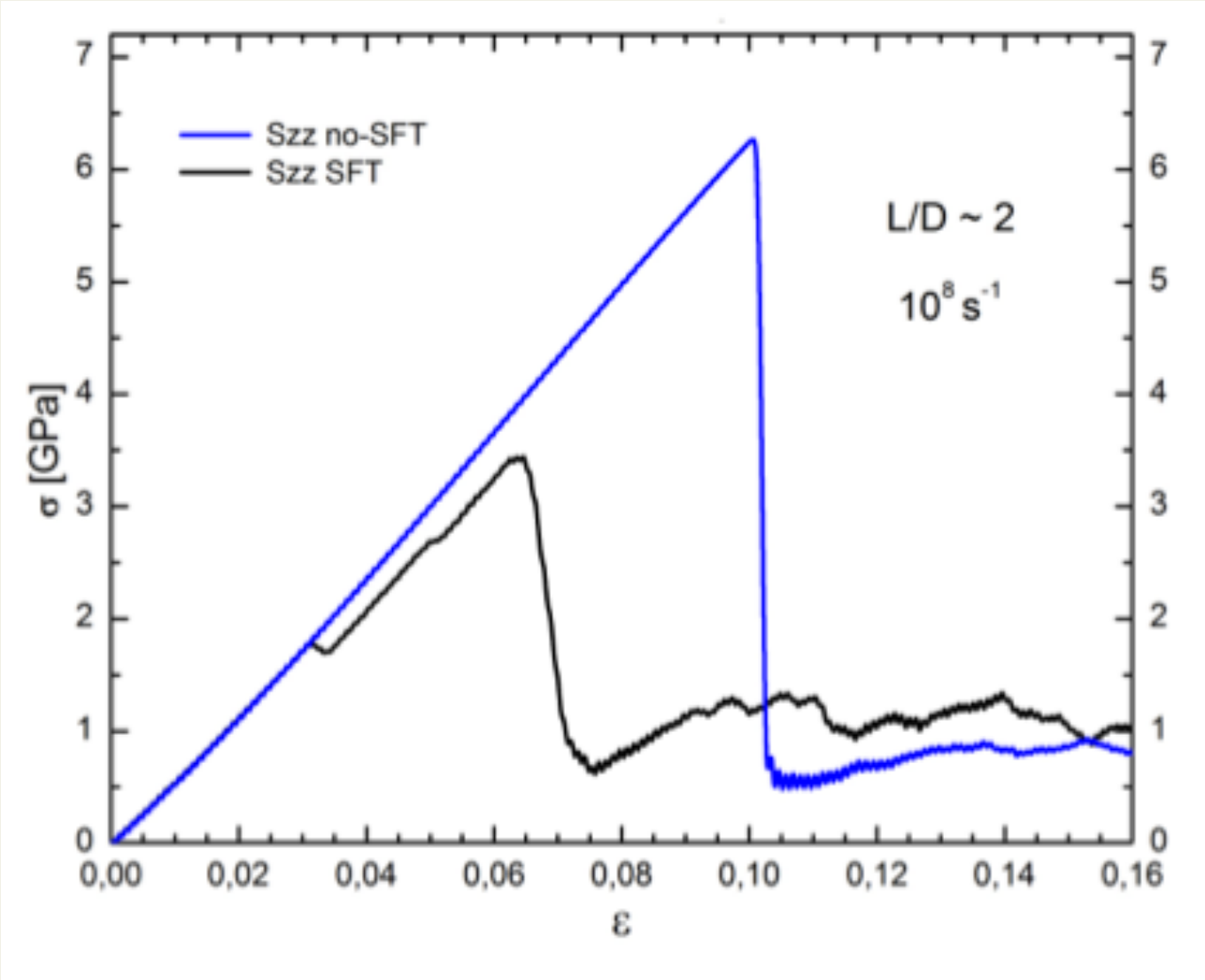
Nine layers of the SFT

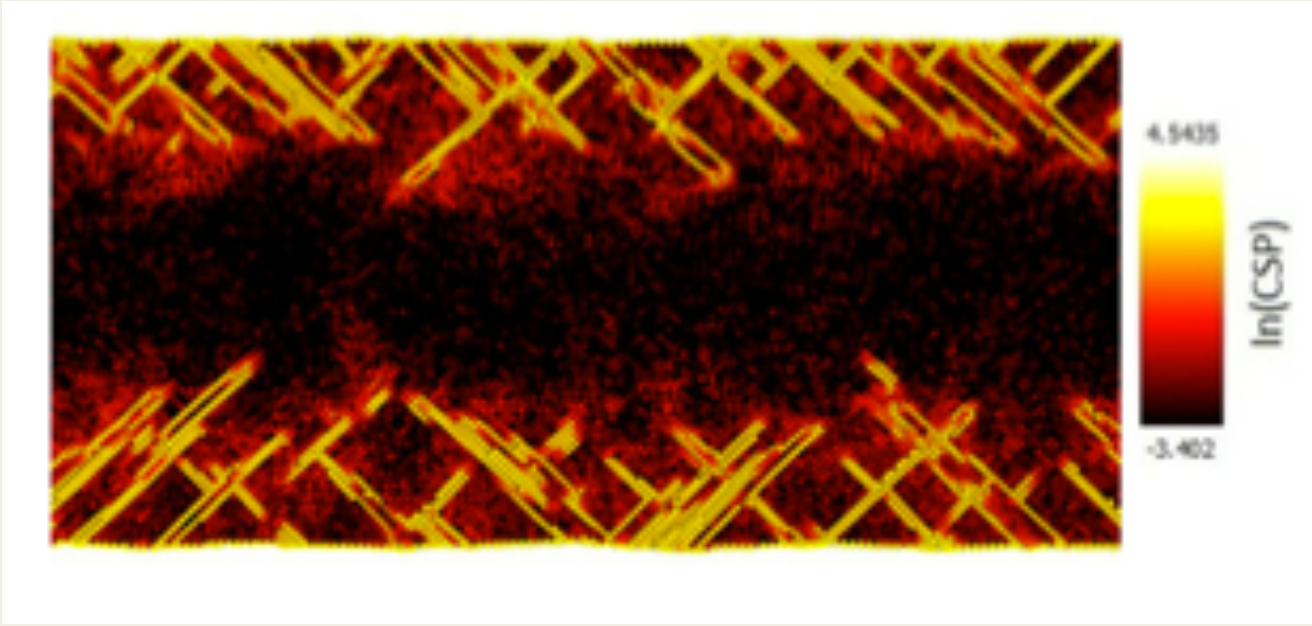


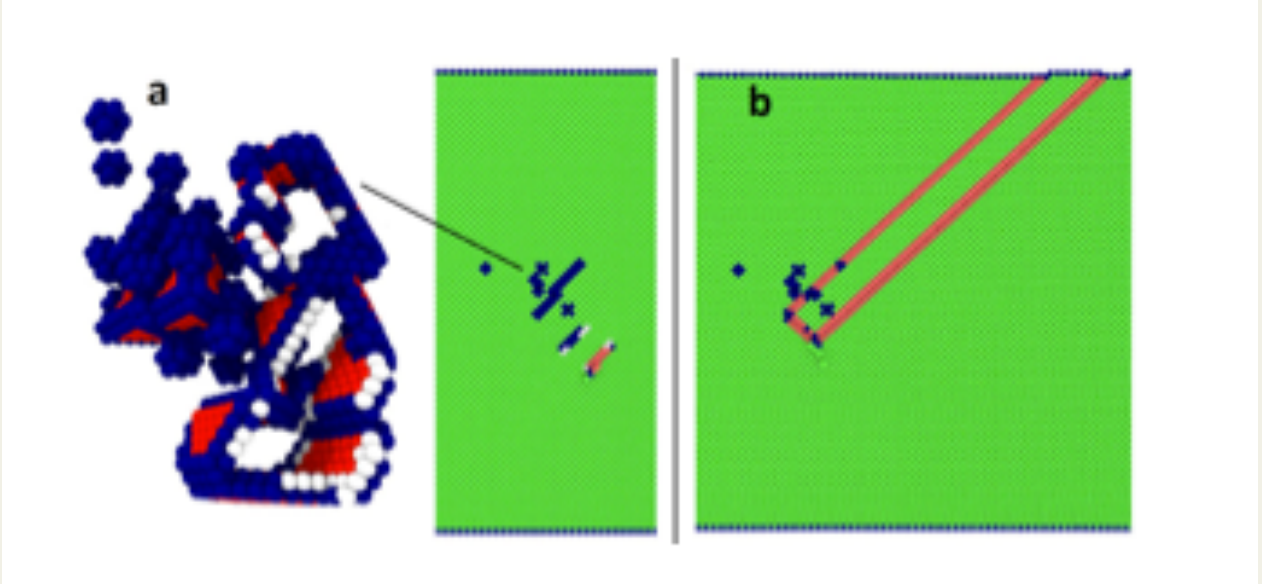
Softening and hardenning of Au nanowires under irradiation

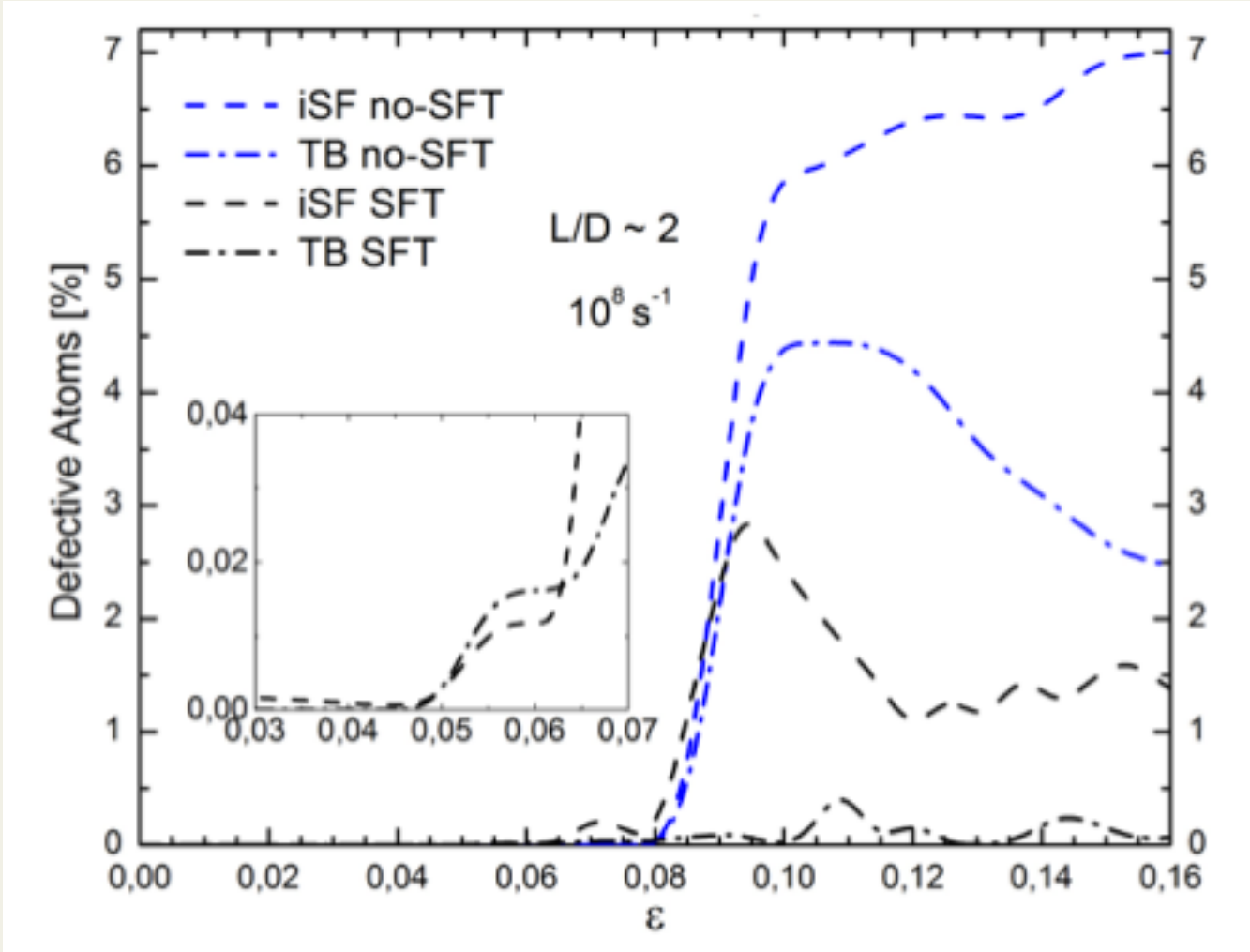
- Mechanical properties of a gold nanowire with pre-existing radiation damage: SFT

-Tensile test: we quantify dislocation and twin density during the deformation


Szz no-SFT
Szz SFT
L/D ~ 2
10^8 s^-1
σ [GPa]
ε
0
1
2
3
4
5
6
7
0,00
0,02
0,04
0,06
0,08
0,10
0,12
0,14
0,16


4.5435
ln(CSP)
-3.402


a
b


iSF no-SFT
TB no-SFT
iSF SFT
TB SFT
L/D ~ 2
10^8 s^-1
Defective Atoms [%]
ε
0,00
0,02
0,04
0,06
0,08
0,10
0,12
0,14
0,16
0
1
2
3
4
5
6
7
0,03
0,04
0,05
0,06
0,07

Conclusions

-stacking fault tetrahedral (SFTs) defect leads to a reduced plastic threshold

- early activation of the SFT as a dislocation source leads to reduced dislocation densities compared to the case without radiation damage

- we observed a total destruction of the SFT, as opposed to a recent paper [1] where it is postulated that SFTs might act as self-generating dislocation sources.

¡Thank you!

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