An atomistic approach to materials: structure of glassy alumina and the mechanical response of copper

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www.gnm.cl

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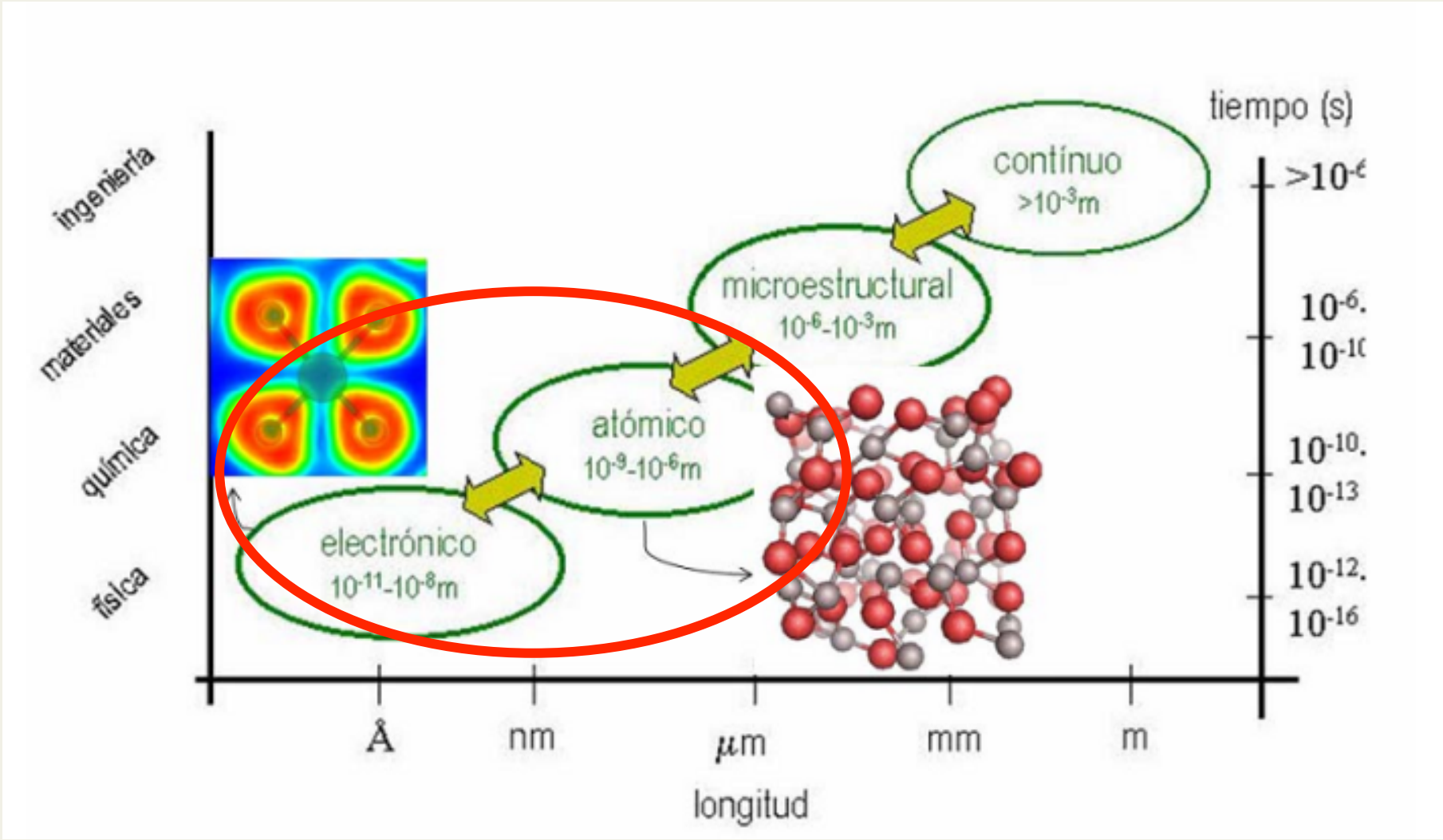
Grupo de NanoMateriales, U. de Chile

www.gnm.cl

- Profs: Eduardo Menéndez, Sergio Davis, Gonzalo Gutiérrez
- Postdoc: Emilio Figueroa, Germán Miño
- Postgraduate students: F. González, Y. Navarrete, N. Amigo, E. Sánchez
- Approx. 10 undergrad per year
- Collaboration in Chile and abroad

Atomistic simulation



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) glasses: structures, dynamical and mechanical properties
b) nano-structured materials: carbon nanotubes
c) materials under extreme conditions
d) Mechanical properties of metals
e) solar cell materials: electronic and optical properties (ab-initio)
f) nuclear materials: radiation damage
g) Biological systems: molecular simulation

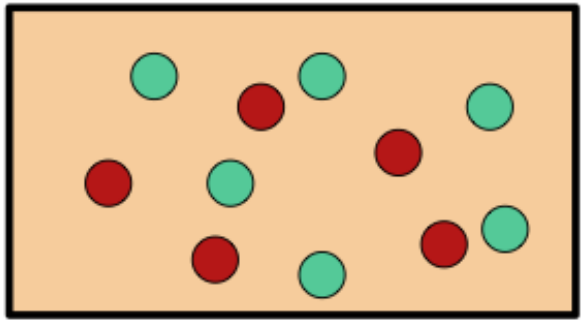
3. Computer simulation techniques
a) Computer programming: Las Palmeras Molecular Dynamics, www.lpmd.cl (Computer Physics Communications, 181(12):2126 – 2139, 2010)
b) Free energy and entropy
c) Algorithms for MD and MC: mpi, CUDA

Outline

- Molecular dynamics simulation
- Amorphous Al_2O_3 by ab-initio MD
- Mechanical properties of copper by classical MD

Molecular Dynamics simulations

Inicial conditions:
$\{\mathbf{r}_i(t_0), \mathbf{v}_i(t_0)\}_N$



N~2000
V
$E_K = 3/2 N k_B T$

Choice of interatomic potential ⇒forces

- empirical pot
- ab-initio $\varepsilon(R)$

$$V(r) = \frac{q_i q_j}{r} - \frac{C_i C_j}{r^6} + B\exp(ar)$$

Numerical solution to the eqs. of motion

Verlet

$\Delta t: 10^{-15}$ s : time step

Physical properties: temporal average over configurations:
$\langle \ldots\ldots \rangle_t$

- Termodynamics prop.
- structural properties
- dynamical prop.

Basic diagnostics

- Pair distribution function
- Angular distribution
- Coordination numbers

Average over positions, velocities and accelerations

- Vibrational density of states *D(w)*

$$Z_{\alpha(\beta)}(t) = \left\langle \sum_{i=1}^{N} m_{i\alpha} \vec{v}_{i\alpha}(0) \cdot \vec{v}_{i\alpha}(t) \right\rangle$$

VACF

$$\mathcal{D}_{\alpha(\beta)}(\omega) = \frac{1}{\sqrt{2\pi}} \int \frac{Z_{\alpha(\beta)}(t)}{Z_{\alpha(\beta)}(0)} \exp(-i\omega t)\, dt$$

- Direct visualization

Structural, elastic, vibrational, and electronic properties of amorphous Al_2O_3 from ab-initio calculation*

Ceramic material with several technological applications
due to high melting point (2327 K),
extreme hardness (Moh 9) y
low electrical conductivity

Structural phase transitions

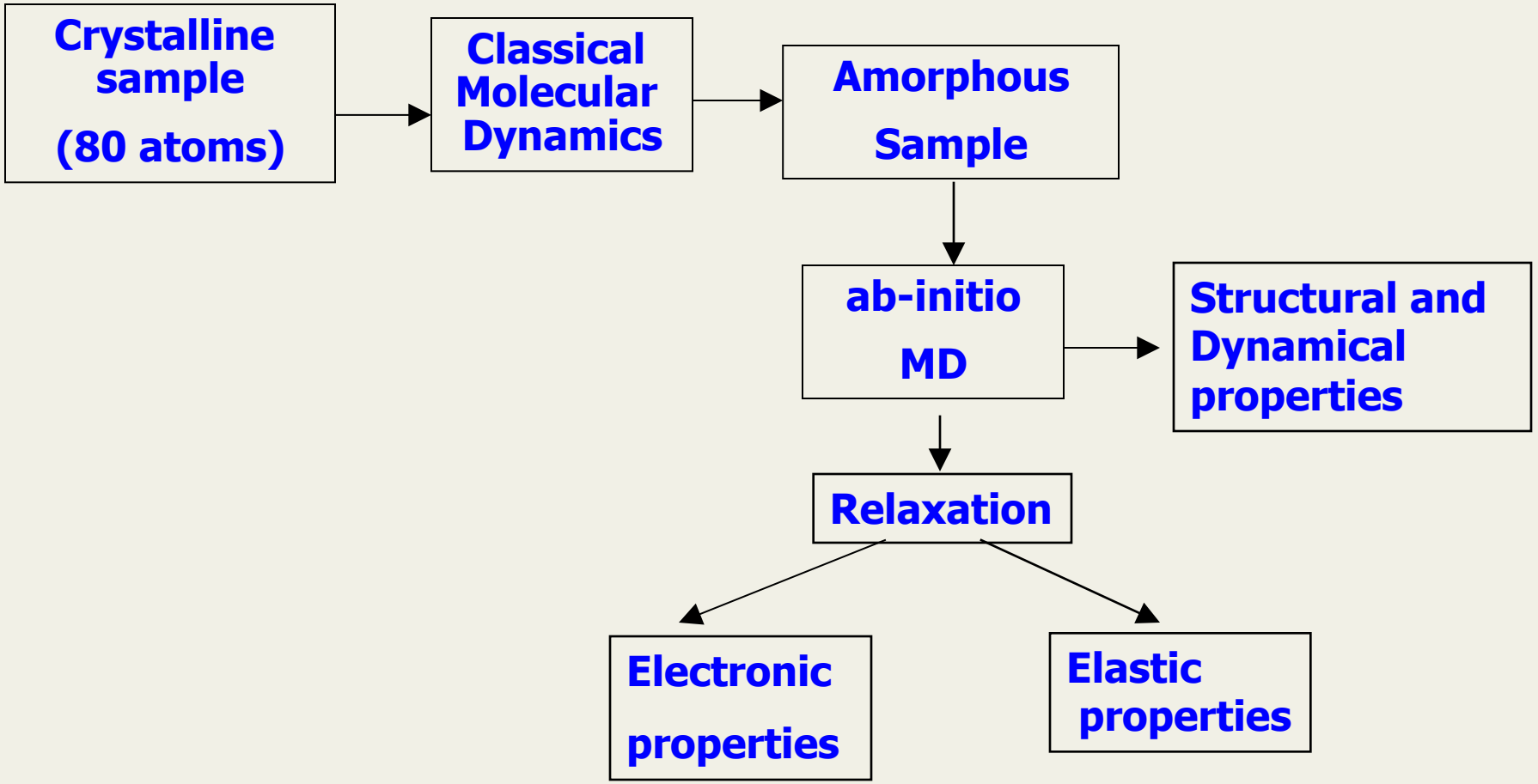
liquid → γ → δ, θ→ α-alumina
amorphous (a.o) → γ → θ→ α-alumina

amorphous alumina? Not many experimental results

* S. Davis, G.G., J. Phys.: Condens. Matter 23, 495401 (2011)

Procedure

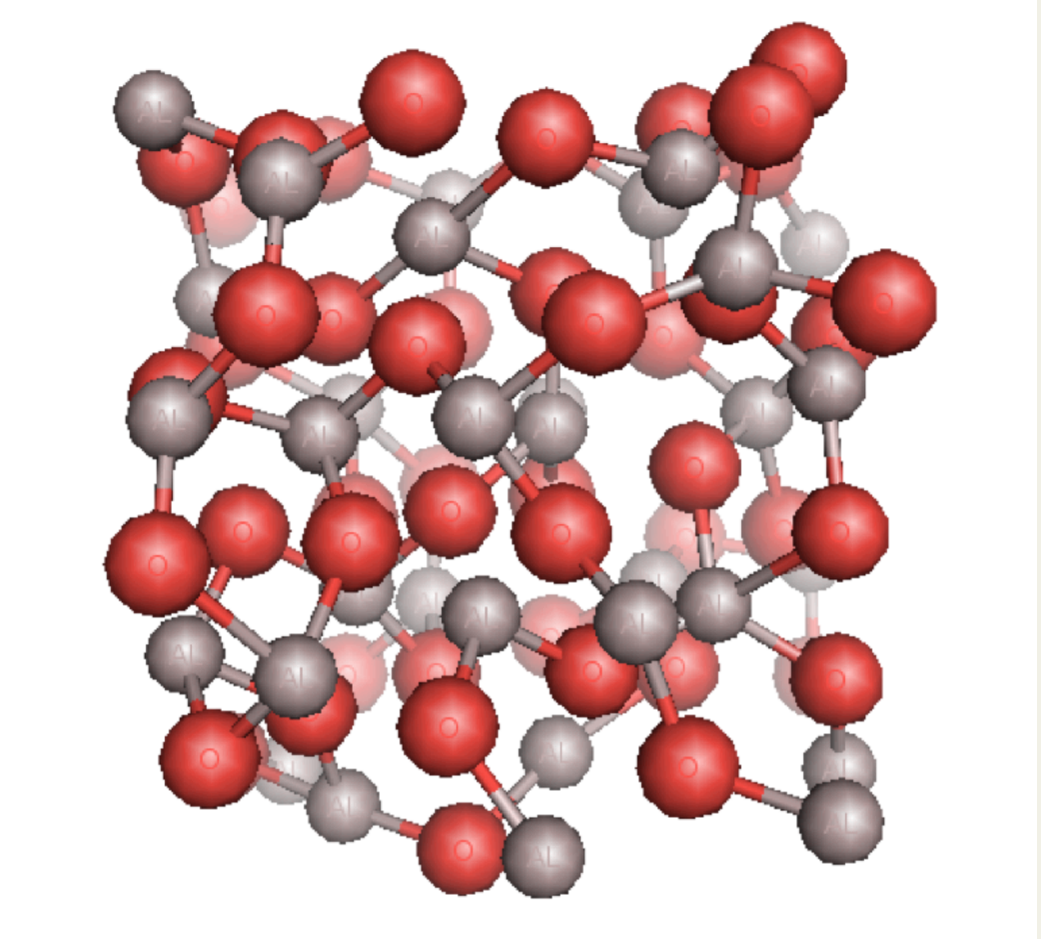
- Combined use of classical an *ab initio* Molecular Dynamics:



Computational details

- *ab initio* MD by using VASP (Vienna Ab Initio Simulation Package)
- Density Functional Theory with LDA (local density approximation)
- Ultrasoft pseudopotentials
- Energy cutoff E_{cut}= 296,77 eV (21,81 Ry)
- Only gamma point, Γ = (0,0,0)
- Time step of 3 fs for atomic motion

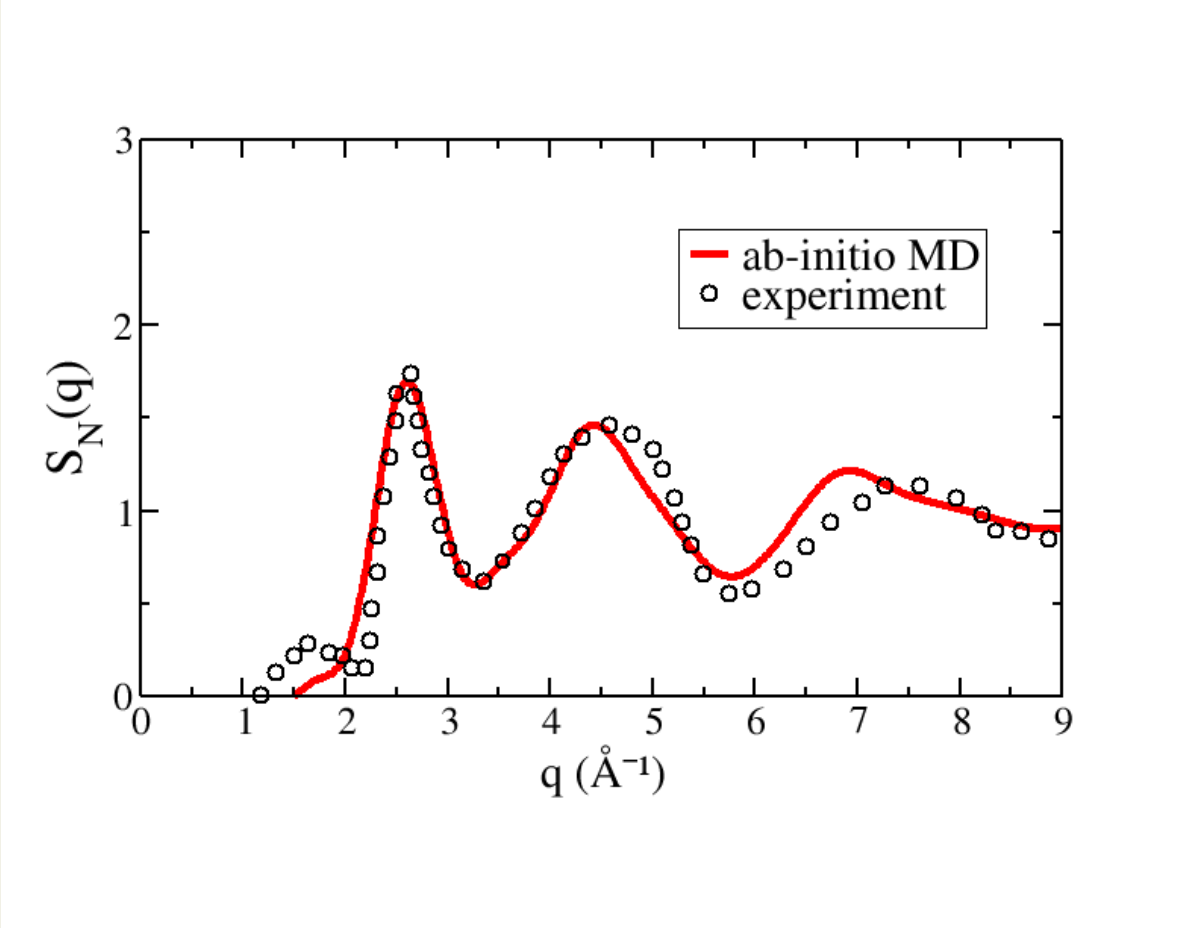
Amorphous Al_2O_3



S. Davis, G. G,
Structural, elastic, vibrational, and electronic properties of amorphous Al_2O_3 from ab-initio calculations

J. Phys.: Condens. Matter 23, 495401 (2011)

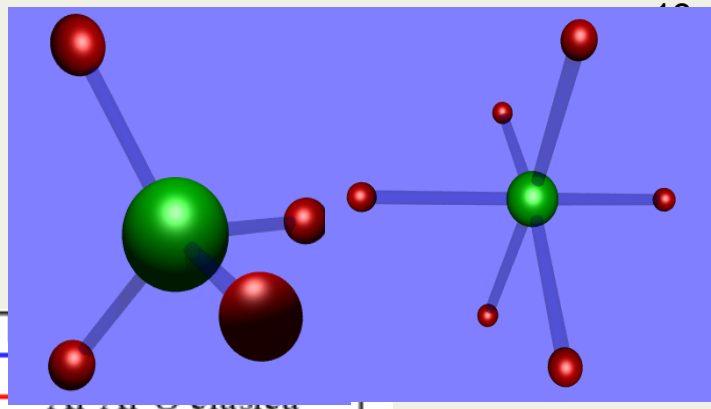
Neutron static structure factor: experiments and simulation

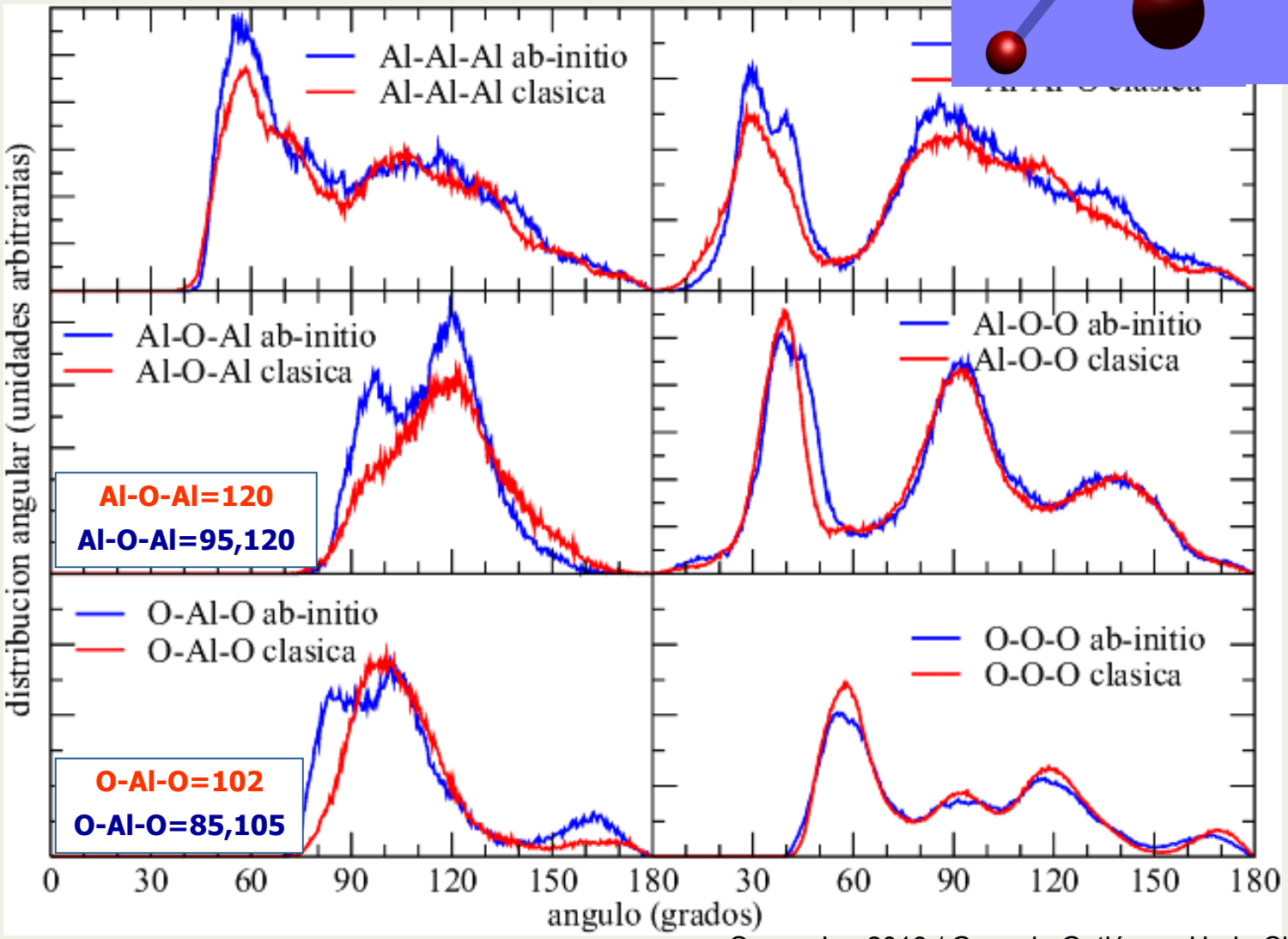


Exp.:
P. Lamparter,
R. Kniep,

Physics B **234**, 405 (1997)

Angular distribution



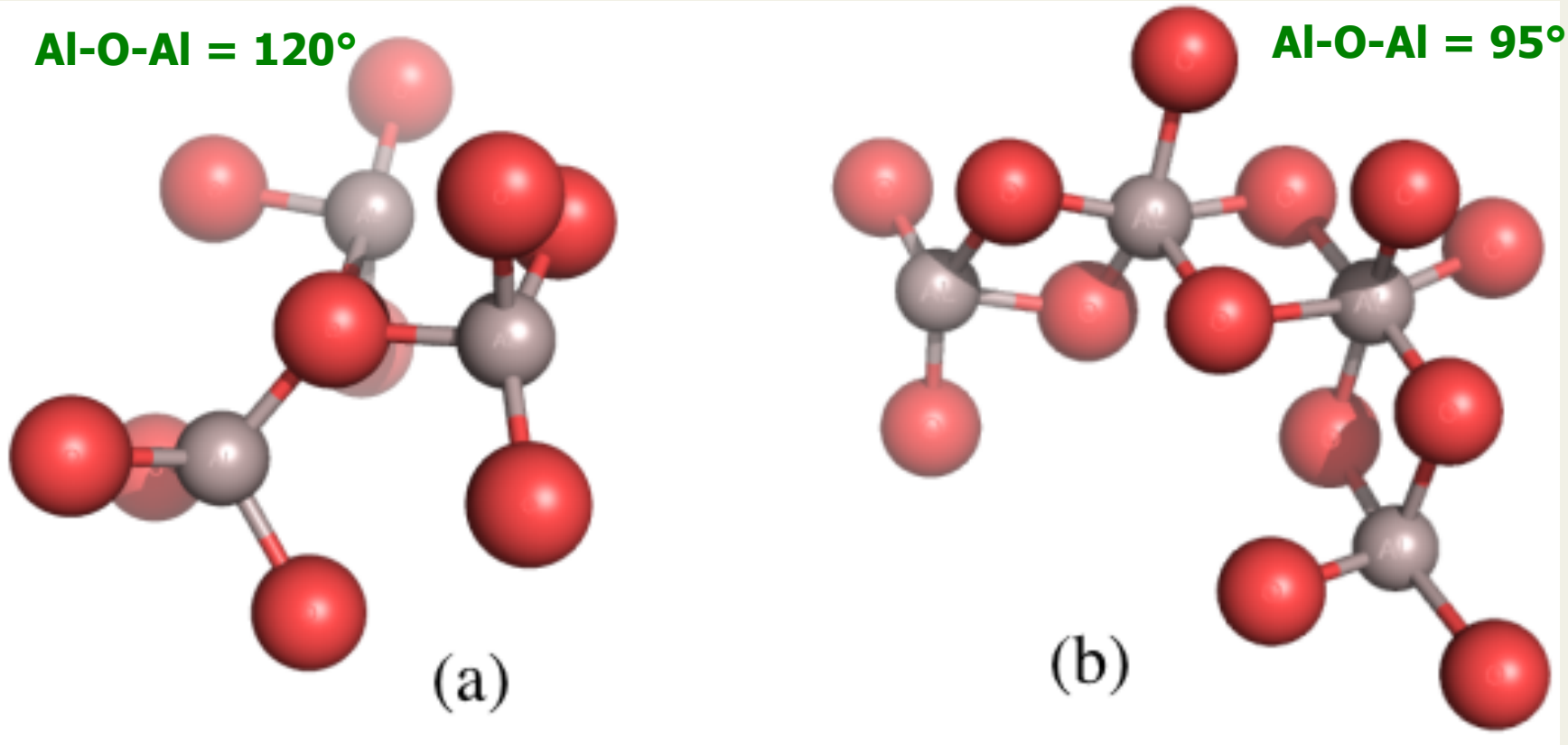


Interatomic distances and coordination numbers

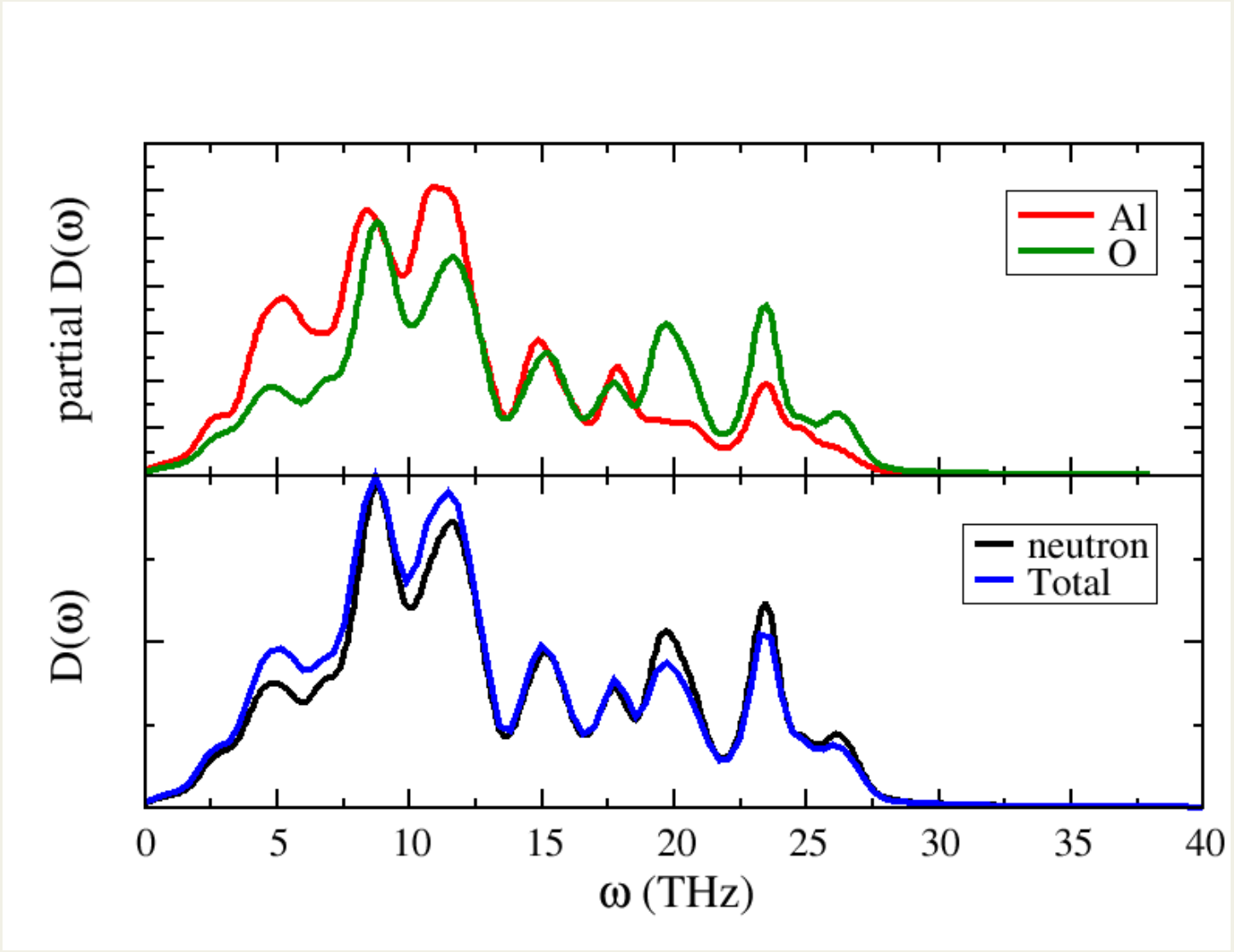
Results	R_{Al-Al} (Ă)	R_{Al-O} (Ă)	R_{O-O} (Ă)
Lamparter y Kniep	3,2 ± 0,55	1,8 ± 0,21	2,8 ± 0,58
Cassical MD	3,24	1,74	2,77
ab initio MD	3,27	1,80	2,91

Results	n_{Al-Al}	n_{Al-O}	n_{O-Al}	n_{O-O}
Classical MD	9,1	3,97	2,65	16,85
ab initio MD	8,9	4,49	2,99	16,46

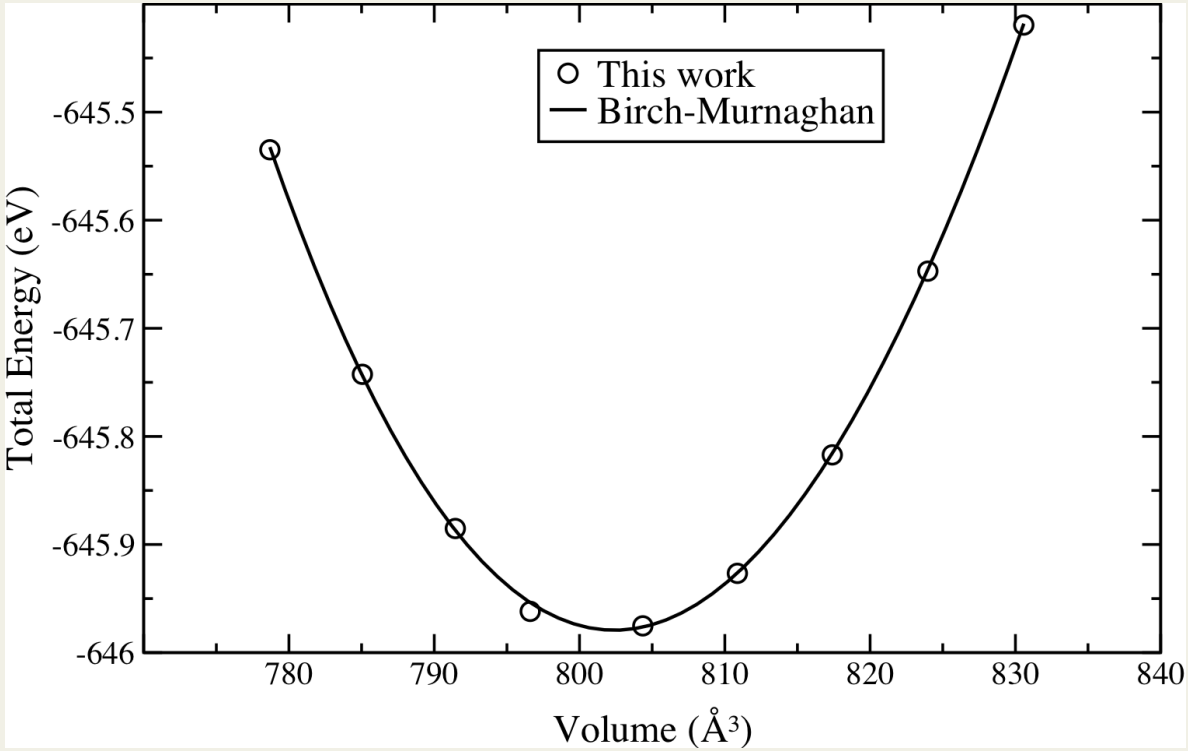
Connectivity between basic units



Vibrational density of states

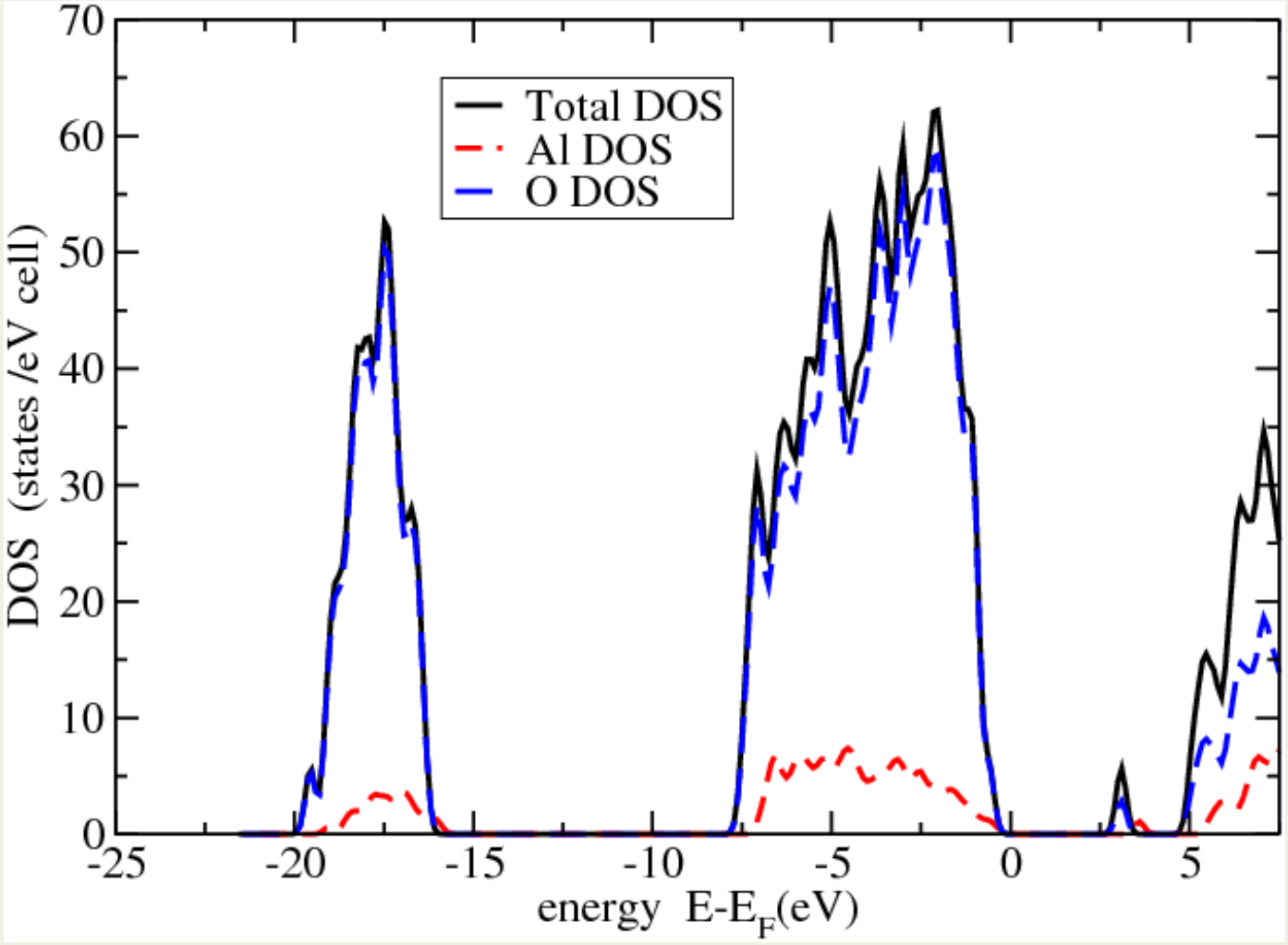


Elastic properties



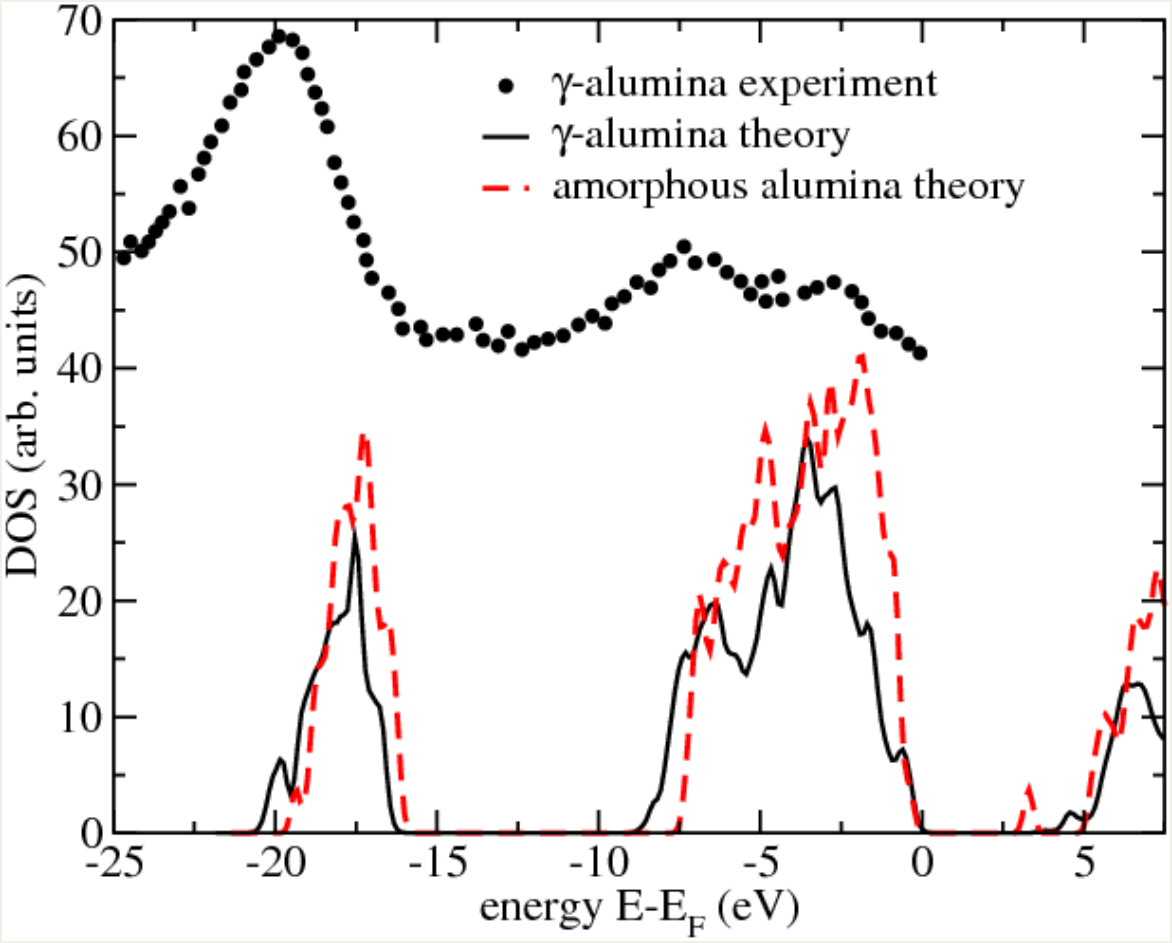
phase	B (GPa)	G (GPa)	E (GPa)	ν
amorph	193.4	141.0	340.3	0.2
Alpha (Wefers & Misra)	253	164	404	0.23

Electronic density of states



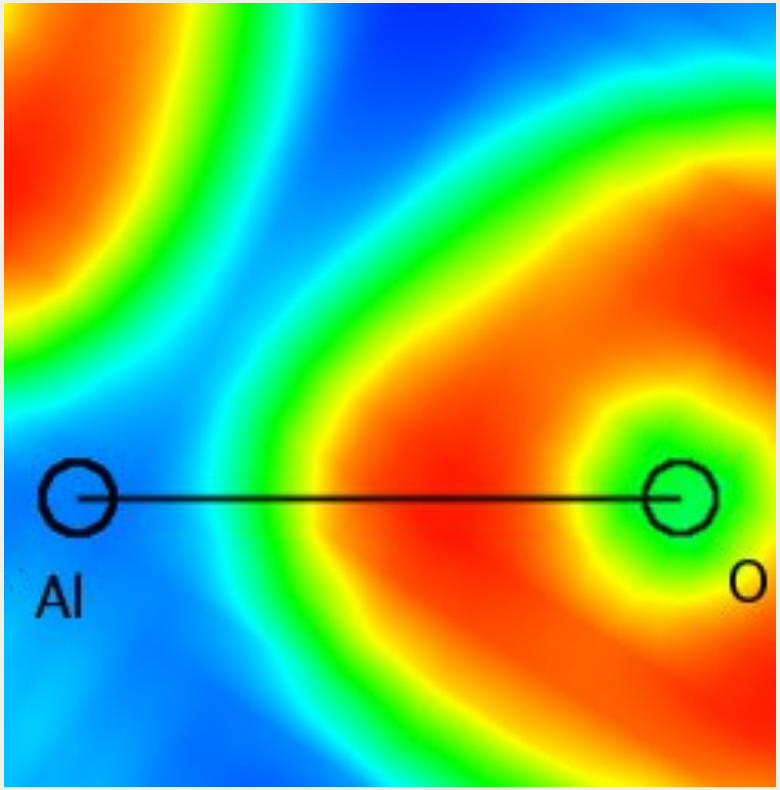
Energy gap
Exp 3.2 eV
Theo. 2.6 eV

Electronic density of states: comparison to γ-alumina



γ-Al_2O_3 Exp: B. Ealet et al. Thin Solid Films **250**, 92 (1994)
Theory: GG, A. Taga. B. Johansson, Phys. Rev. B **65** 012101 (2002)
GG, E. Menéndez, Phys. Rev. B **72** 035116 (2005)

Electron localization function



Charge transfer calculated via Voronoi analysis:
Al ~ 2.89
O ~ -1.92

Different alumina phases

Phase	Density g/cm^3	Al Coordination Number	Bond length Al-O (A)
amorphous[b]	3.17	4(76%), 5 (22%)	1.76
	3.9	4(23%), 5(51%), 6(21%)	1.77
	4.2	4(15%), 5(21%), 6(64%)	1.79
a, ab-initio[d]	3.17	4(50%), 5(42%), 6(5%)	1.81
liquid[a]	3.17	3(13%), 4(66%), 5(20%)	1.76
gamma[c]	3.66	4(37%), 6(63%)	1.94 +/- 0.3
theta	3.65	4(50%), 6(50%)	1.9 +/- 0.3
alpha	3.98	6 (100%)	1.97

Our results:

a) PRE **61**, 2723 (2000),
b) PRB **65**, 104202 (2002), unpublished (2008)
c) PRB **65**, 012101 (2002), PRB, **72**, 035116 (2005)
d) J. Mat Sc. 45, 5124–5134 (2010);
J. Phys.: Condens. Matter 23, 495401 (2011)

Conclusions

- Using of ab-initio MD appear new features, absent in (simple) empirical interatomic potential
- The building blocks of the system are **AlO_4** and **AlO_6**
- The connectivity of this units is both by the corners (majority) and by the edges (minority)
- The v-DOS present two bands. The low frecuency band is related to the inter-unit vibrations, and the high band to the intra-unit vibrations
- B = 193 GPa, the lower of all polymorph
- The e-DOS is similar to the one of the crystalline γ-Al_2O_3, with a gap of 2.9 eV

Mechanical properties copper: atomistic simulation

(work in progress)

N. Amigo, GG, M. Ignat

(in the framework of IM2-U. Chile project:
M. Ignat, A. Valencia, G. Gutiérrez, S. Davis)

Copper Project

Determinación de Propiedades Mecánicas de Productos de Cobre

CODELCO
Orgullo de Todos

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

Marzo 2012

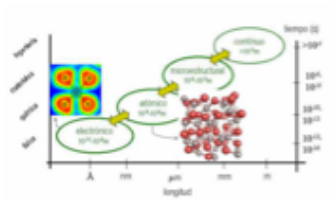
Miguel Ignat: Análisis propiedades mecánicas

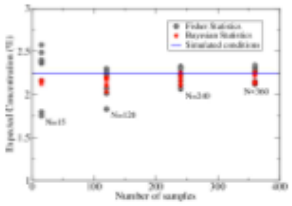
- Docteur Ingenieur (1977), Docteur en-Sciences (1983)

Álvaro Valencia: Análisis Termodinámico

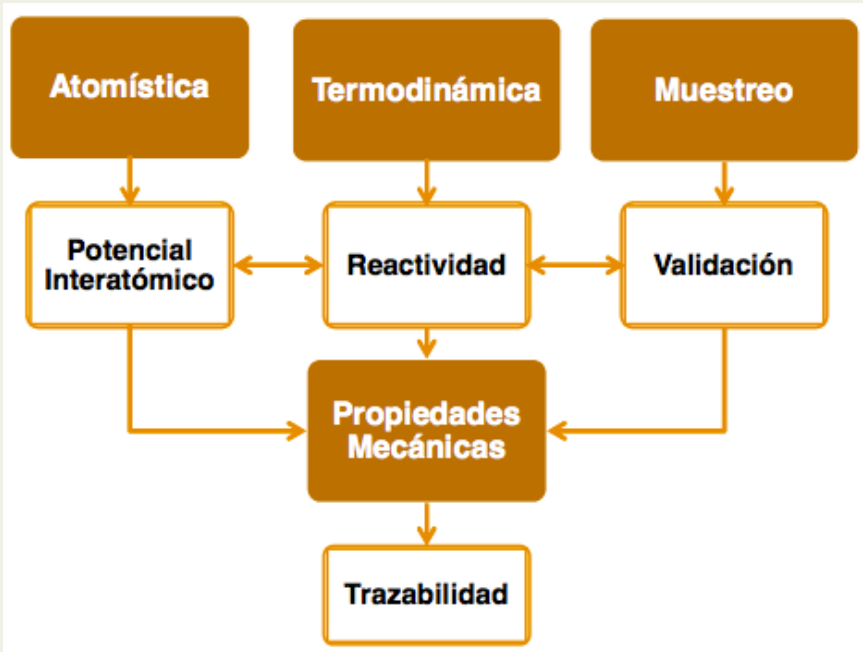
- Dr-Ing. Ruhr-Universität Bochum, Alemania, 1993.

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

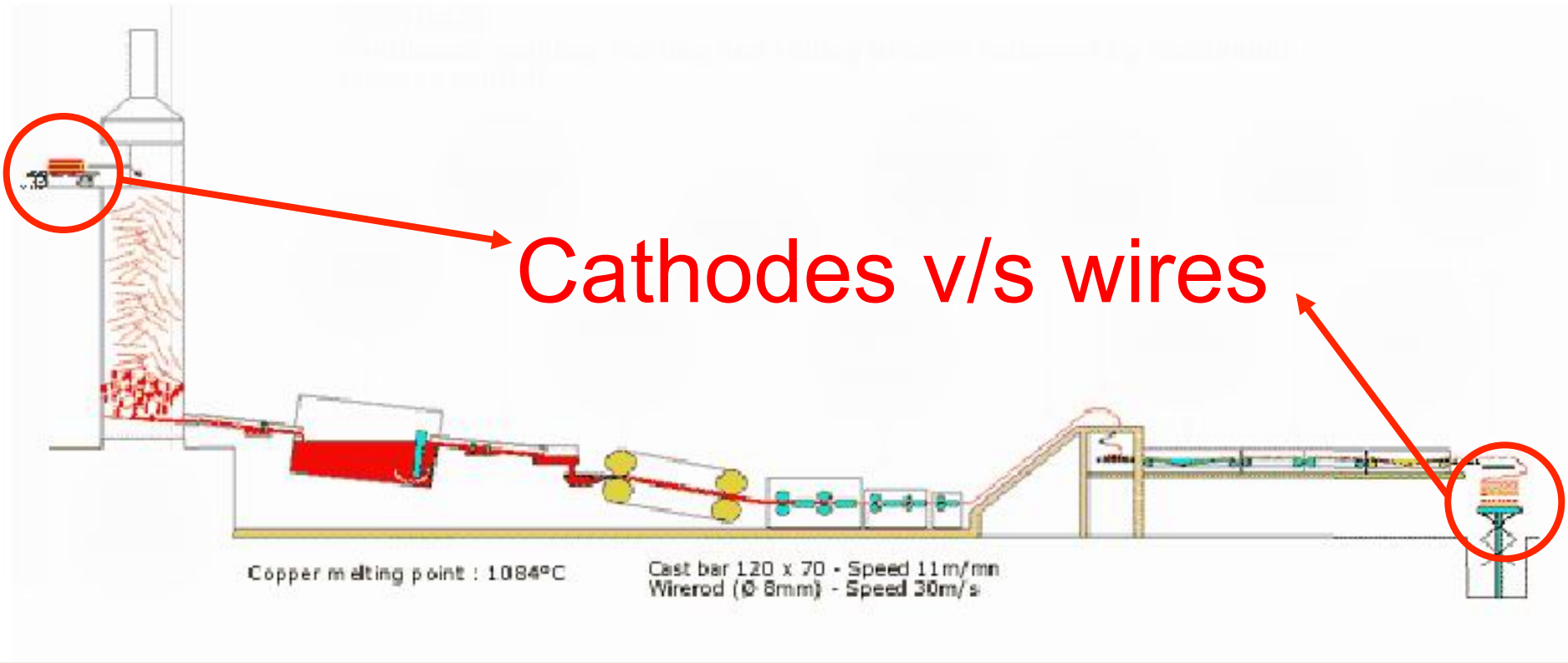




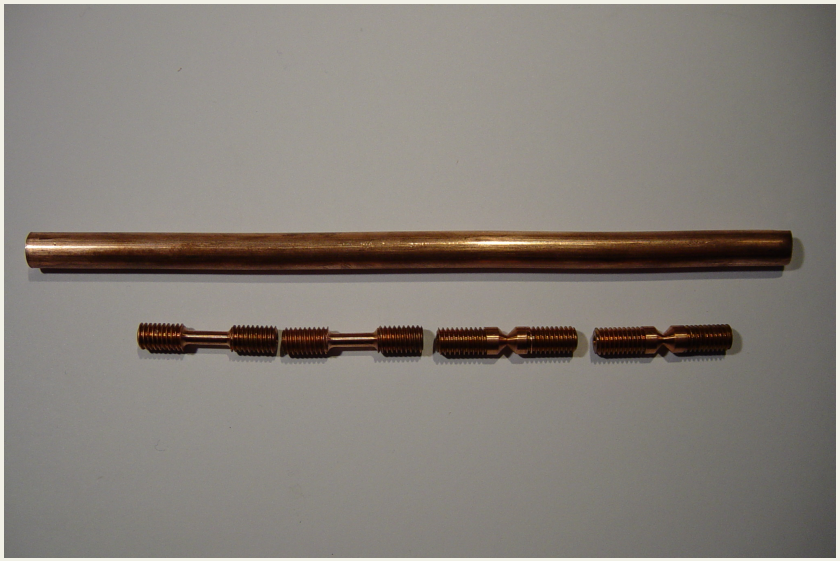
- Sergio Davis: Estadística de Muestreo
  - Ph.D in Applied Material Physics, Royal Institute of Technology (KTH), Estocolmo, Suecia (Septiembre 2009)

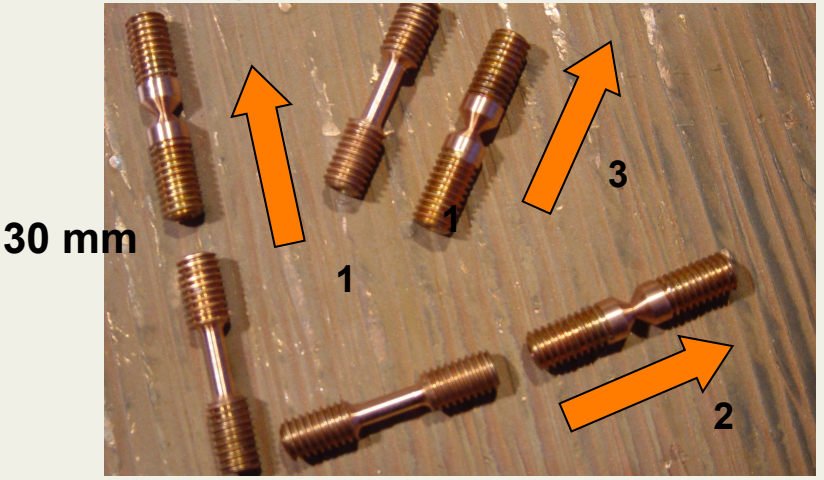


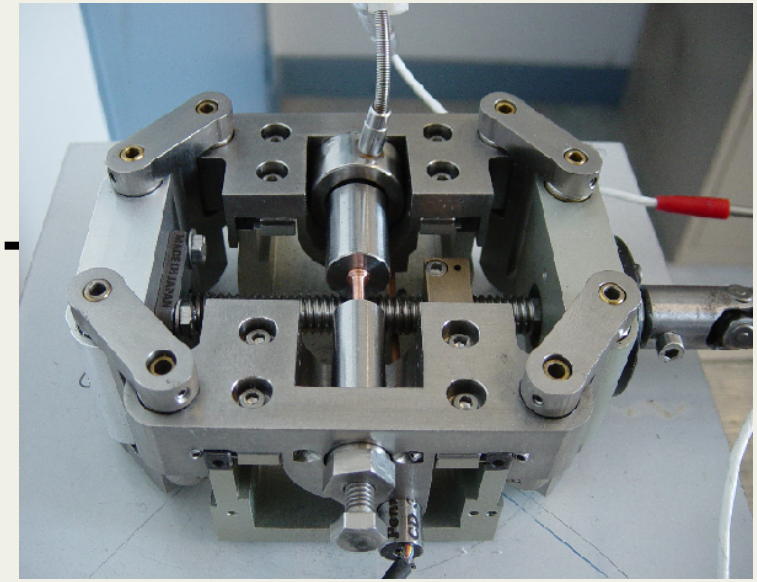
From Cathodes to wires



Experiments: M. Ignat + Alice Moya and Tomás Jil







mechanical test + analysis →effects of impurities

Tensile test: stress-strain curves

- Ley de Hollomon

$$\sigma = k\epsilon^n$$

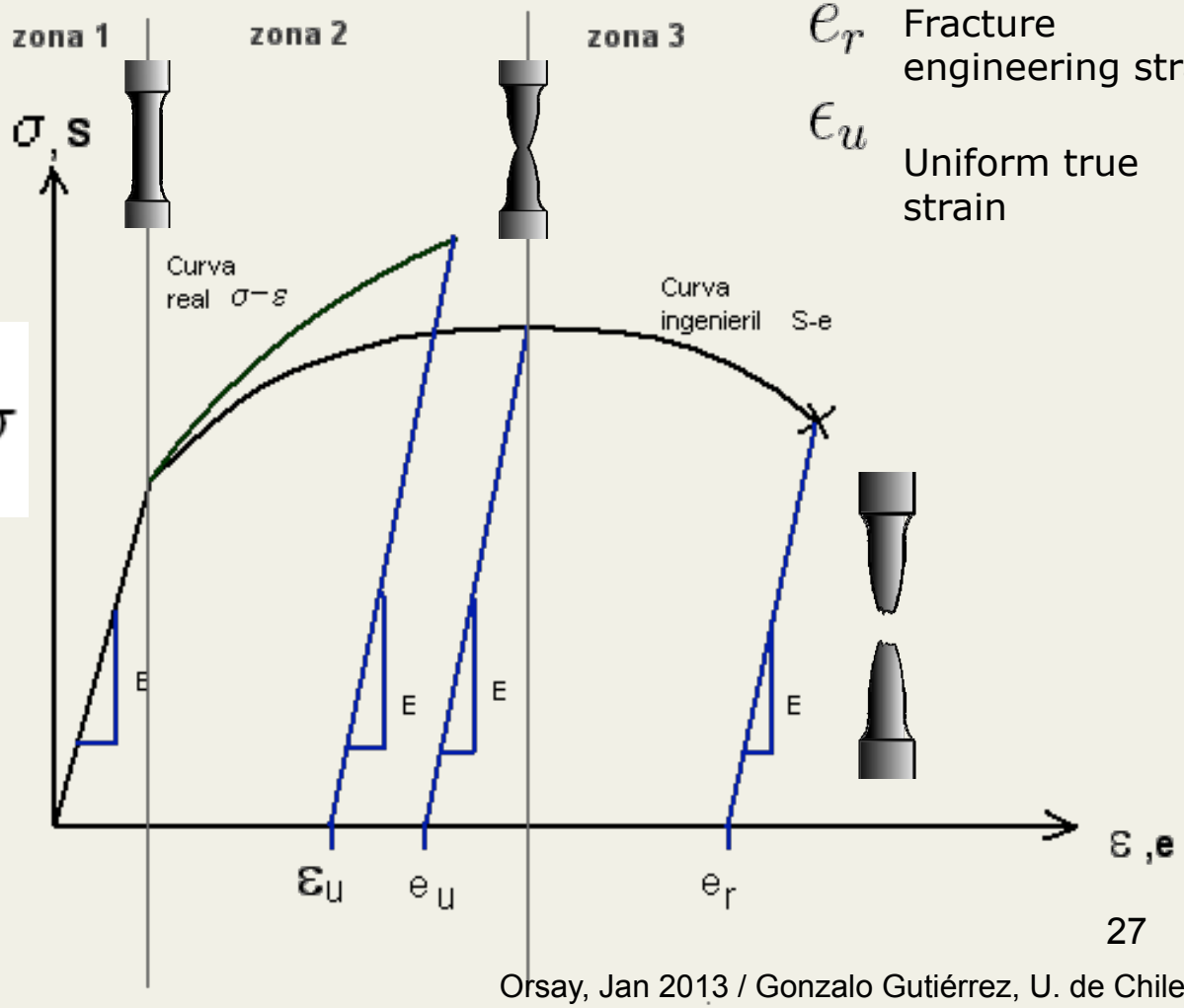
$$\frac{dS}{de} = 0 \Rightarrow \frac{d\sigma}{d\epsilon} = \sigma$$

$$\Rightarrow n = \epsilon$$

e_u Uniform engineering strain

e_r Fracture engineering strain

ϵ_u Uniform true strain



Atomistic simulation in Cu

Goal:

to study the effect of impurities in the mechanical behavior of copper, at an atomic level.

In particular Ag, As, Fe, Pb, S y Cu_2O

a) how does the strain-stress curve change due to impurities?

b) what are the relationship between mechanical properties, impurities and microstructure (grain boundary)?

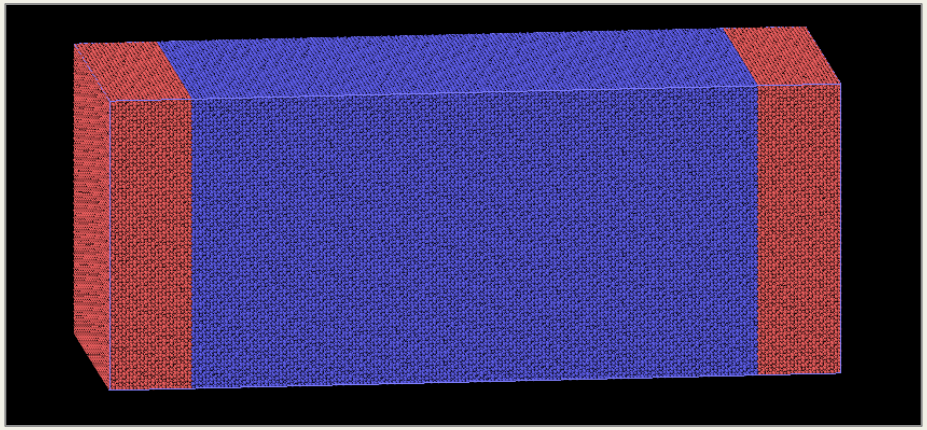
Methodology

Classical molecular dynamics
Interatomic potential: embedded atom (many body effect)
Programs: LAMMPS / LPMD (our own code)
Thousand and millions of particles

So far:
Elastic properties
Strain-stress curve
-monocrystal
-polycristal

Mono-crystal (T = 0 K)

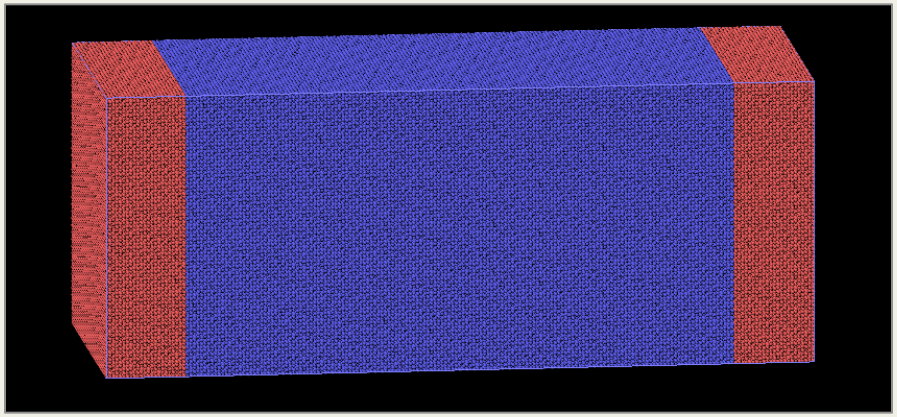
- 660 000 atoms
- 361 [Å] long
- 144 [Å] heigh and width

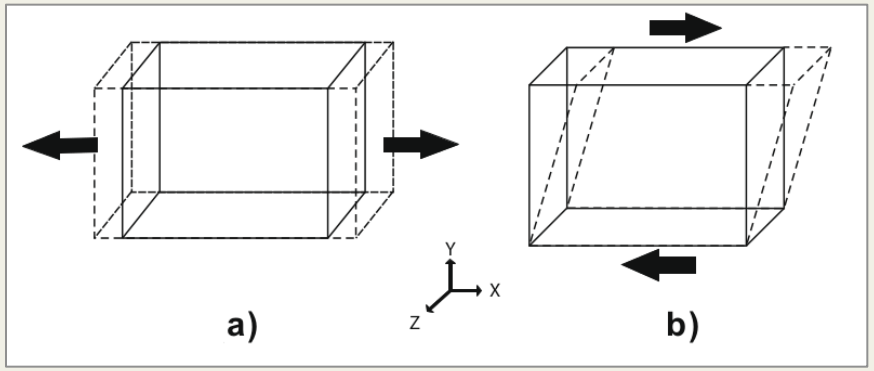


Elastic constants

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

(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))

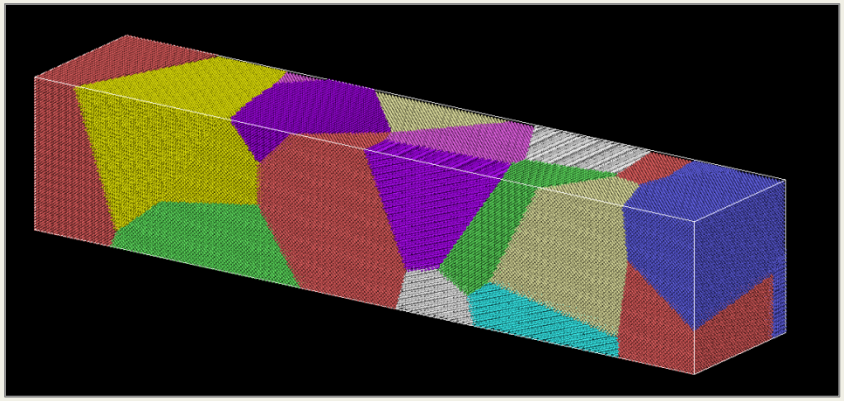


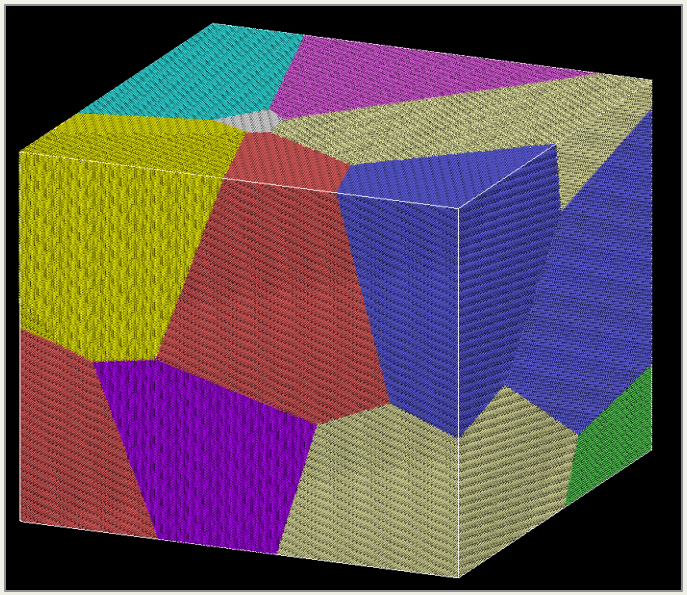


Constant	Exp [Gpa]	Simulation [Gpa]
C_{11}	176.2	171.0
C_{12}	125.0	126.3
C_{44}	82.0	79.9

Copper poly-crystals

- 1.3 million atoms
- 20 grains
- 722 [Å] long
- 140 [Å] h and w



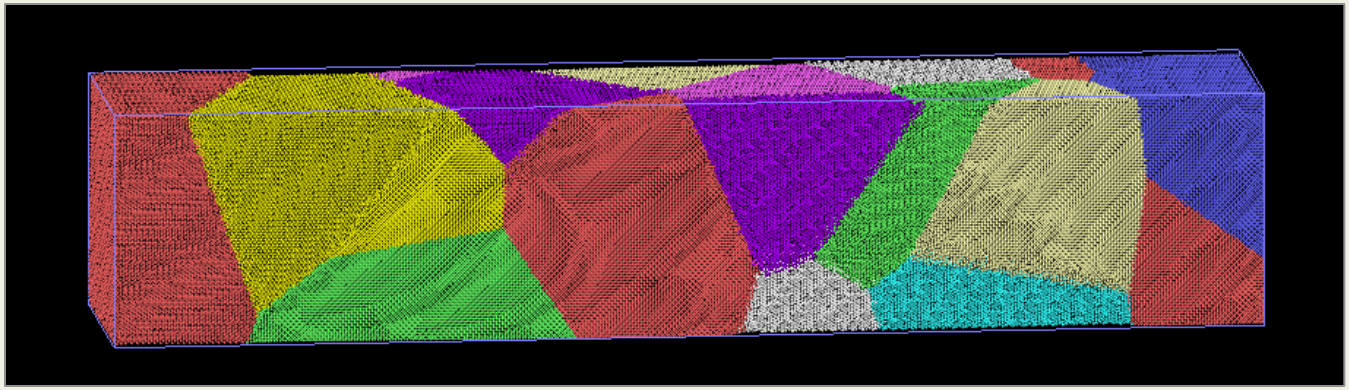


- 20 million
- 20 grains
- 614 [Å] edge

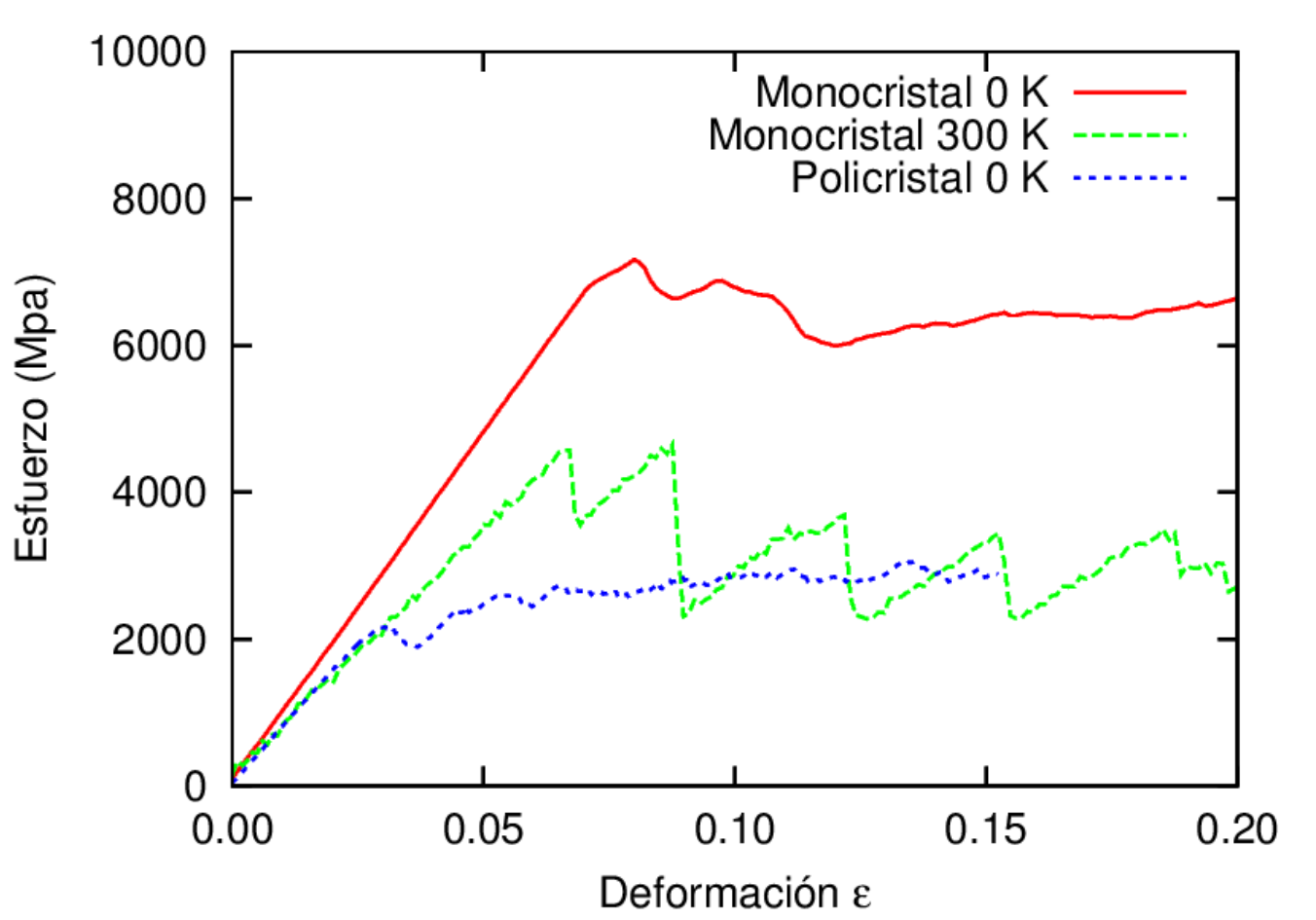
Poly-cristal

- 1.3 millones de atoms
- 20 grains (~10-15 nm diameter)

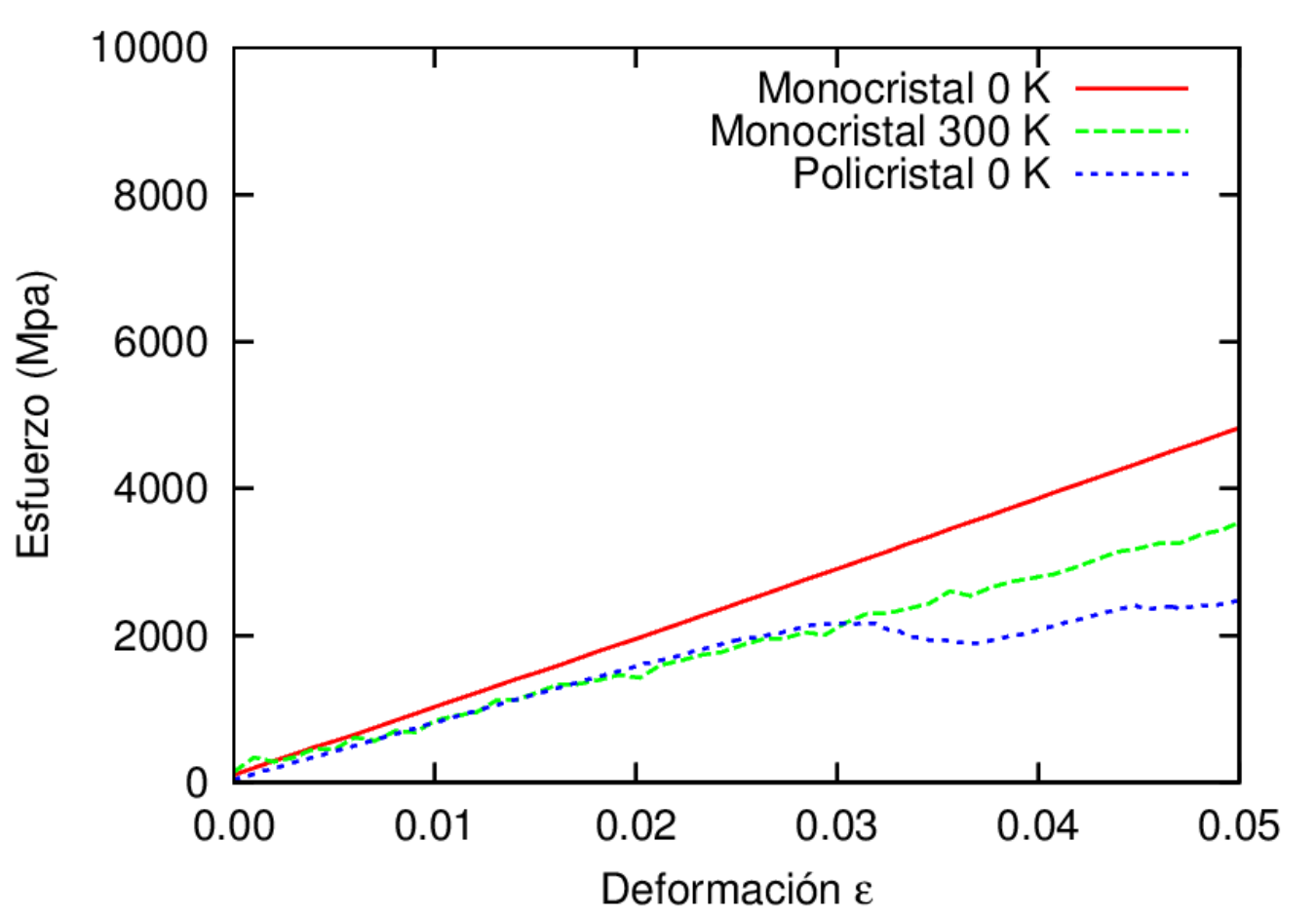
- 720 [Å] l
- 144 [Å] h and w



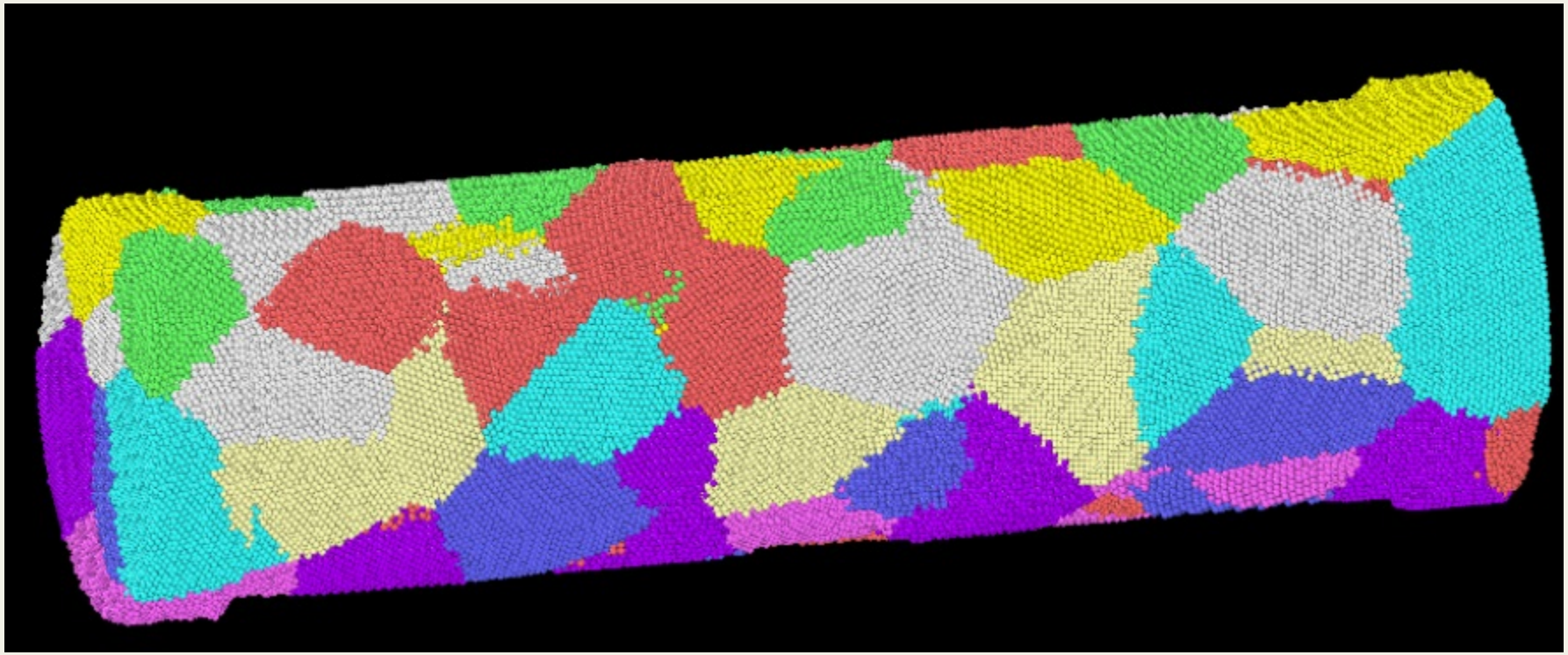
Strain-stress test



Zoom at small strain



Cu and Cu-Ag

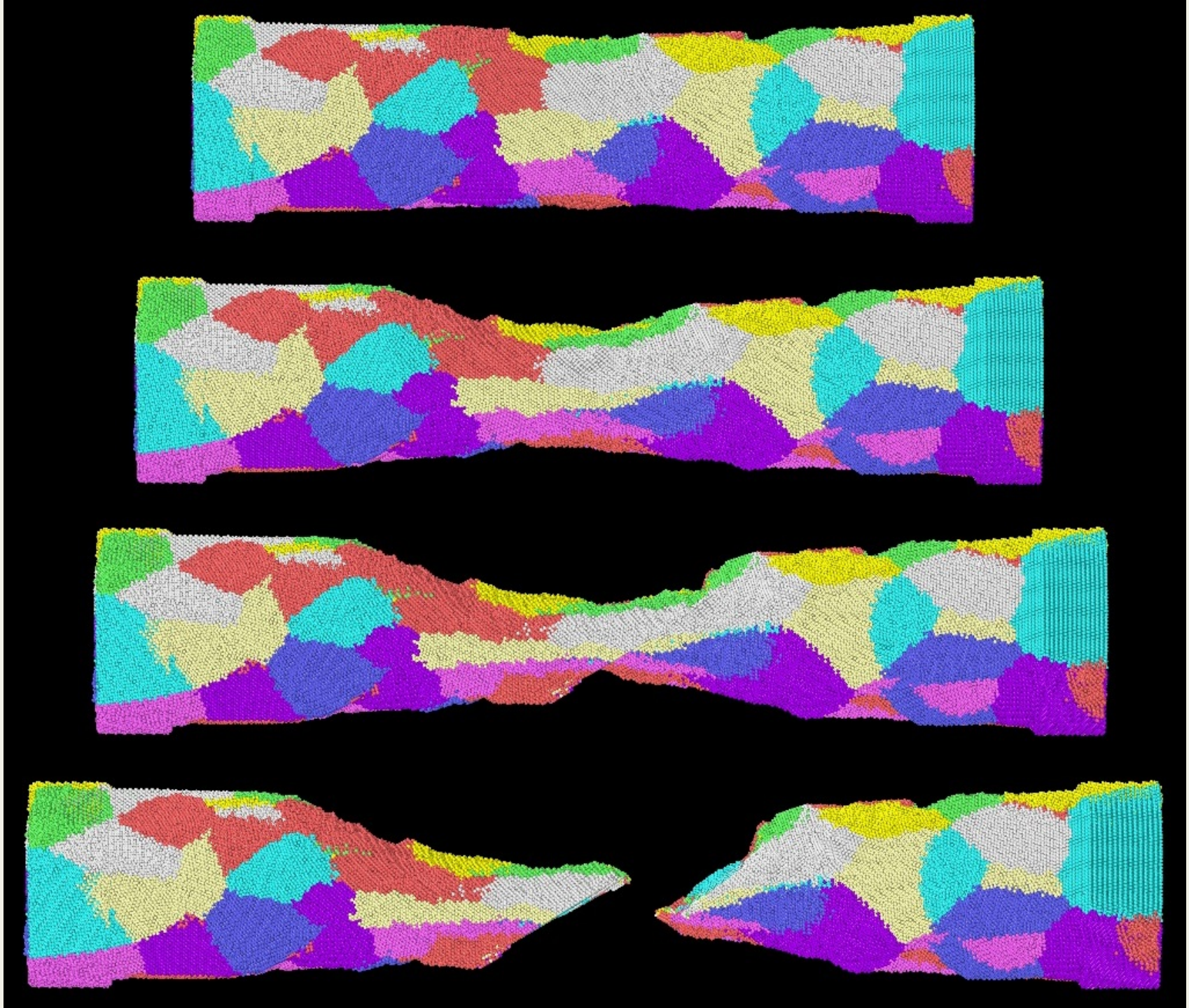


System 1: pure Cu

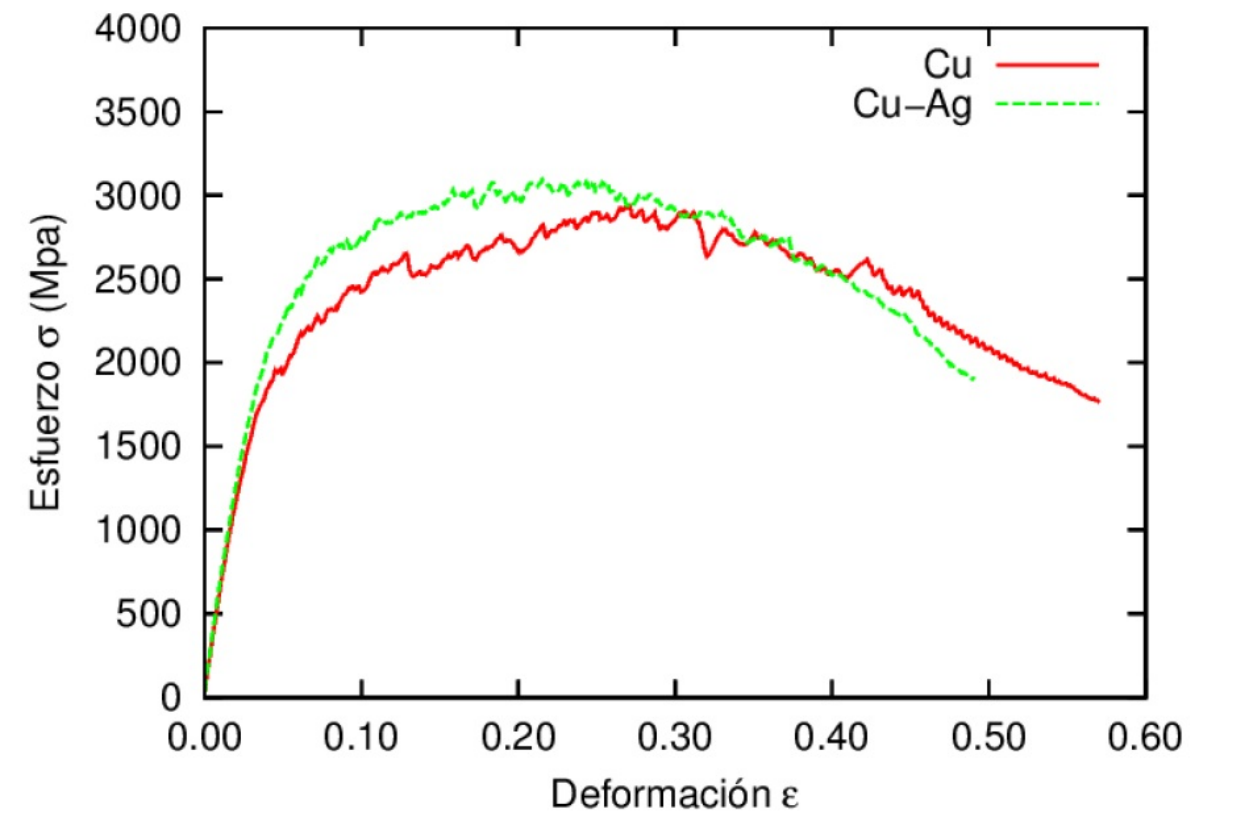
- Cu poly-crystalline cilindrical shape
- 125 grains
- 500 000 atoms approx.
- Long: 470 [Å] , radius: 65 [Å]

System 2: Cu-Ag

- same as system 1
- Ag interstitial impurities, at concetration of 1.64% (w/r to the total number of atoms)



Strain-stress curve



Composición	E [GPa]	σ_{elas}[MPa]	σ_{ult} [MPa]	σ_f[MPa]	ε_f
Cu	62.4	1292.7	2924.3	1740.3	0.57
Cu-Ag	67.4	1464.9	3081.4	1876.5	0.49

Conclusions (preliminary)

- The strength of poly-crystalline copper increases when Ag interstitials atoms are present

- the tensile strength also increases

- Ag impurities results in a decreases of ductility in Cu.