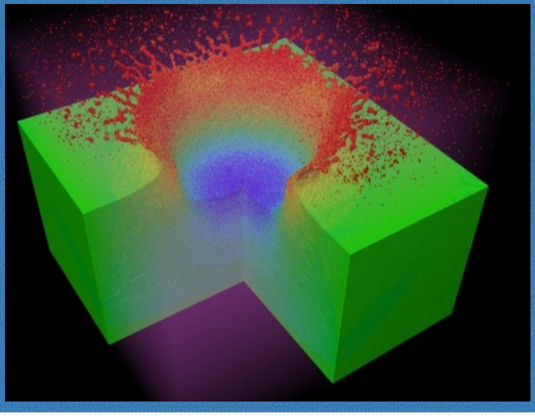
Introduction to Molecular Dynamics (MD) Simulations Part IIb: Advanced Applications



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https://sites.google.com/site/simafweb

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Agencia CyT, Argentina

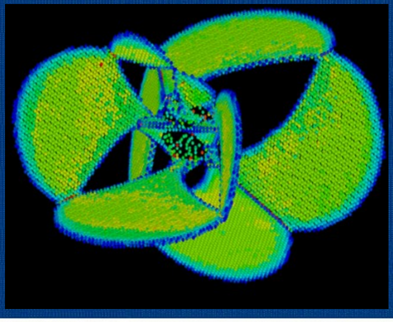
FING, U Mendoza

SIIP, UN Cuyo

Aplicaciones de simulaciones y programación CUDA: estudios a escala atómica, fenómenos climáticos y ópticos

Centro de Investigaciones Hidráulicas e Hidrotécnicas (CIHH)

UTP, Panamá
September 2019



COLABORATIONS: C. Ruestes, E. Millan (UN Cuyo), **B. Planes, J. Grossi, A. Araguna, E. Aparicio, G. Mora,** E. Miranda **(U. Mendoza)**, N. Gunkelmann, C. Anders, H. Urbassek (TU Kaiserslautern), R. Gonzalez-Valdez (U. Mayor, Chile), F. Valencia, M. Kiwi, F. Munoz, E. Figueroa, S. Davis, G. Gutierrez (U. Chile), M.A. Meyers, Y. Tang, E. Hahn, S. Zhao, K. Olney, D. Benson (UCSD), B. Remington, J. H G. Moraawreliak, R. Rudd (LLNL), M. Ruda, G. Bertolino (Instituto Balseiro, Argentina), A. Stukowski (TU Darmstadt, Germany), P. Erhart (Chalmers U., Sweden), A. Higginbotham, J. Wark (University of Oxford, UK), R. Gonzales, A. Rivera, A. Prada (UP Madrid), S. Ramos, E. Crespo (U. Comahue), J. Kohanoff (QUB, N. Ireland).

SiMAF

Two questions …

SiMAF

Given all the approximations and limitations involved …

- Can we hope for quantitative agreement between classical MD and experiments when electronic effects are important?

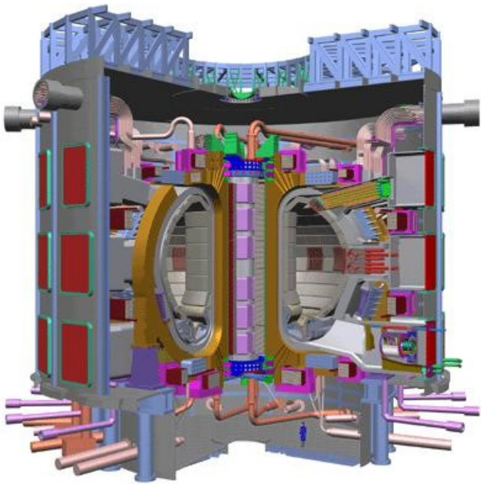
OR …

- Is classical MD just pretty movies and pictures?

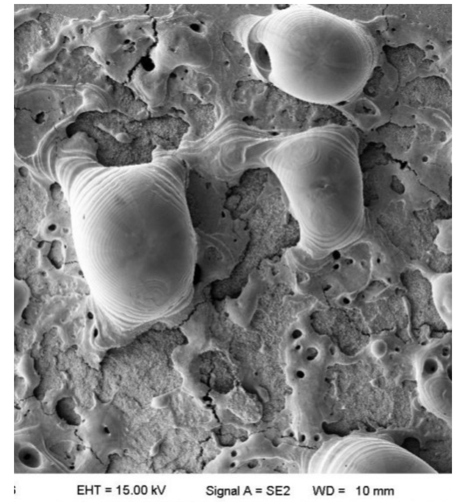
Materials for future fusion reactors: need to understand nanostructures

P. Piaggi (I. Sabato), R. Pasianot (CAC), R. Arrabal, N. Gordillo (UPM, Spain)

Clean, sustainable energy!

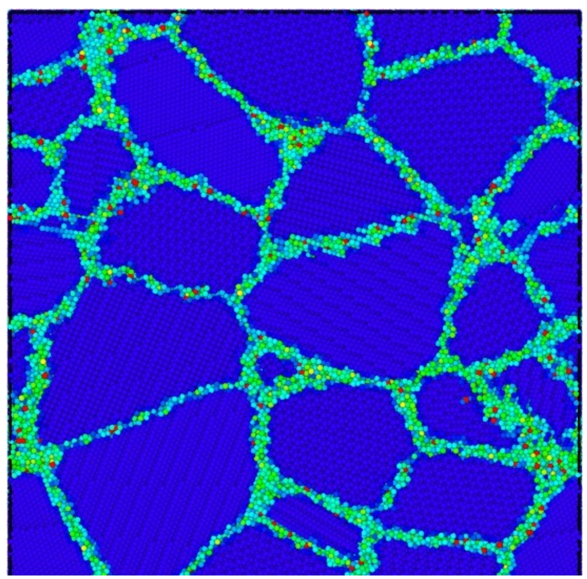


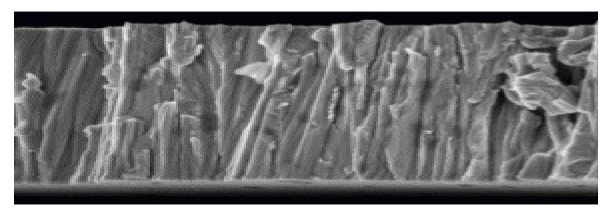
Need to find new materials for harsh environment

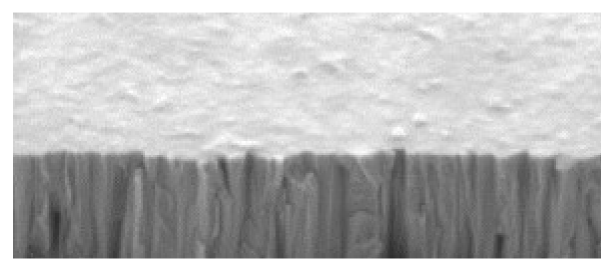


Nano-W displays better mechanical properties and radiation resistance than coarse-grained W.

Any phase transitions near GBs? WCH precipitates?

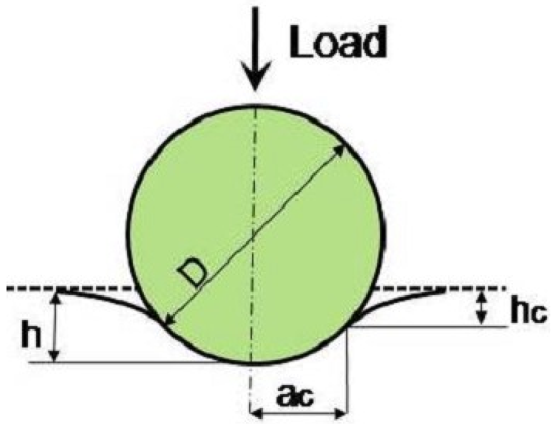






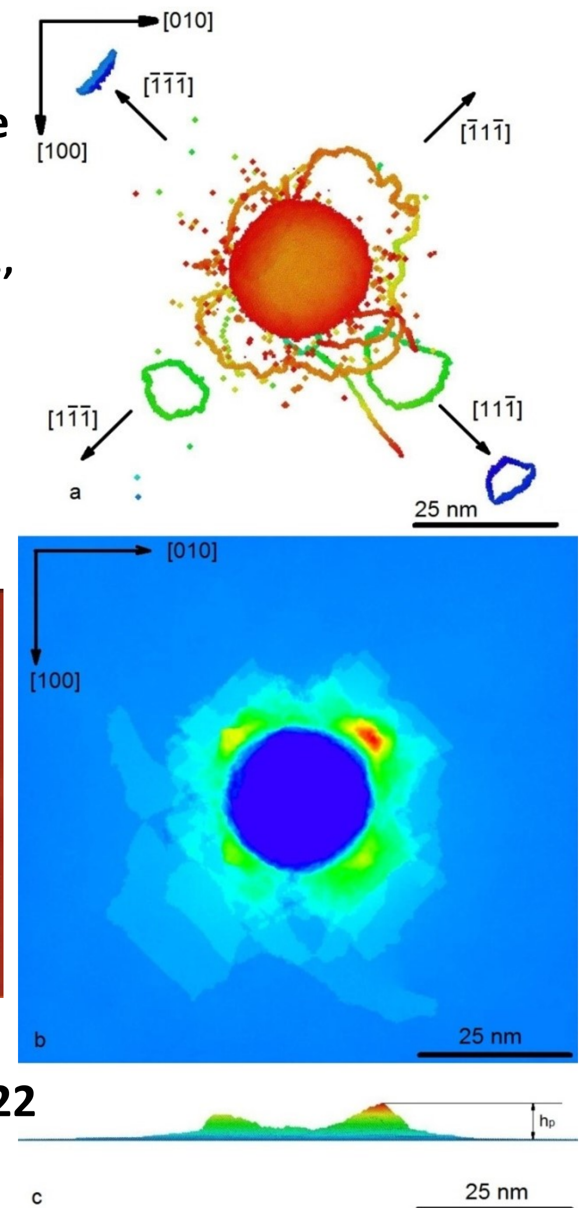
Nanoindentation: mechanical properties and nanoscale surface modification

collisions against surface at 3-30 m/s

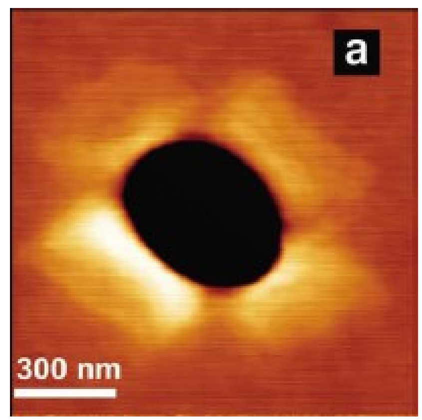


Dislocations determine surface features

Remington, Ruestes, *et al.*, Acta Mat. (2014) Comp. Mat. Sci. (2015)



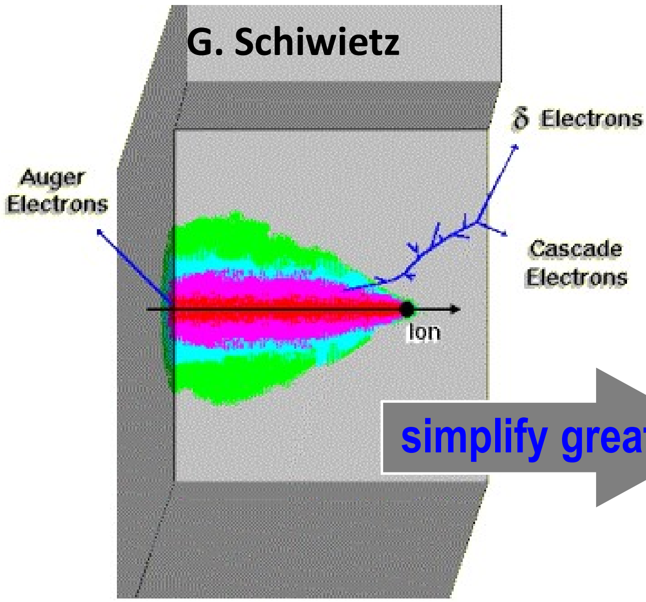
Ta: simulations (UNCuyo) and experiments (UCSD)



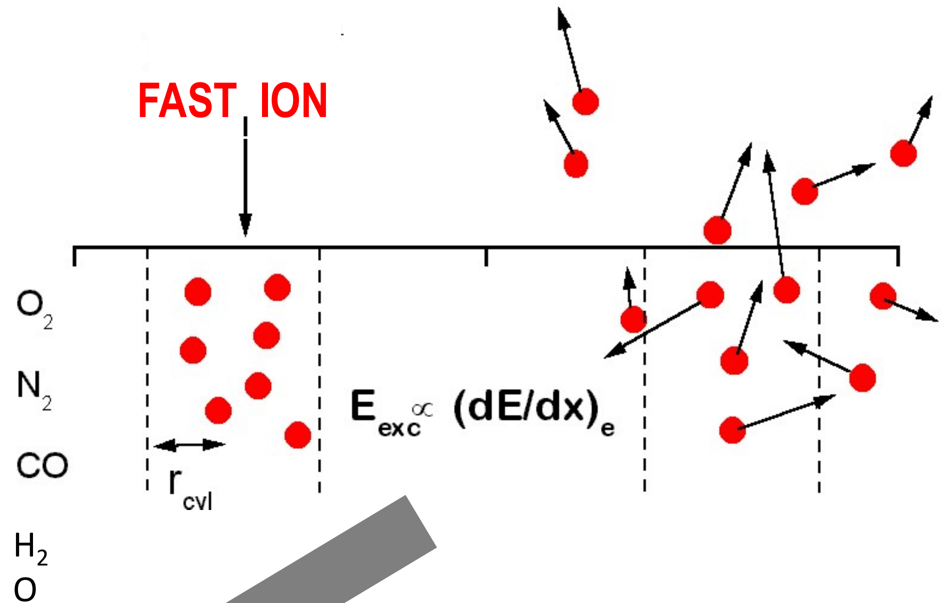
Biener *et al.* PRB 76 (2007) 165422

Better than approximate hardness from elastic constants

Radiation damage caused by fast ions
→ Ion track evolution and modeling



simplify greatly



Many "analytic" models

Coulomb Explosion

Thermal Spikes (many flavors)

Fleisher, Price and Walker, J. App. Phys. 36, 3645 (1965)

Trautmann, Klaumunzer and Trinkaus, Phys. Rev. Lett. 85, 3648 (2000)

MORE ....

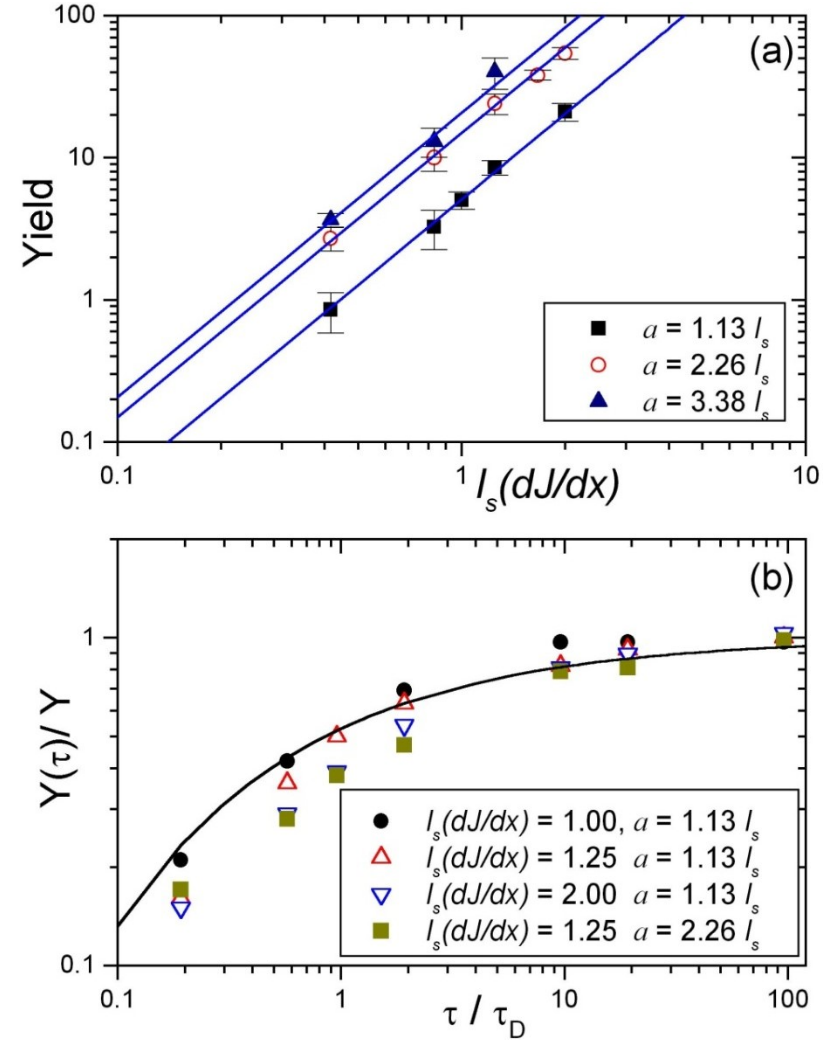
but MD is better

MD can predict experimental results

tracks [Devanatham *et al.*, NIMB (2008)]

sputtering [Bringa and Johnson, PRL 88, 165501, (2002)]

Coulomb explosion leads to heating of the lattice as in TS



$Y \sim (dJ/dx)^2 \, ln(a)$

Bringa and Johnson, PRL **88**, 165501 (2002)

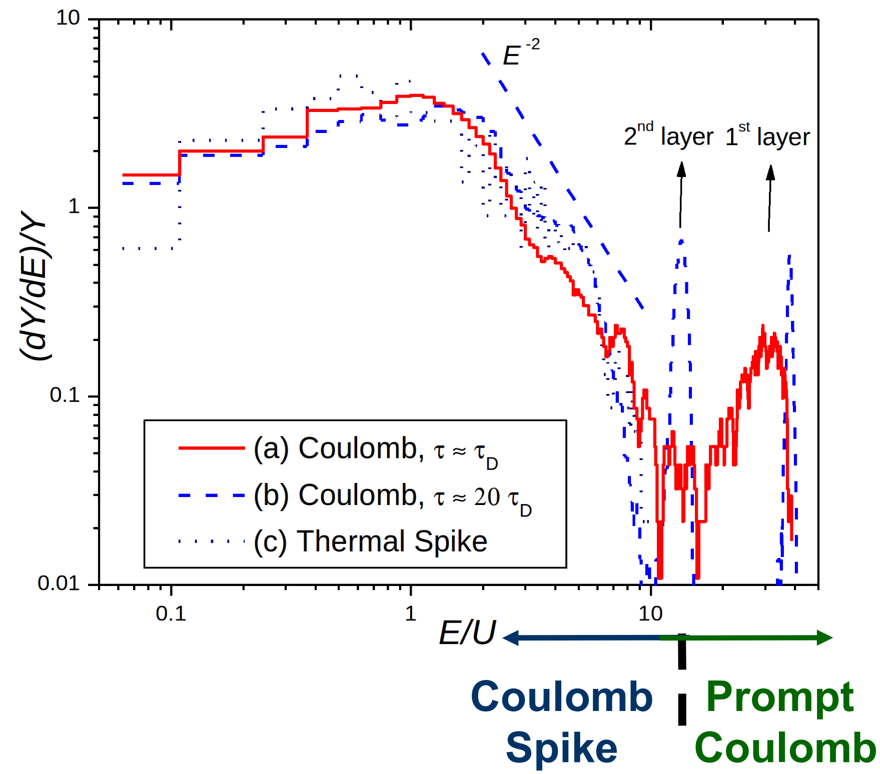
Is there a thermal spike (TS)? YES!

Analyzing MD data, there is a clearly defined energetic track with:

1) $(dE/dx)_{eff} = A\,(dJ/dx)^2$

2) r_{cyl} = Constant

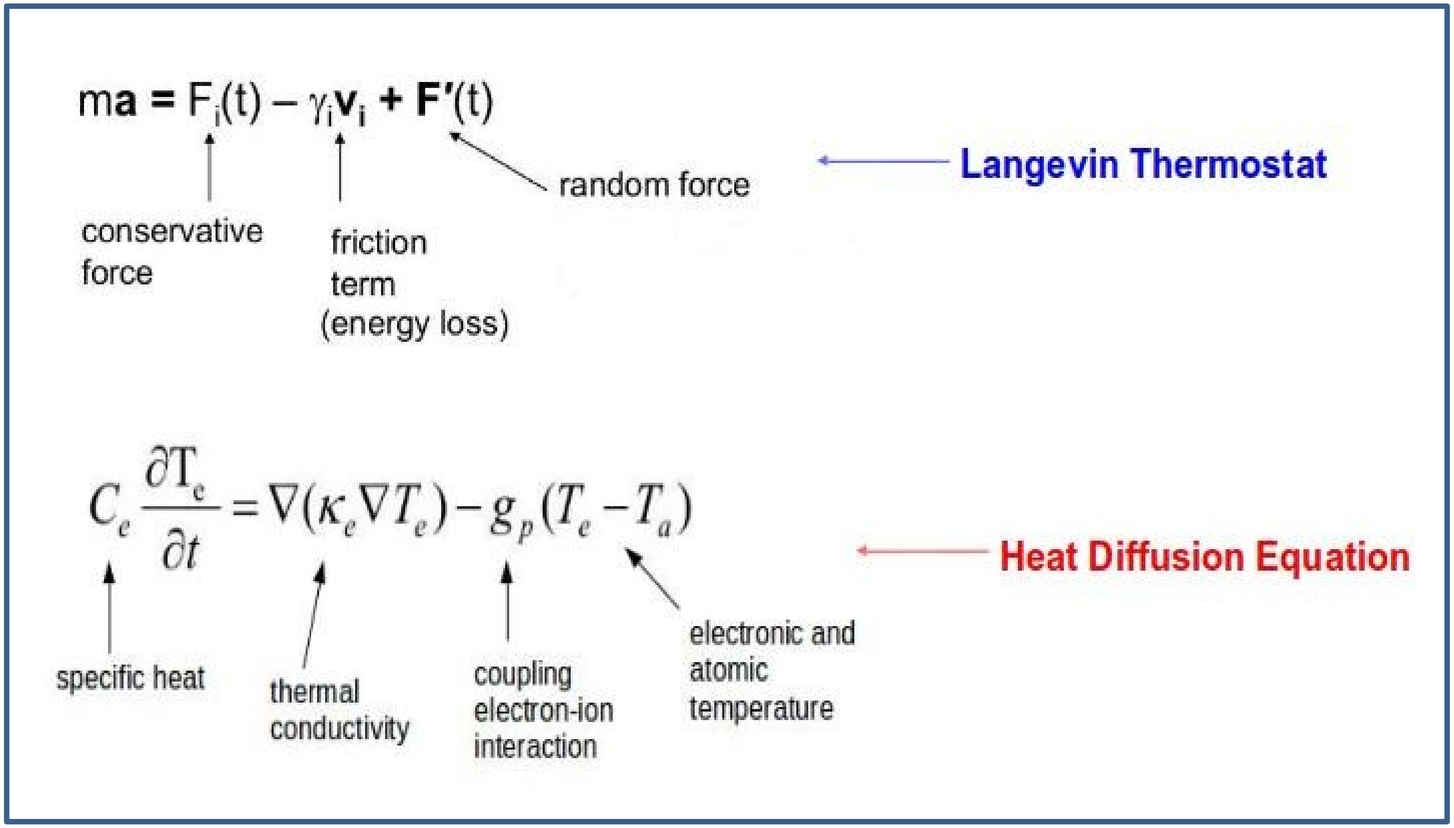
$\Rightarrow$ $Y_{MD\text{-}CE} = Y_{MD\text{-}TS}$



Two Temperature model (TTM) + MD

Electron-atom energy transfer is based on a local, inhomogeneous Langevin thermostat.

D.M. Duffy and A.M. Rutherford, J. Phys. Cond. Matter, 19 (2007)

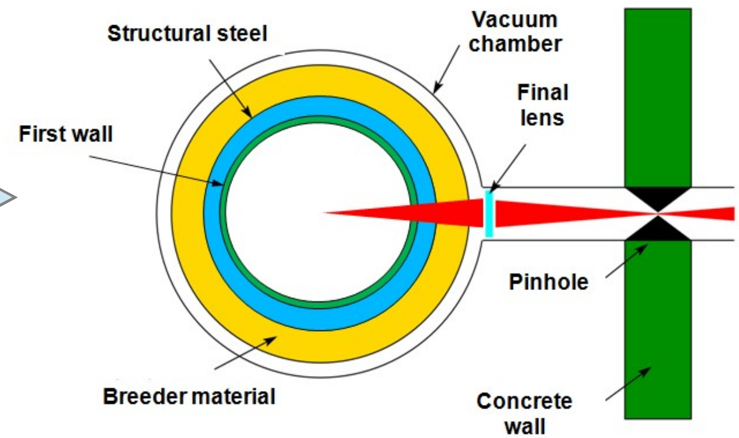


Unknown:
e-ph coupling and conductivity for nanostructures?

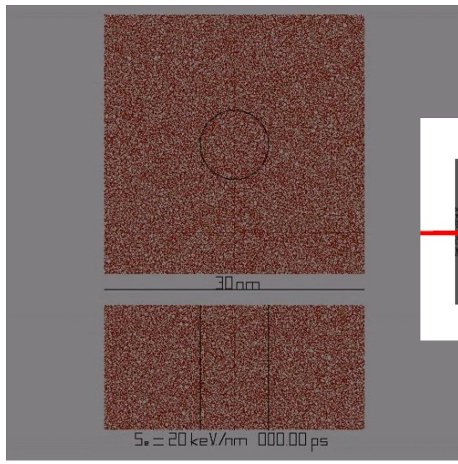
Several versions of TTM-MD (i.e. Tamm *et al.*, PRL 120, 185501 (2018)).

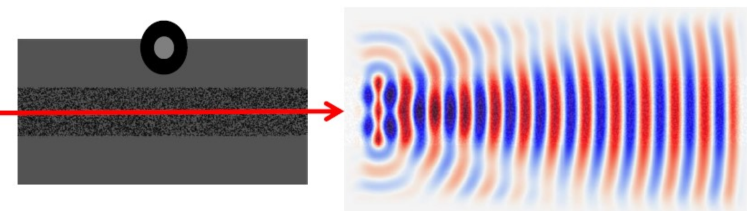
Tracks in oxides (mostly silica)
Silica: A → A phase transition

Energy production:
Fusion reactor lenses



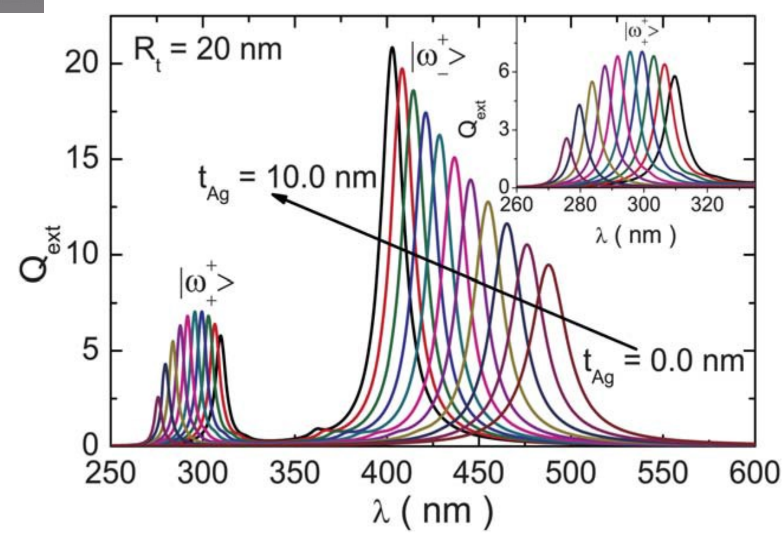
Electro-optical devices:
irradiation modifies
optical properties
(A. Prada-Valverde *et al.*,
Scientific Rep (2017))





(nano-guides)

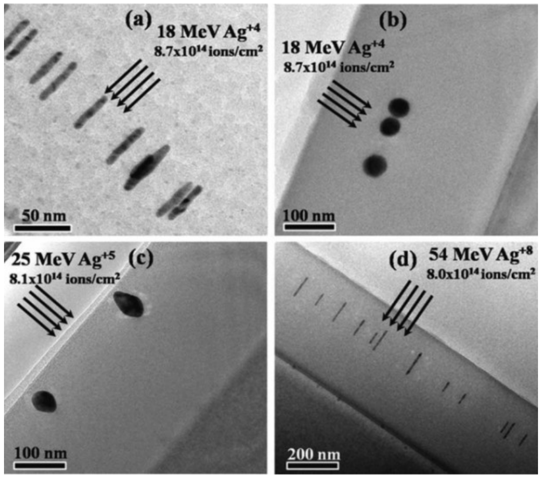
Nanoparticles (Au-Ag):
Tuning of optical properties
(O Pena *et al.*)



Collaboration with UP Madrid
Maherit, 100-1000 cores

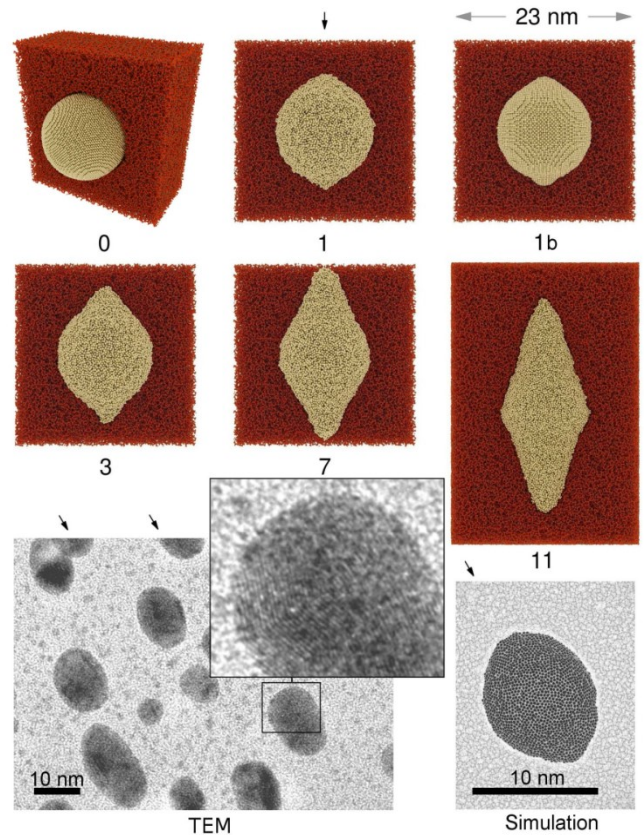
Swift Heavy Ion irradiation: NP shape control

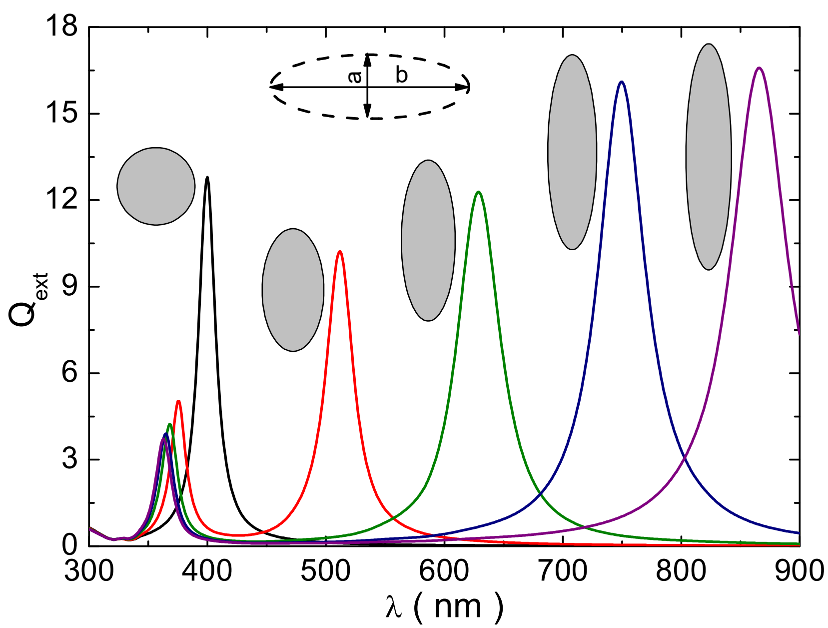
Phase transitions in nanoparticles? (e-ph coupling)



E.A. Dawl et al. ,
J. Appl. Phys. 105
(2009) 074305

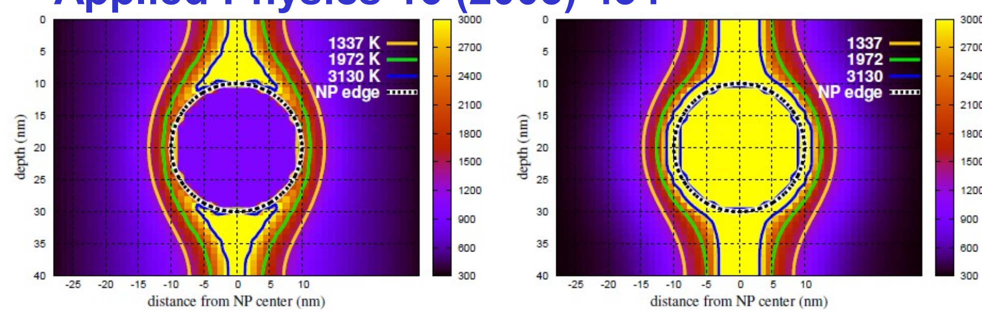
A.A.Leino et al.
Materials
Research Letters
(2013)





Shape-induced peak shift

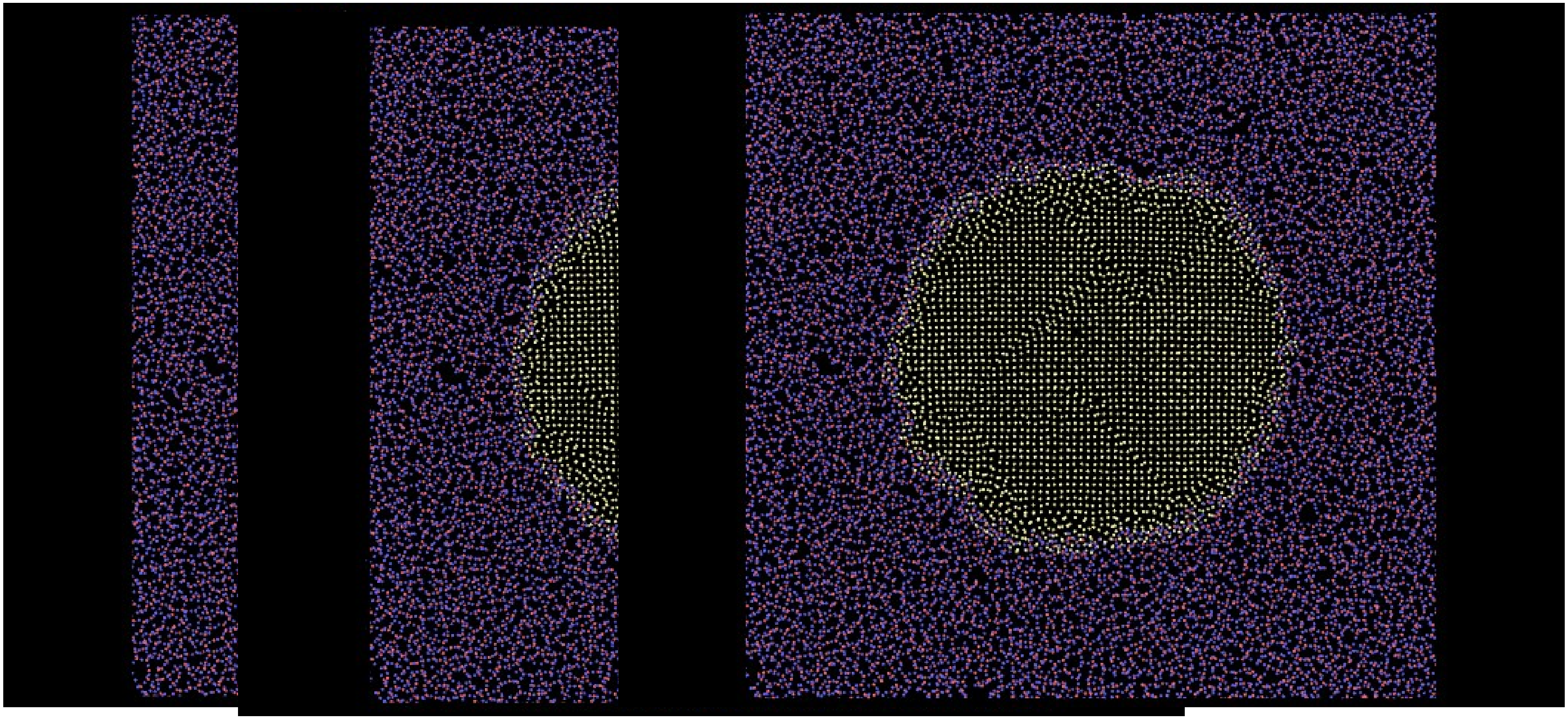
Ch Dufour et al. Journal of Physics D in Applied Physics 16 (2003) 434



Final configuration after structural relaxation and single track NP melting is lower than bulk melting (as expected)

How to add energy? Test several options, with lower T for Ag

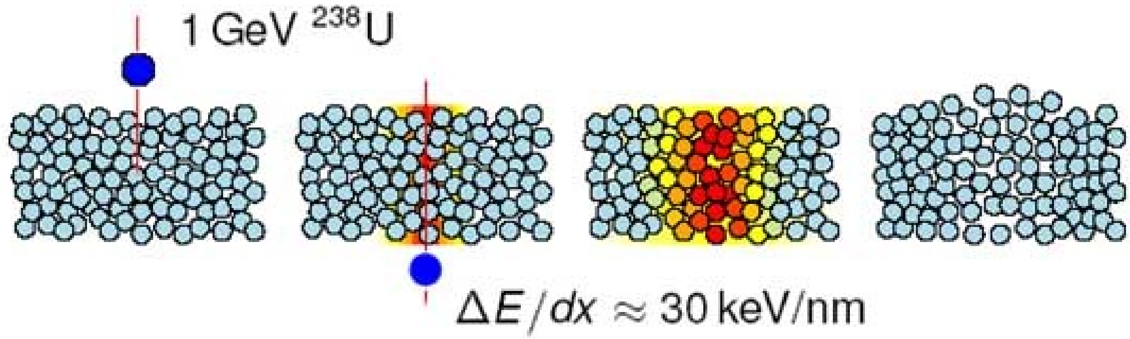
No elongation for single track, in agreement with experiments.
~4% elongation after 3 tracks (A. Prada, A. Rivera, O. Pena -UPM-)

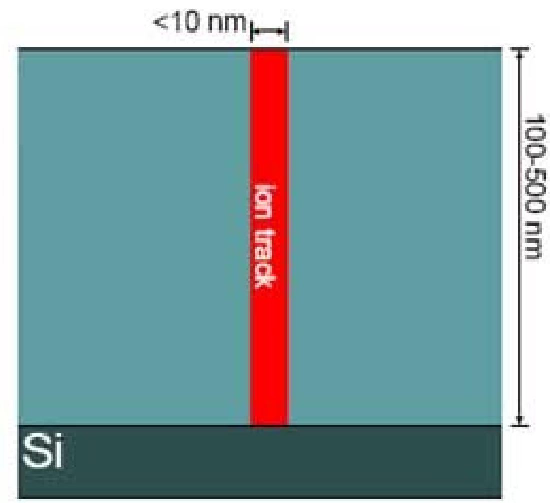


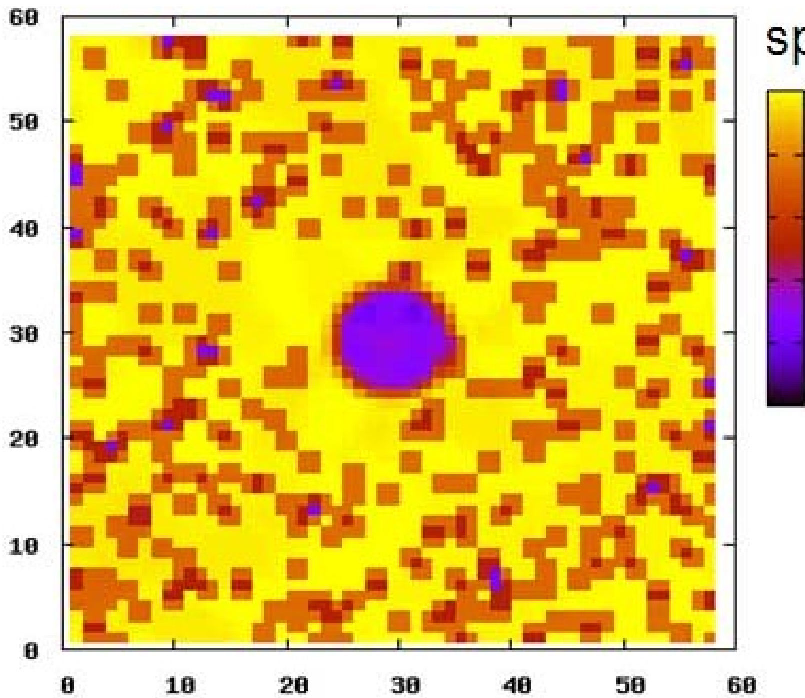
Scientific Reports (2017) x 2

Trazas ionicas en ta-C crean nano-alambres conductores
$sp^3 \rightarrow sp^2$ phase transition

ta-C = tetrahedral amorphous C = diamond-like C = dlC

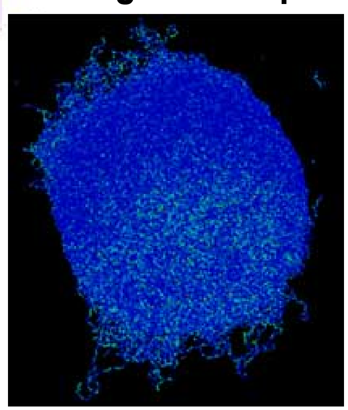


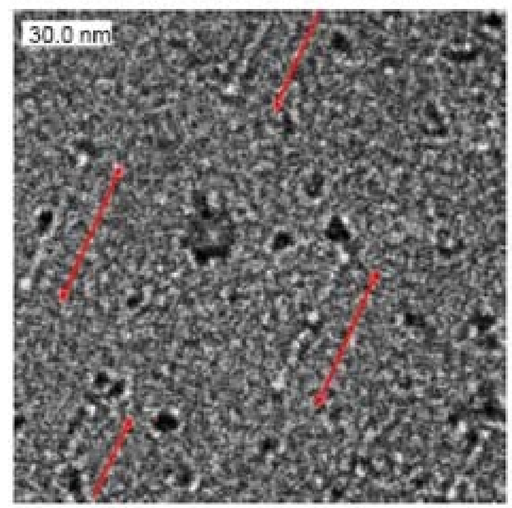




Schwen & Bringa, NIMB 2007

Simulaciones y experimentos muestran creacion de region rica en ligaduras sp^2

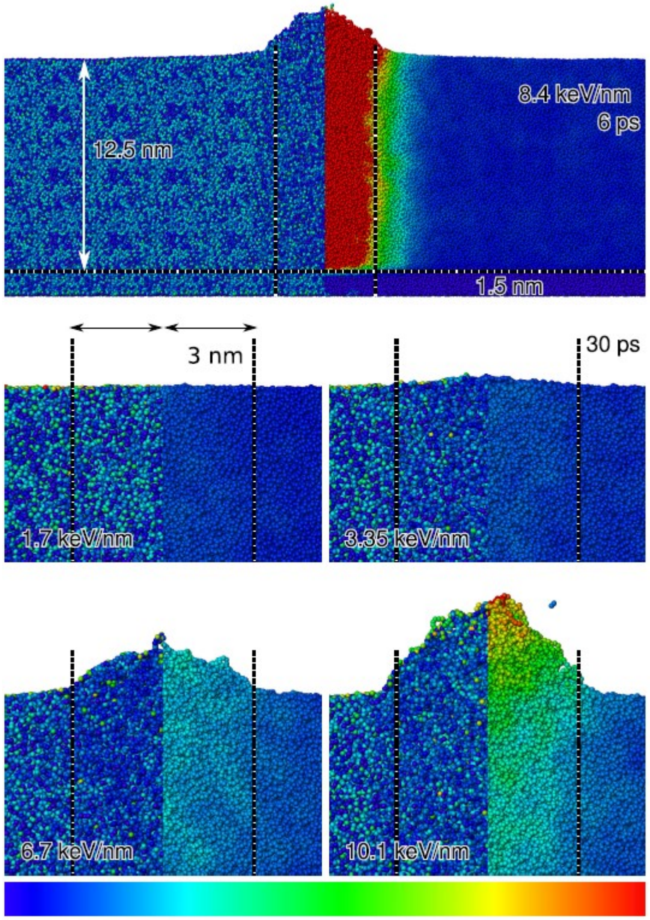


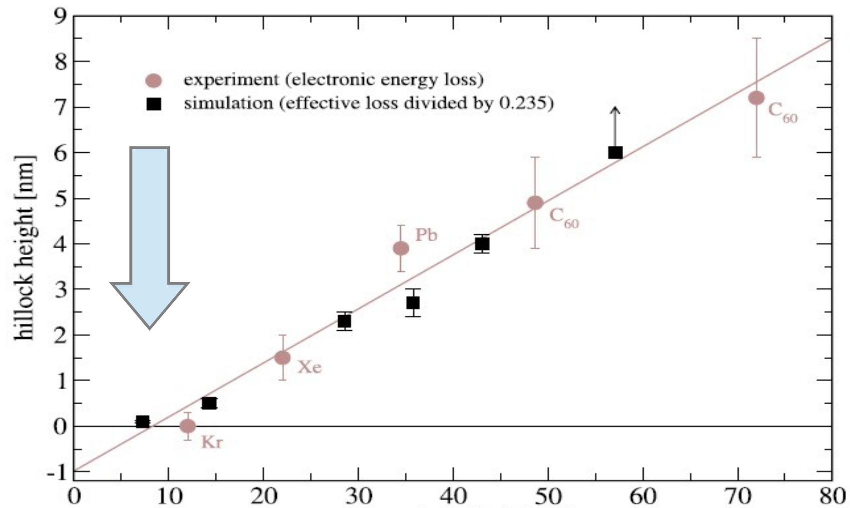


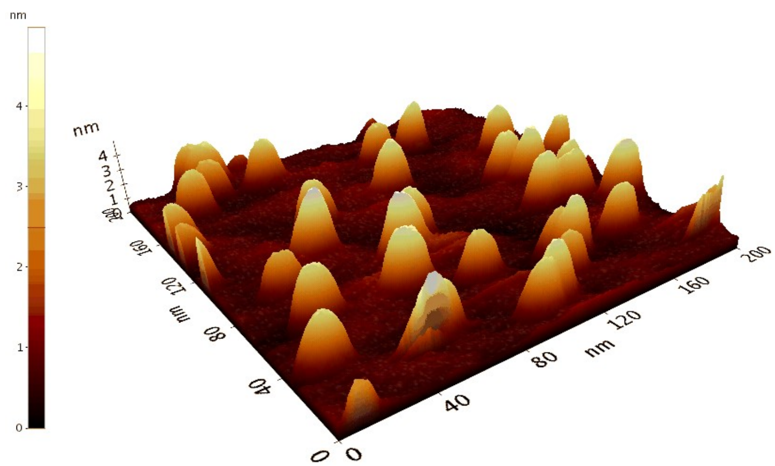
Cosmic ray destroying a carbon grain

Nanostructuring in dIC by ion irradiation: phase transition leads to hillocks

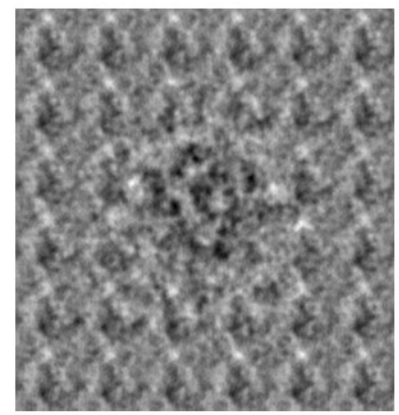
SiMAF







Sim. Defocus 3.6

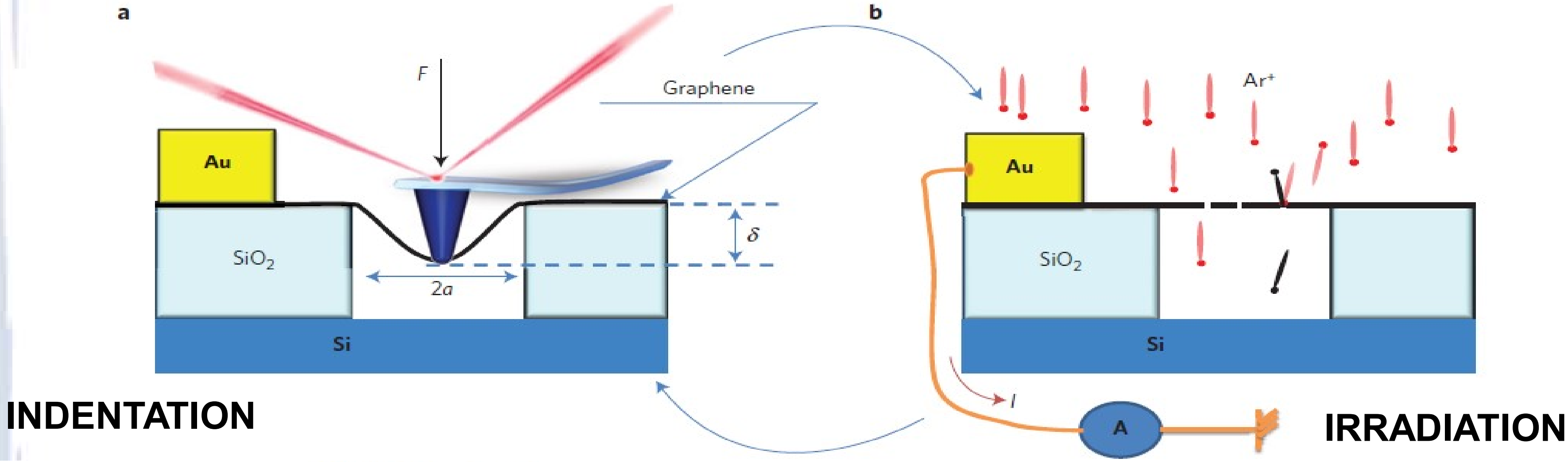


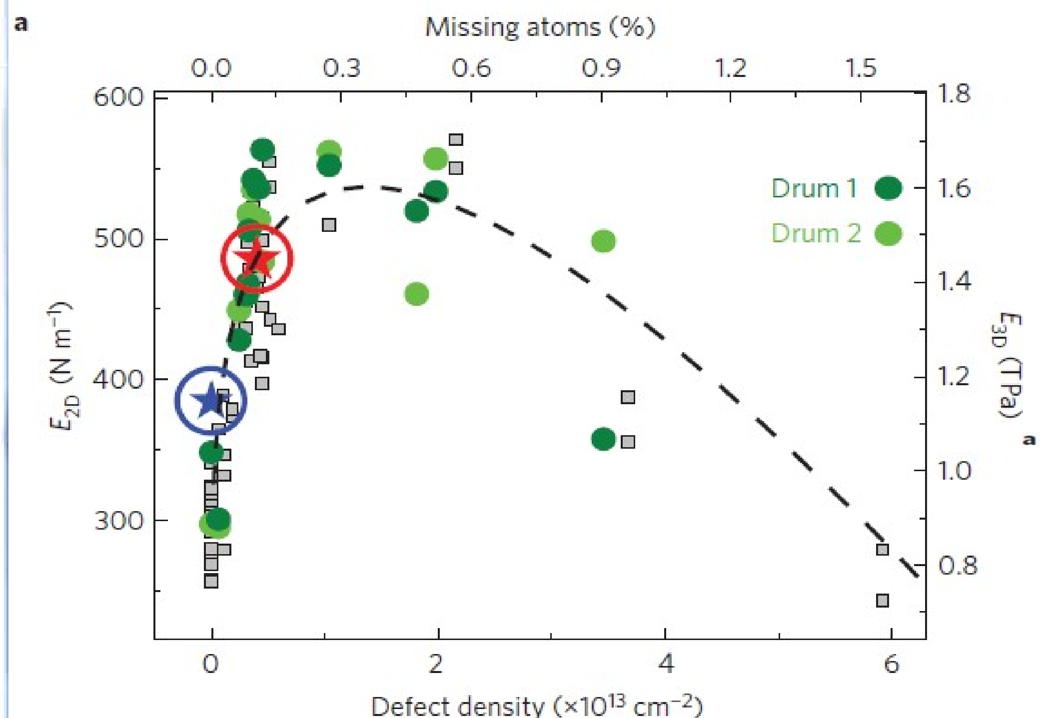
ICB/LANL/GSI

Schwen *et al*., APL **101**, 113115 (2012): thermal spike can explain experiments

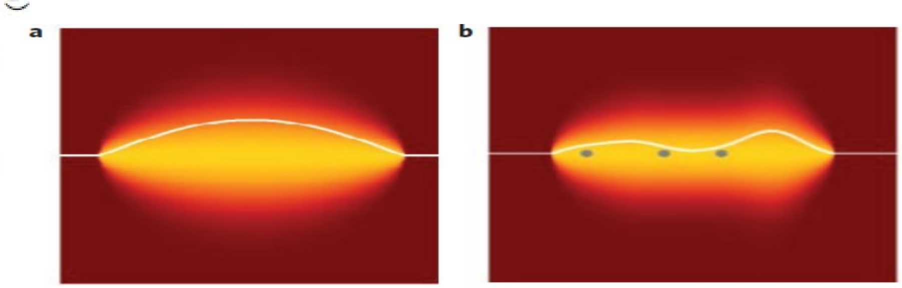
+10 keV/nm to form hillocks. "Effective energy" dE/dx ~0.2 $(dE/dx)_{exp}$

Experiments: irradiation of graphene by 140 eV Ar ions





Graphene stiffness DOUBLES at very low defect content (~0.2%). **Possible explanation**: phonon localization leads to roughness, which increases effective elastic modulus.



Lopez-Polin *et al*, Nature Phys. **11**, 26 (2015)

Graphene irradiation and nanoindentation

Lopez Asencio, Ruestes, *et al.*, PCCP (2016)

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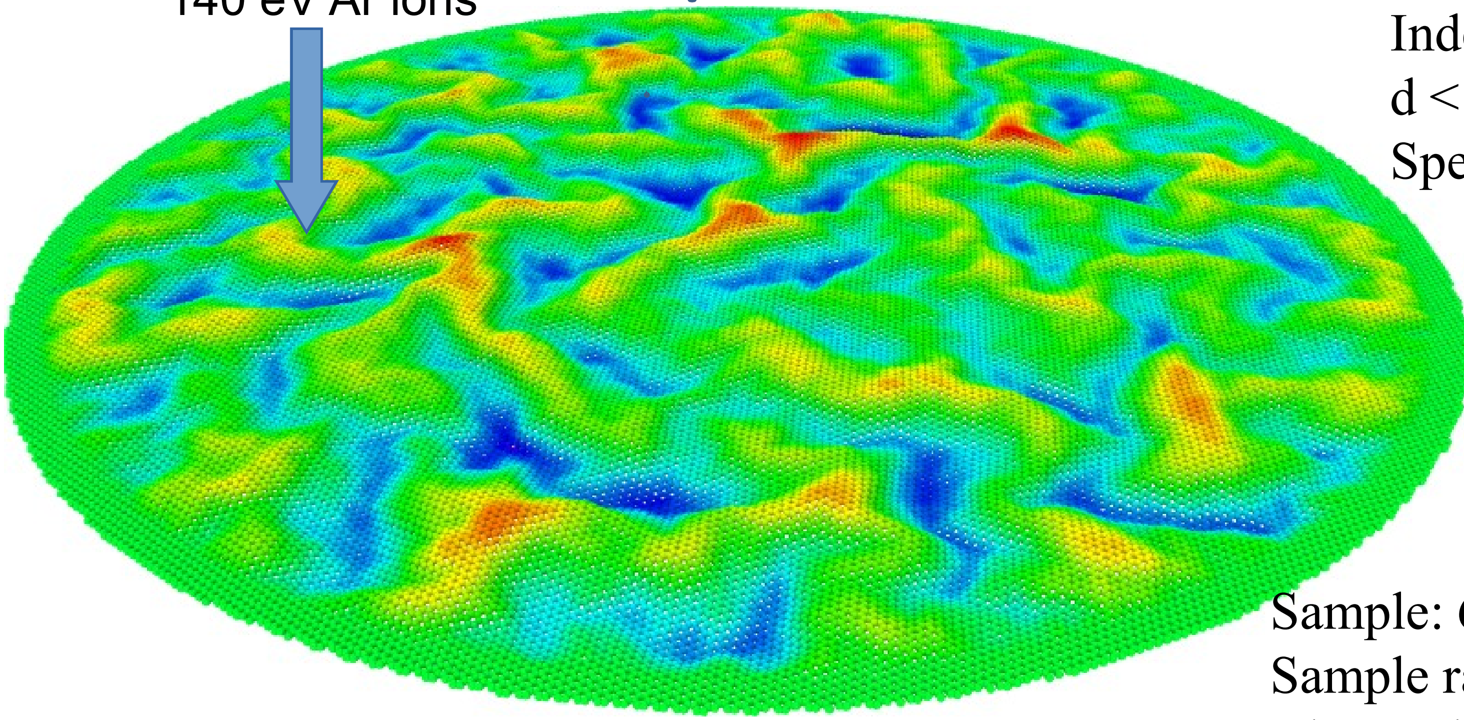
140 eV Ar ions



Indenter: 10 nm radius

d < 5 nm

Speed 5 m/s

Sample: 674644 C atoms

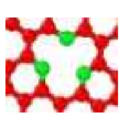
Sample radius a=75 nm

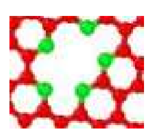
Clamped boundary conditons

Tersoff/ZBL interactions

Irradiation

MonoV DiV TriV 4+V





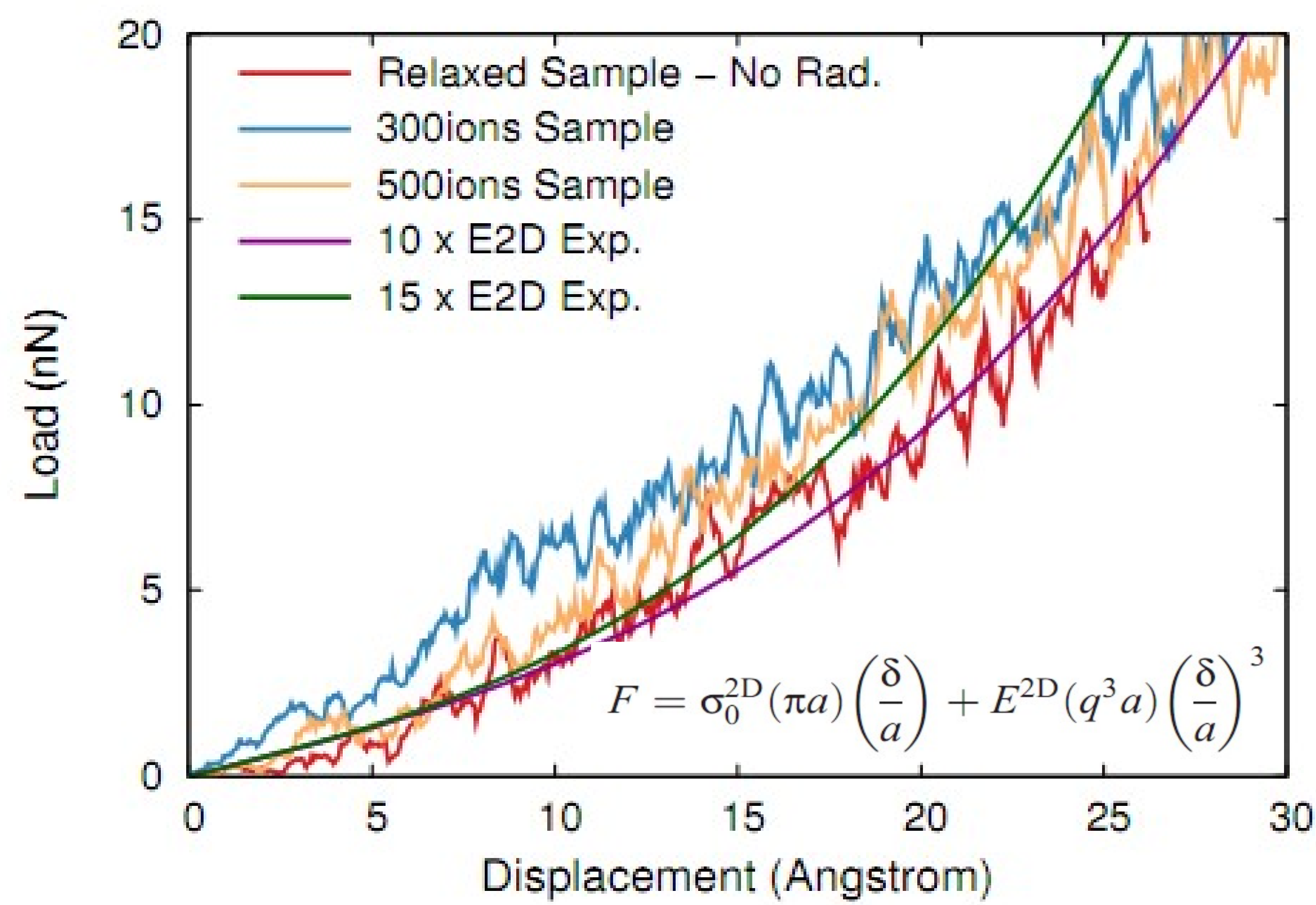
Coordination number:

Green → 2 , Red → 3

Irradiation produces mostly single vacancies, in agreeent with experiments

Simulated nanoindentation: is the elastic modulus increasing with dose at low dose?

SiMAF

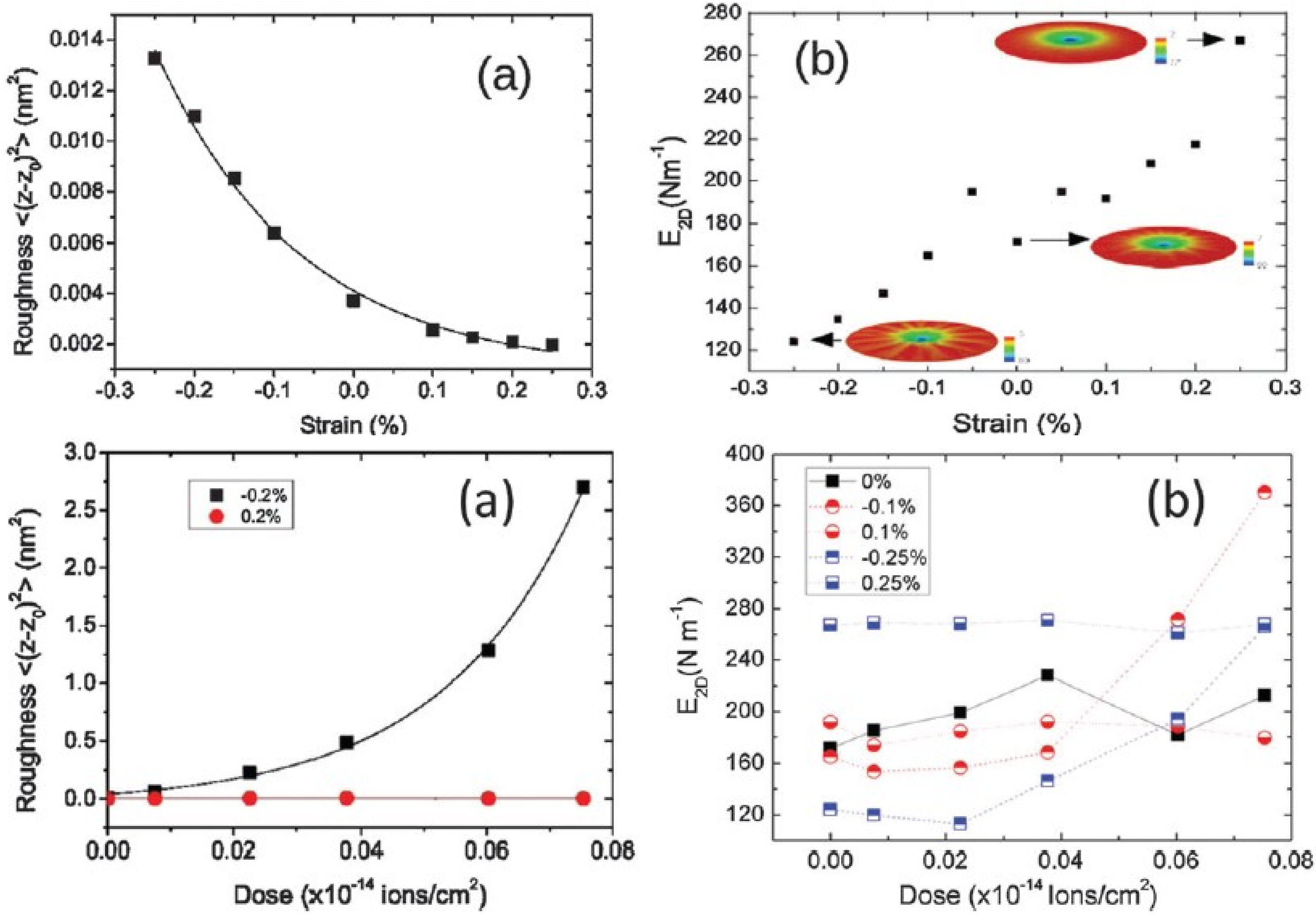


No clear evidence for modulus increase...

Are there any simulation details which make comparison with the experiment impossible?
Test sistem size, indentation rate, temperature, etc.

Newly published simulations using quasistatic indentation and small samples do observe modulus increase

Simulated nanoindentation: is the elastic modulus increasing with dose at low dose? PCCP (2016) NEED LARGE SAMPLES



Alternative explanation for modulus increase!

Nanocrystalline diamond coatings

- Biocompatible
- Excellent tribological properties
- Also used in sensors, water treatment, etc.

Diamond for head of heart pump

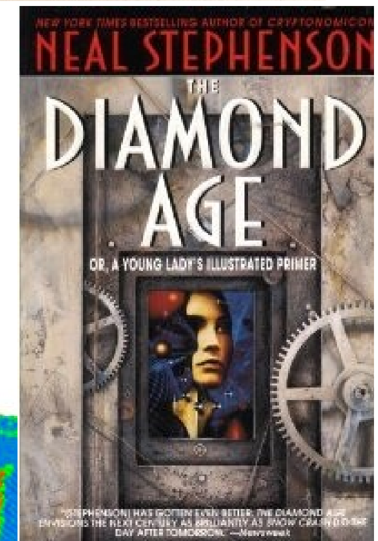
http://www.thindiamond.com/

What are we doing?

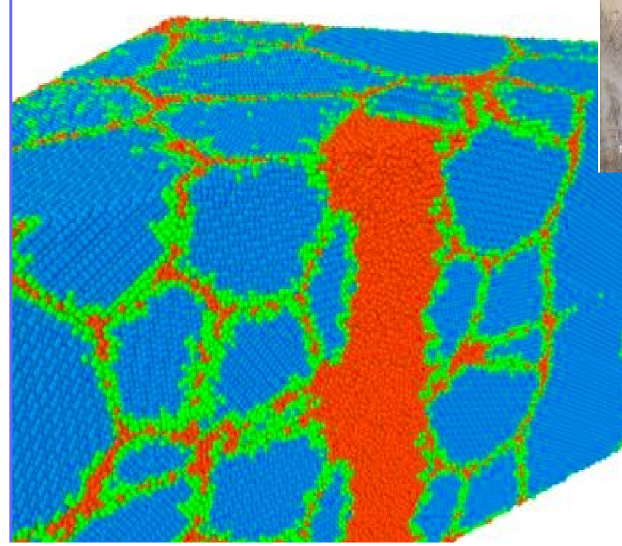
Study mechanical properties as function of grain size (R. Perriot, LANL, USA)

Study chemical and mechanical modifications by irradiation (M. Kiwi, R. Gonzalez, F. Valencia, U. Chile).

Compare with experiments (A. Rivera, R. Gonzalez-Arrabal, UP Madrid).

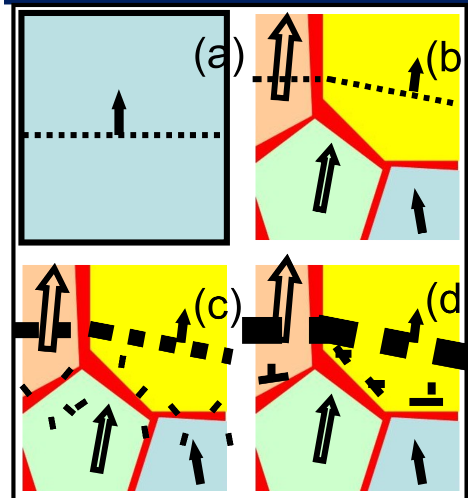


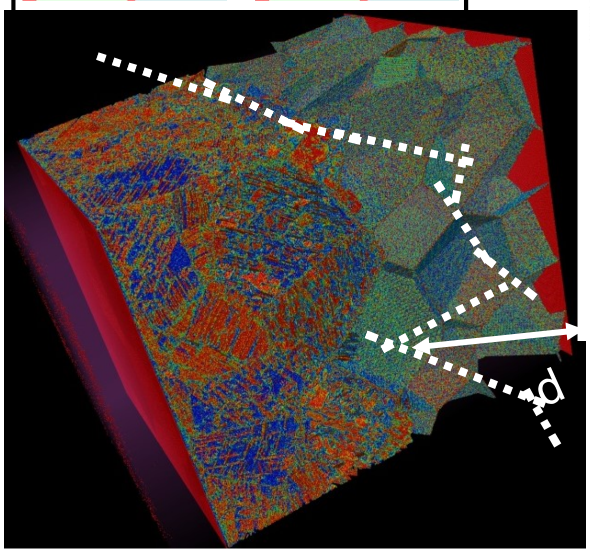
Published 1995: Matter compilers (3D printers), smart paper, carbon-based materials, etc.



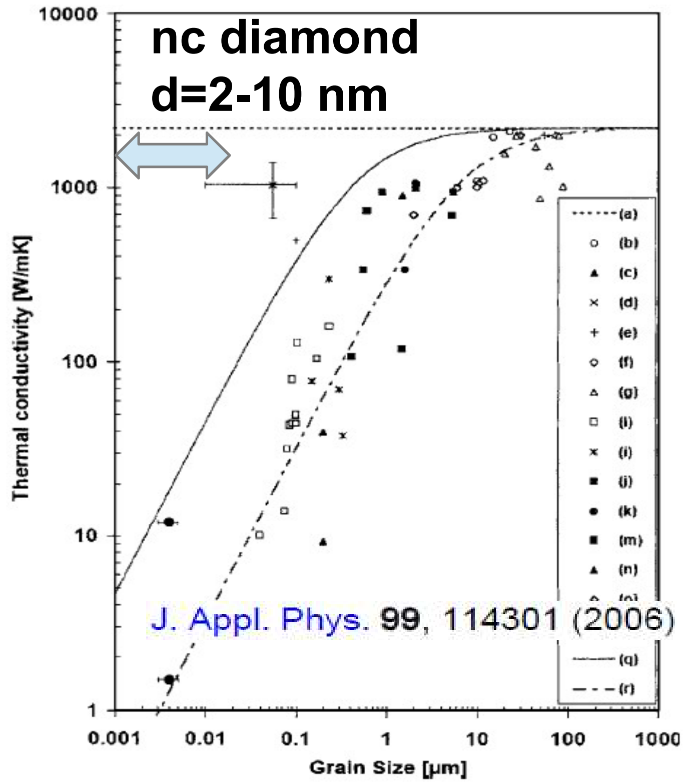
Valencia *et al*, Carbon (2015)

Nanocrystalline diamond has several technological applications GBs in nc diamond change transport properties tremendously





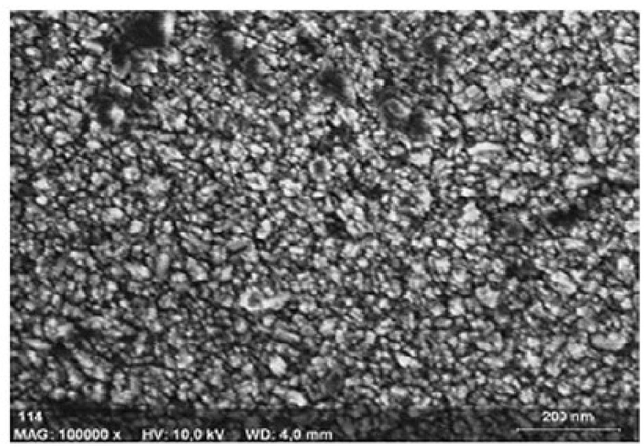
Pressure wave: elastic anisotropy and scattering by GBs, Bringa *et al.*, JOM (2005).



Kapitza resistance for grain size d:~a/(b+ c d) a,b,c constants

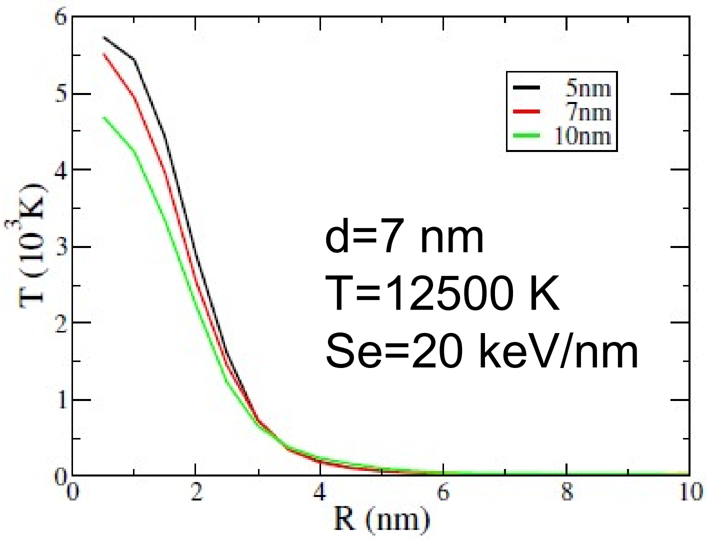
MD (2 grains, Σ GB), Watanabe *et al*. JAP (2007)

O.A. Williams, Diamond & Related Materials 20 (2011) 621

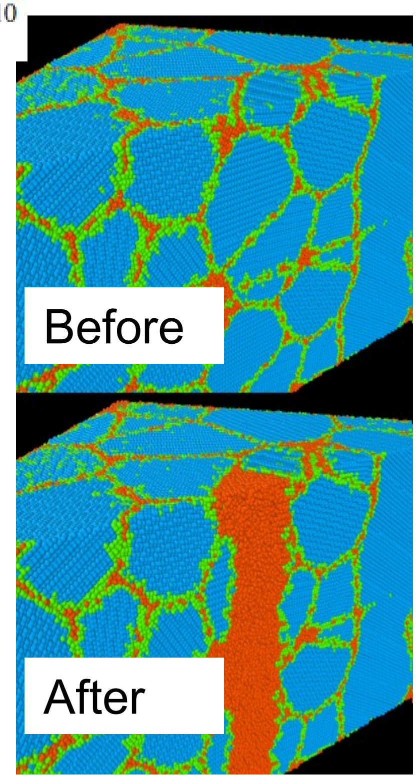


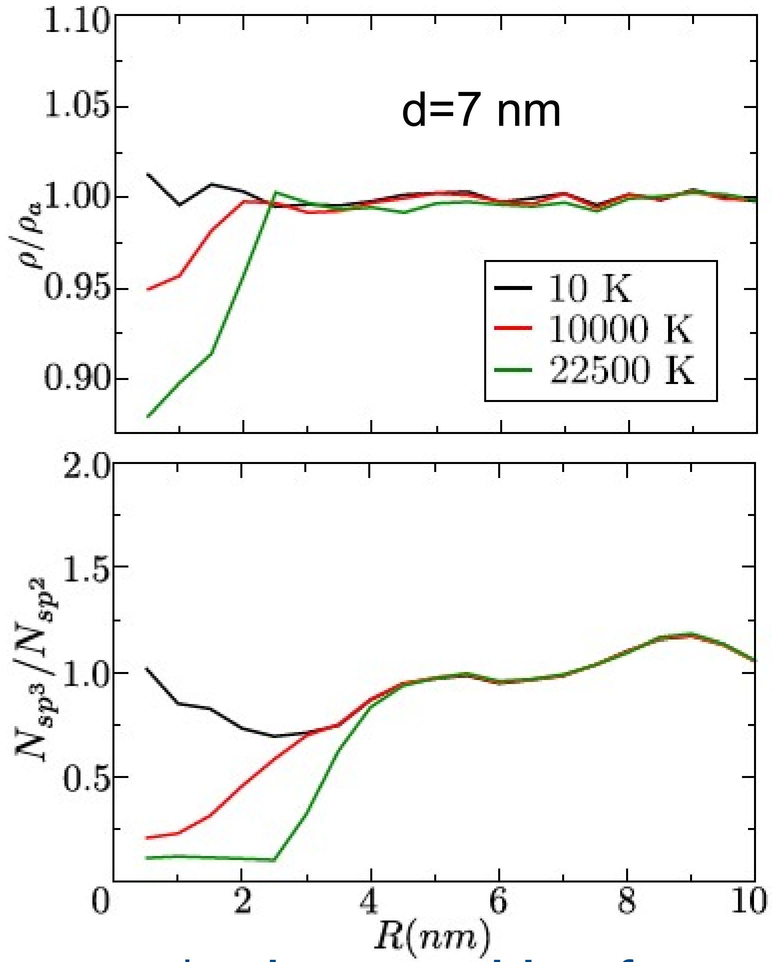
Confinement effects in irradiation in nc diamond

Defects survive because of nanoscale grains



Valencia *et al.*,
Carbon (2015)
Carbon (2017)

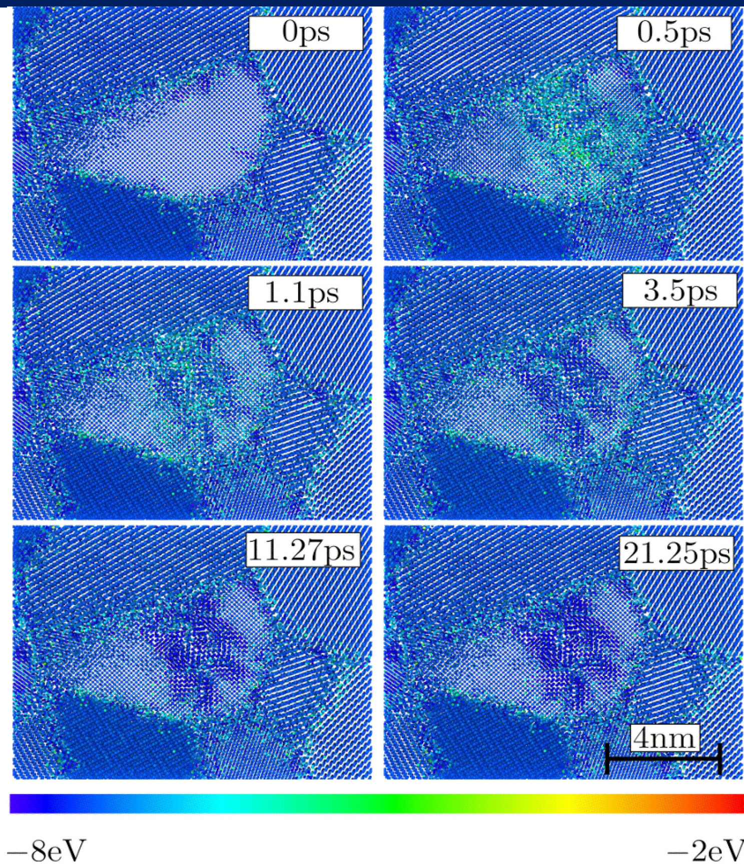




GBs reduce thermal conductivity, as expected in nc diamond [Dong *et al.*, Sci. Rep. **4** (2014) 7037] ⟶ T is much higher for smaller grains ⟶ longer spike lifetime

Nanoscale **phase transition:** from diamond to graphitic.
Density decrease expected from hybridization ratio.

Confinement effects in irradiation in nc diamond
Deffect production due to nanoscale grains



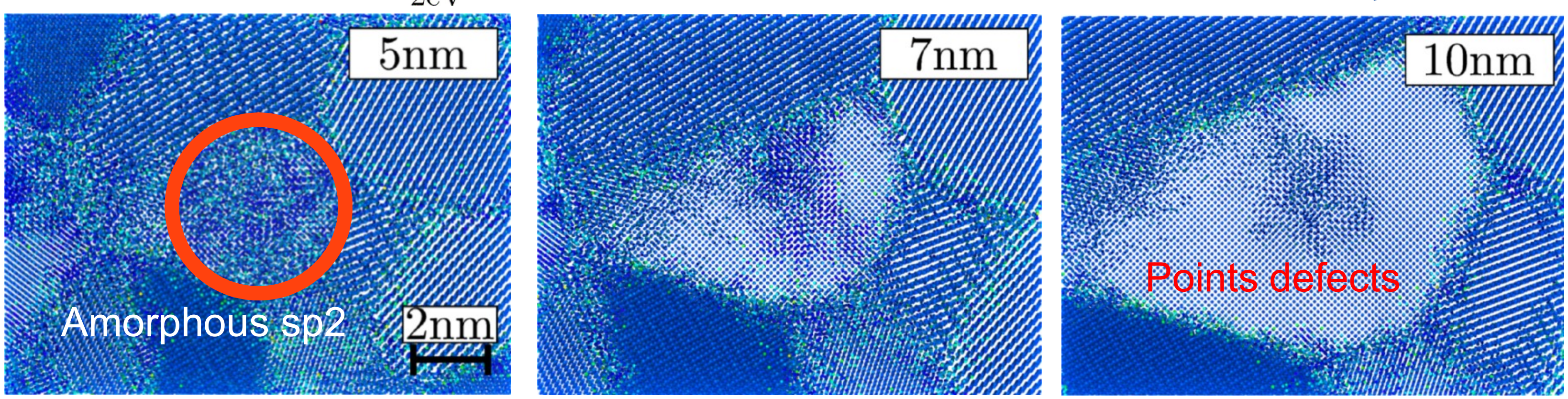
In most materials, GBs are assumed to reduce radiation effects, but for nc diamond and SHI, GBs enhance radiation effects!

Damage threshold:
Single crystal ~ 50 keV/nm
Nc (10 nm) ~ 15 keV/nm

No experiments yet :(

Grain Size (T=10000 K)

Valencia *et al.*, Carbon (2015)

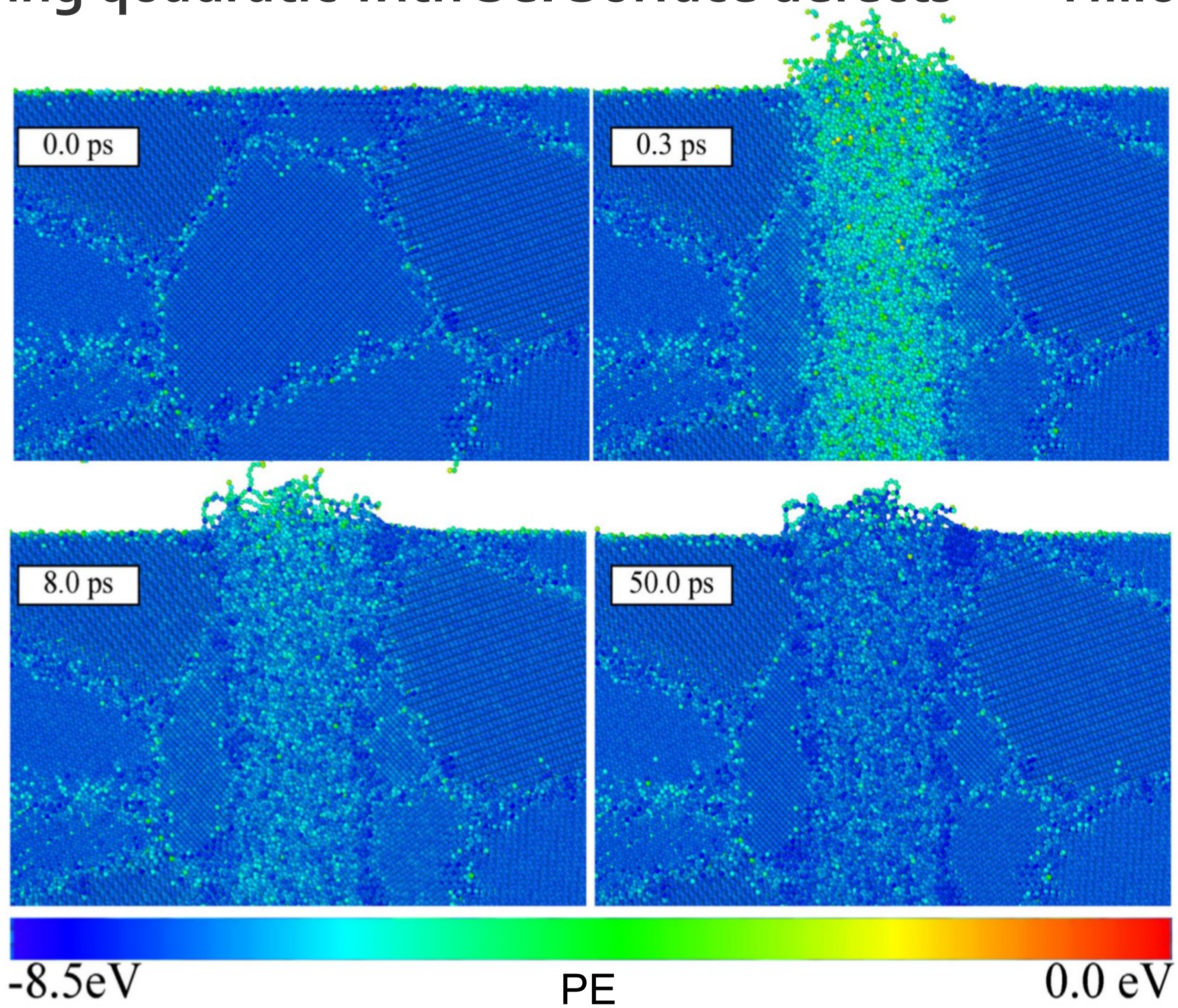


Time evolution of the thermal spike at nc diamond surface

Valencia *et al.*, Carbon (2017)

Sputtering quadratic with Se. Surface defects → Hillok → Crater

5nm grains
15keV/nm

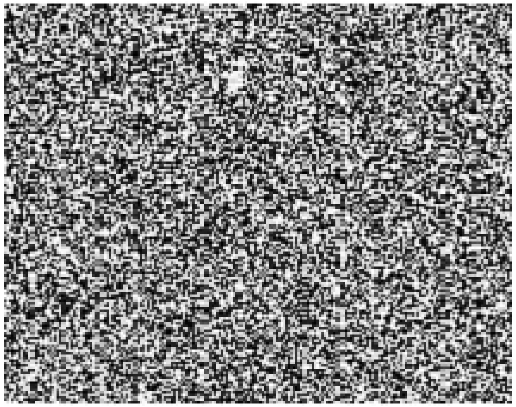


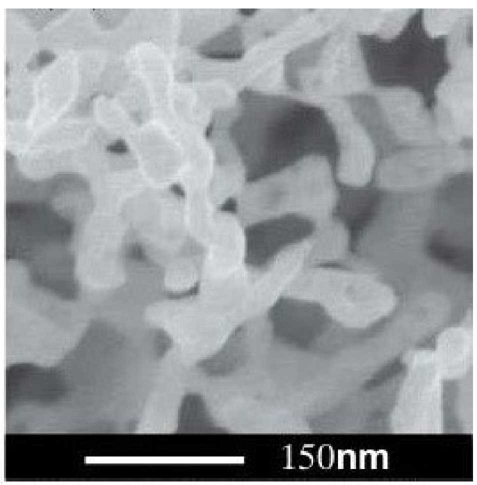
Irradiation changes mechanical properties (in progress)

Complex initial defect structure: "Reaction-diffusion equation" to obtain initial foam

D. Schwen, A. Caro (LANL), D. Farkas (Va Tech)

http://en.wikipedia.org/wiki/Spinodal_decomposition

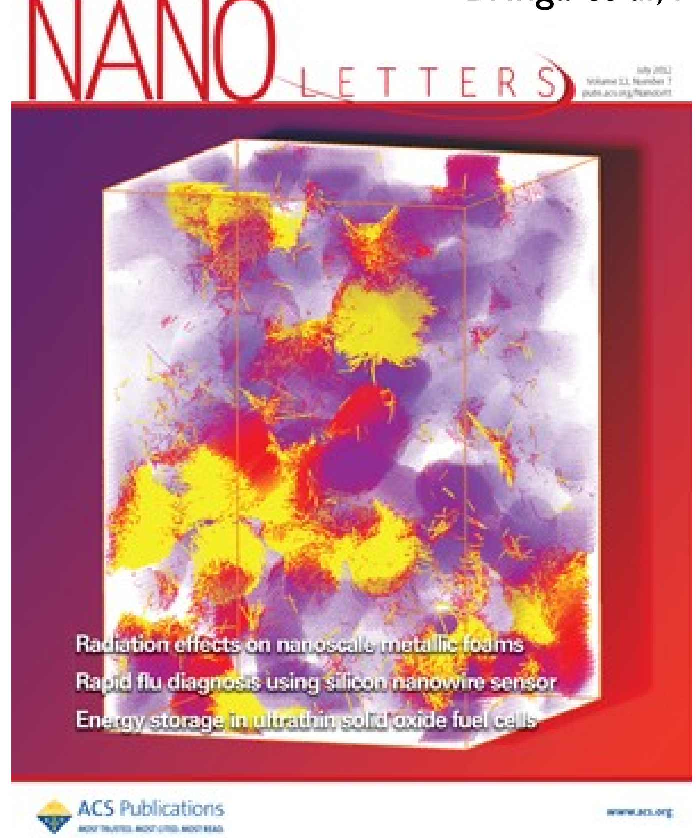




Plasma exposed W-C surface Takamura et al., Plasma and Fusion Research 1, 51 (2006)

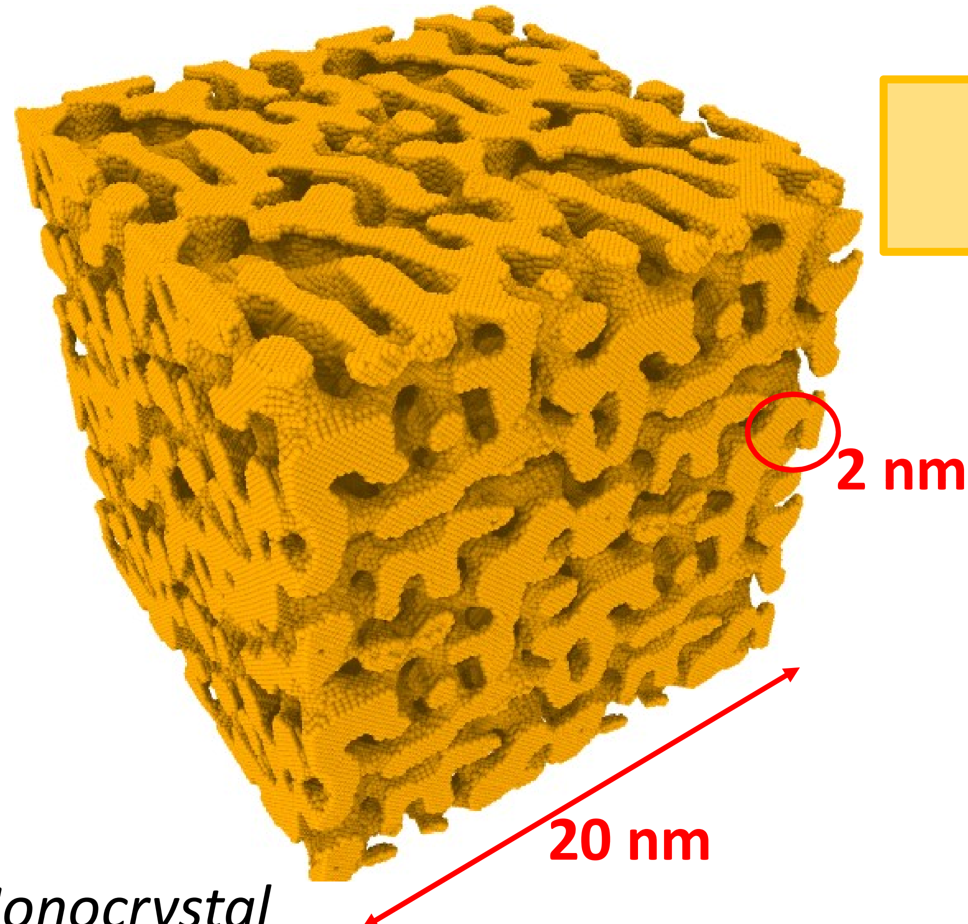
Uses Cahn-Hilliard Equation, to generate 3D foam. OpenCL code by Schwen needs modifications for future research

Bringa *et al*, NanoLetters (2012)

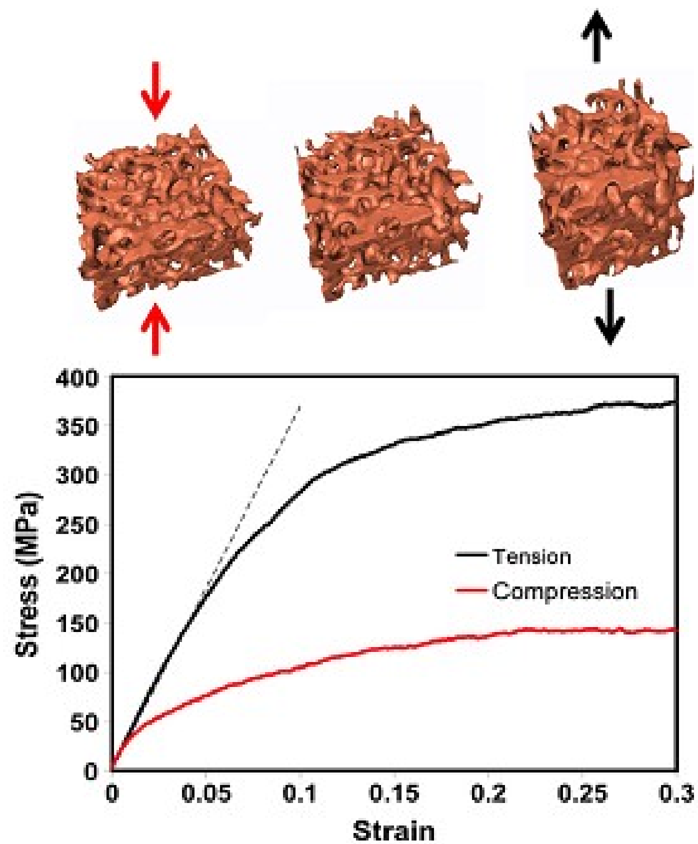


“Model” Nano-foams

1e6 atoms x 1 ns
~12 hours in 10 cores



Monocrystal (defect free)

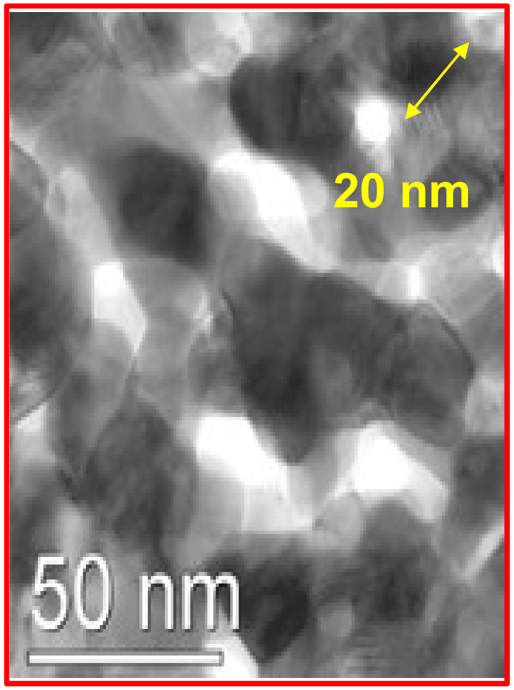


Farkas et al. *Acta Materialia* **2013**
Bringa et al. *Nano letters* **2012**

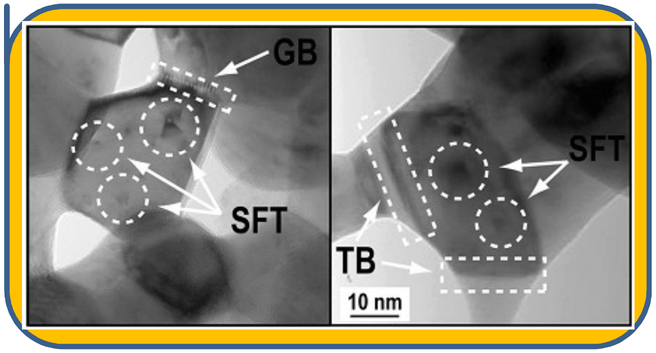
Realistic Nanofoams

~1500 hours in 100 cores, ~50 TB

~200 nm



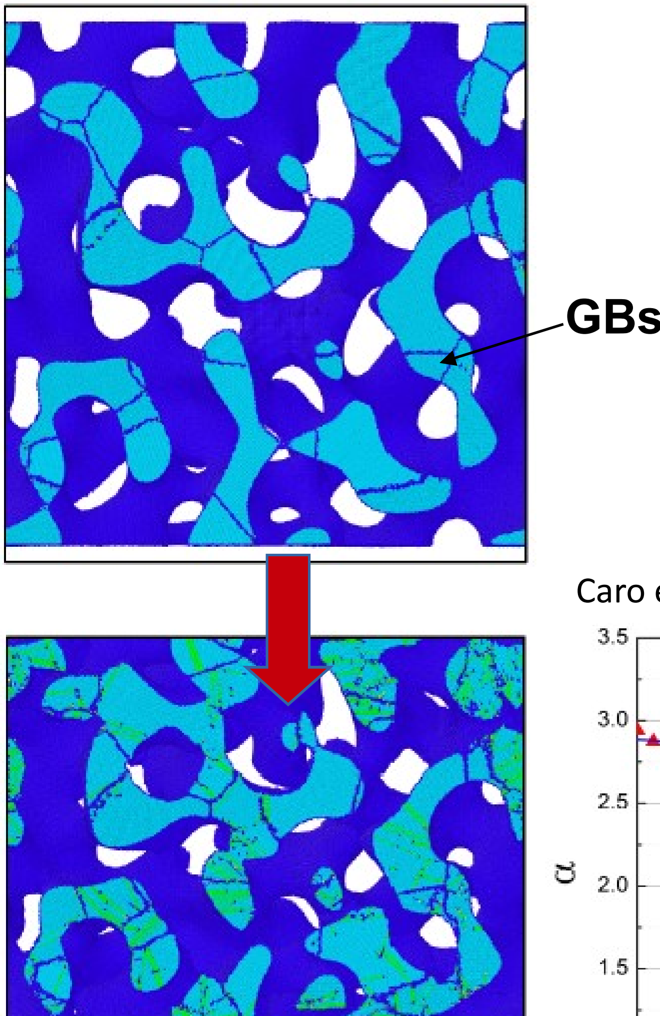
Polycrystal nanofoam with defects



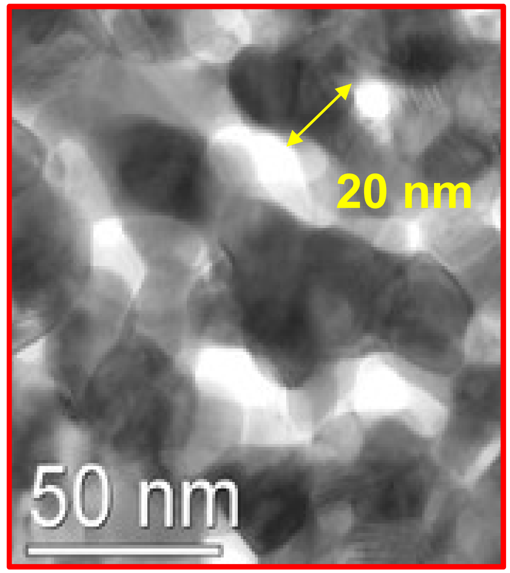
Interesting science with possible technological applications.
Where is the cross-over with models for macrofoams?

Caro et al. *Appl. Phys. Lett.* **2014**
Zepeda-Ruiz et al. *Appl. Phys. Lett.* **2013**
Fu et al. *Appl. Phys. Lett.* **2012**

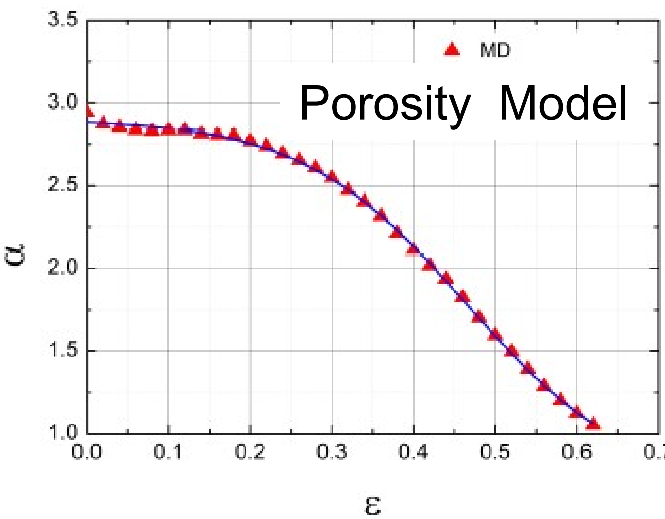
Loading of high porosity ncAu foams (2-15 nm filaments)
C. Ruestes *et al*, Comp. Mat. Sci. (2018)



70% porosity foam
Elastic and plastic behavior



Caro et al. *Appl. Phys. Lett.* **2014**

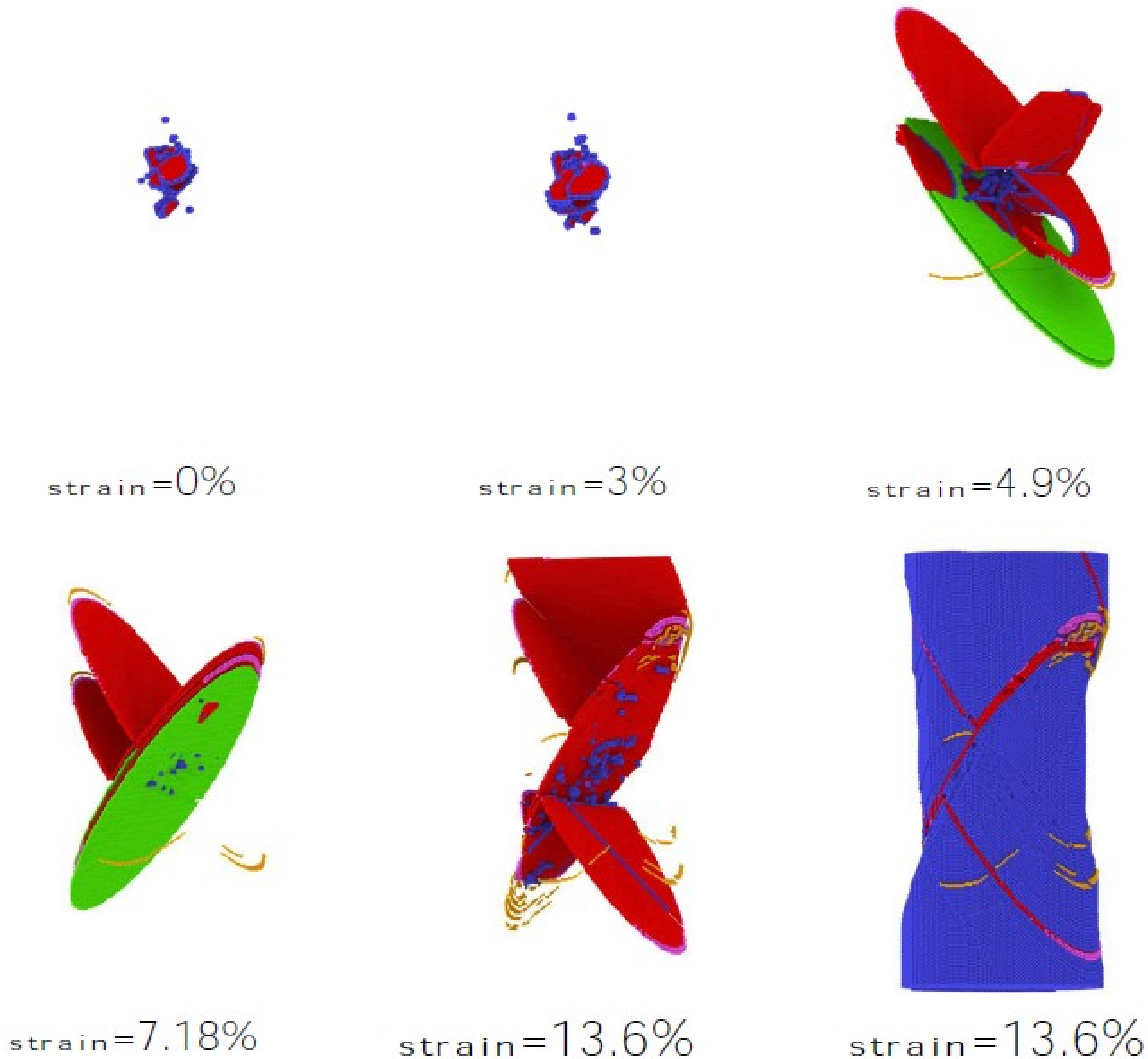


Loading: “realistic” foam includes full dislocations in addition to SFs and twins. New porosity evolution model.

Recovery: survival of SF intersections. Huge residual strain. Analysis in progress.

Deformation of NW with radiation-induced defects, including SFT

Uniaxial tension along [001], another case



Nucleation of SFs at SFT surface leads to "small" relaxation and limited twin formation. Shear localization clearly observed.
Unlike what happens under compression [Zepeda-Ruiz *et al*., APL (2013)], SFT disappears!
Dozens of papers showing SFT+dislocations: Wirth, Bacon, Osetsky, Martinez, etc → SFT removal

Figueroa *et al*, JNM **467**, 677 (2015)

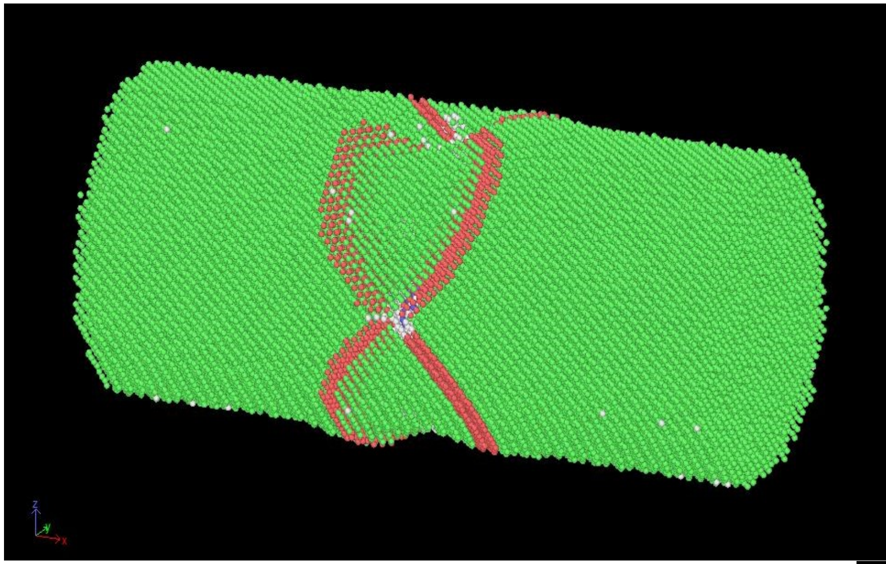
Gold Nanowire Irradiation

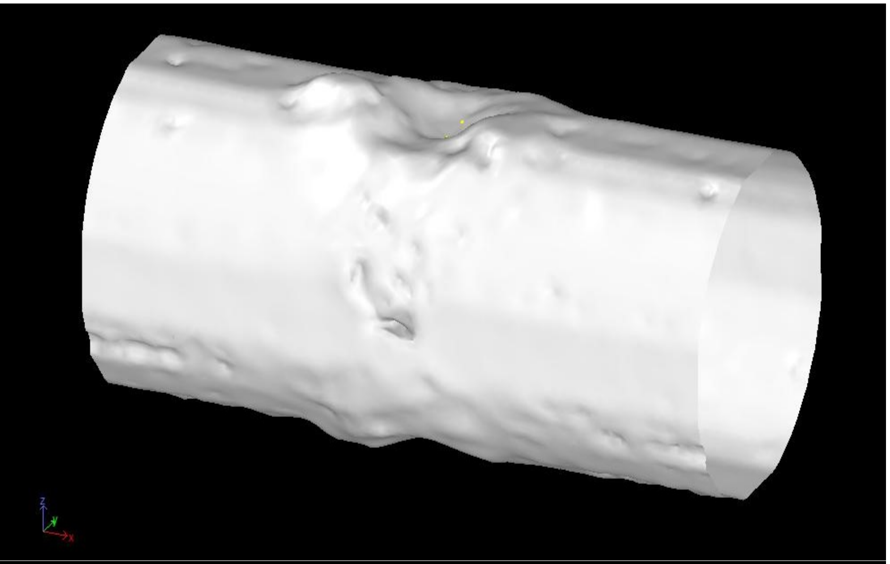
Joás Grossi

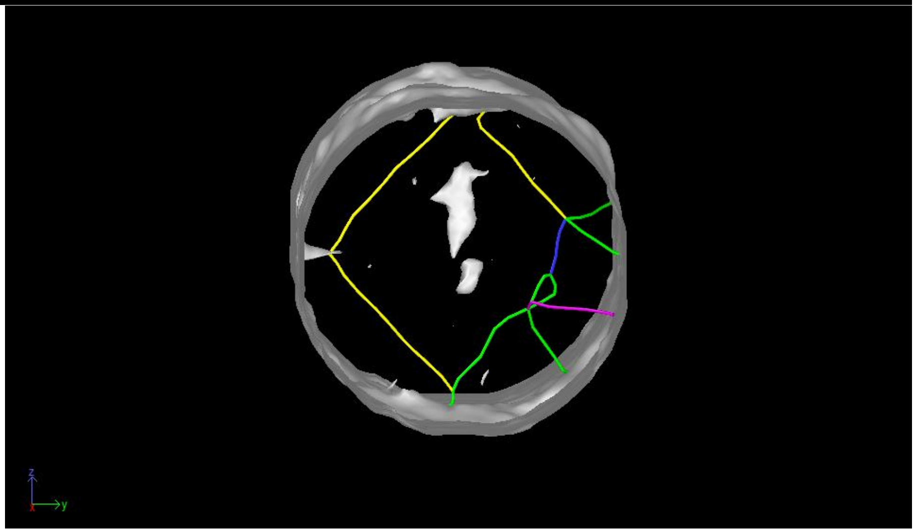
- Thermal spike to mimic an ion through a nanowire (20nm length, and 10nm diameter)
- The track (5nm diameter) was set to 10000, 20000 and 30000K
- Different mechanisms of defects formation were observed depending on track temperature.

Irradiation - Results

Joás Grossi



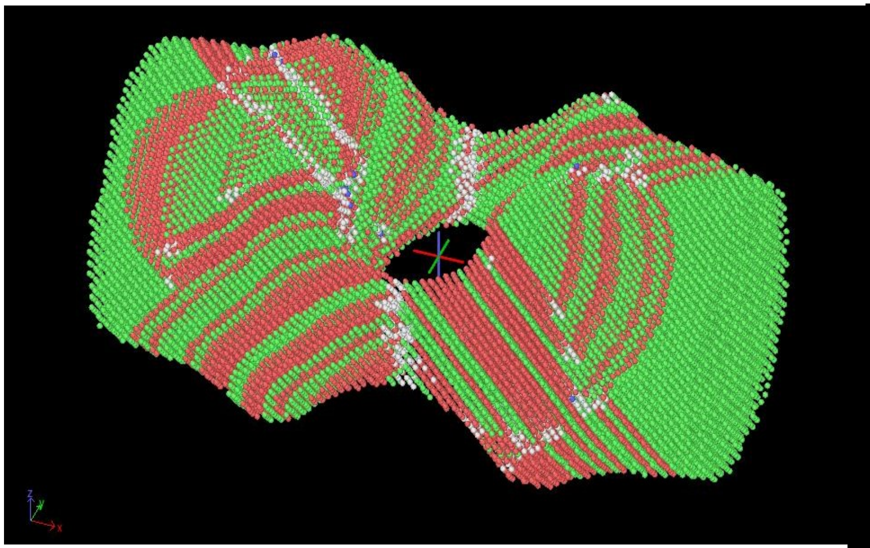


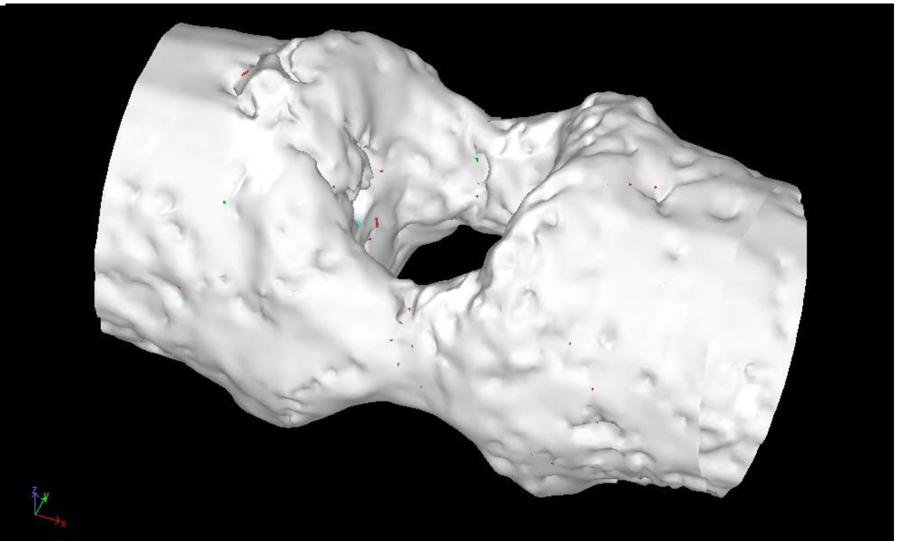


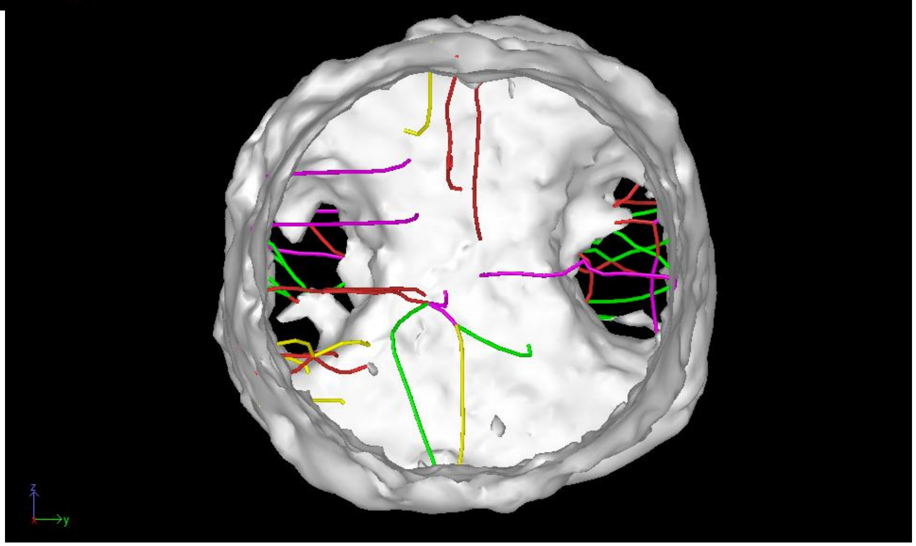
final stage of the wire -
track was set to 10000K

Irradiation - Results

Joás Grossi



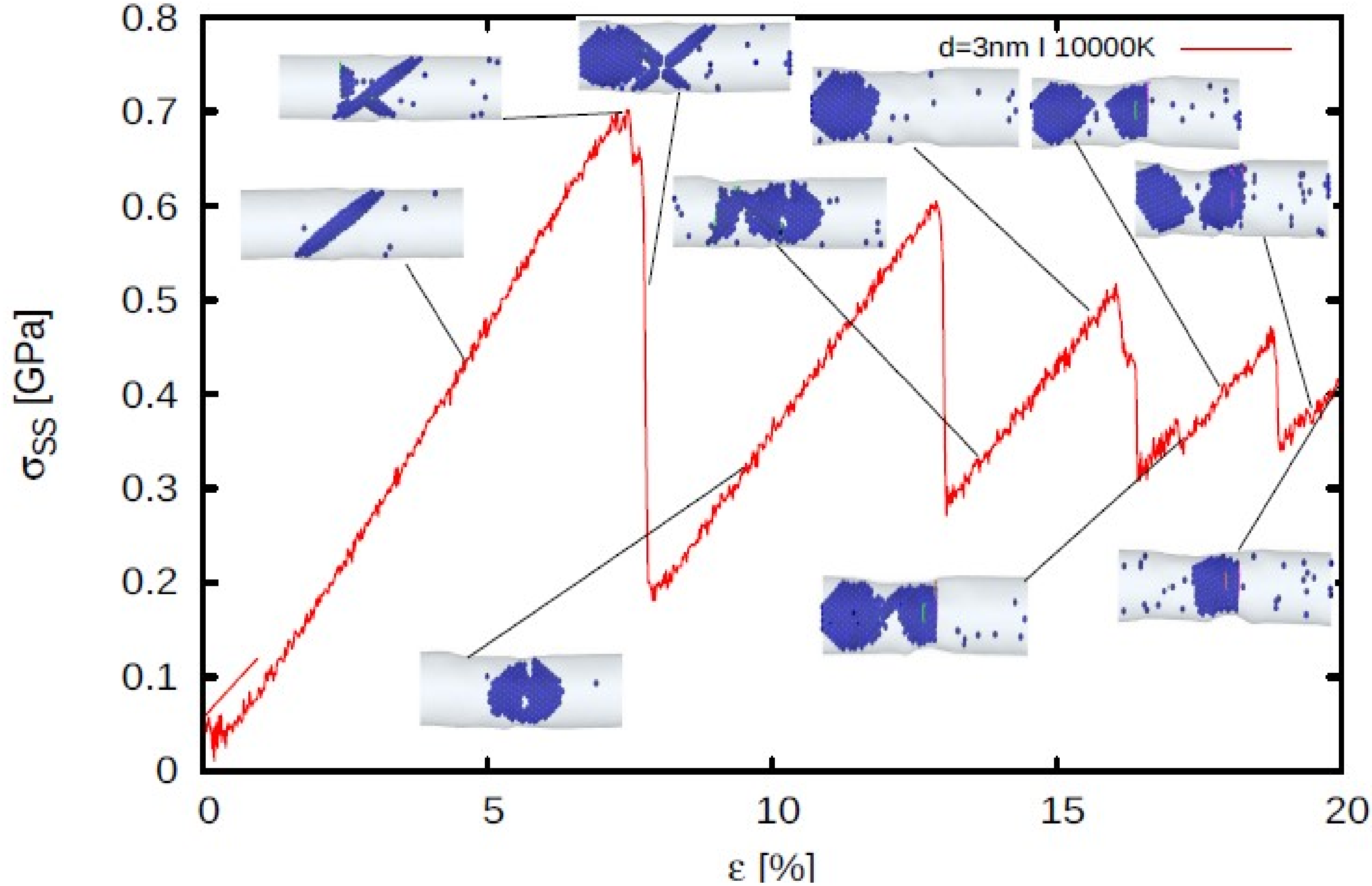




final stage of the wire - track was set to 20000K

Deformation of NW with radiation-induced defects (electronic)

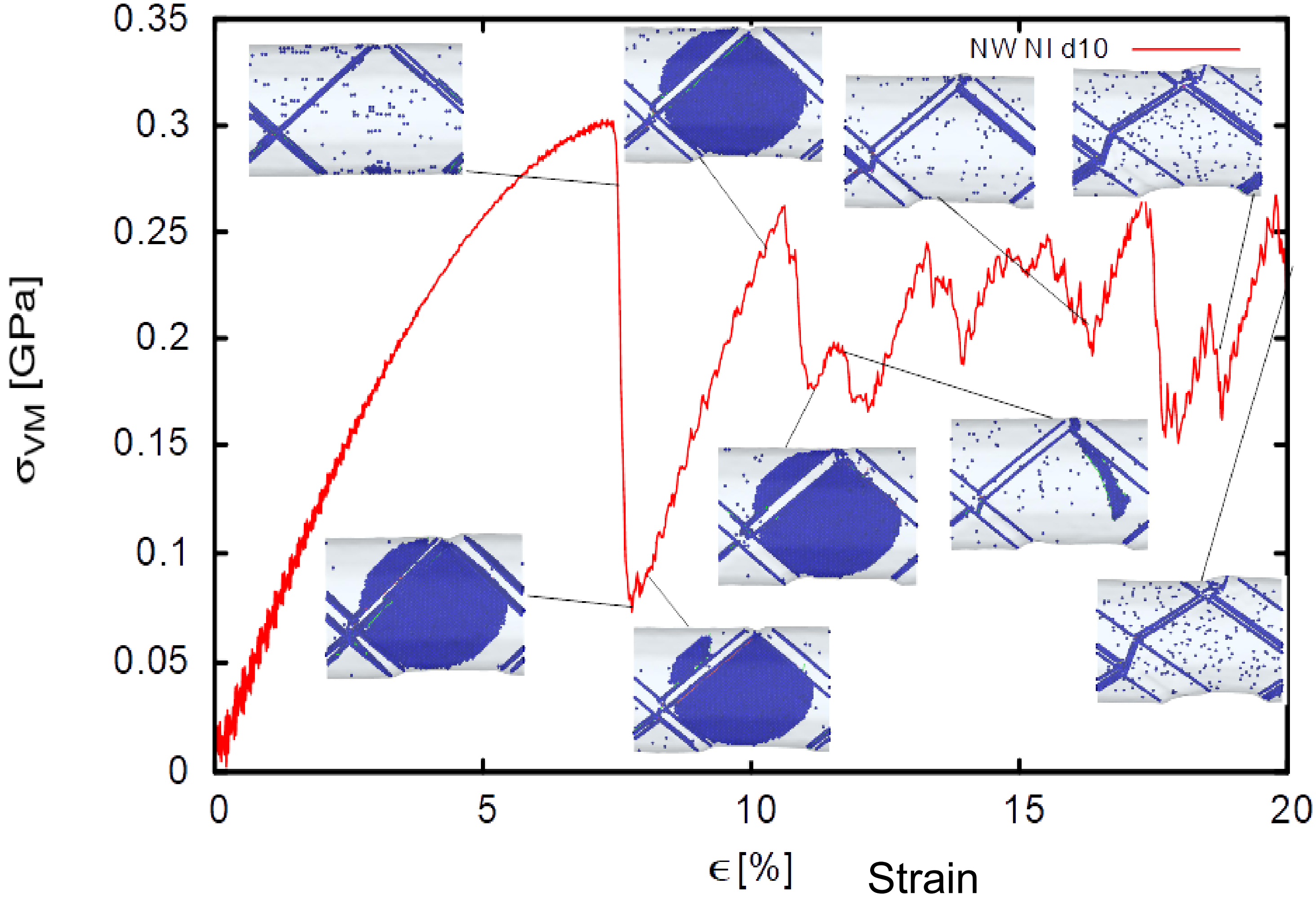
Uniaxial tension along [001], Au nanowire, 3nm diameter



Low electronic stopping power leads to initial stacking fault. Under tension, there is necking but no failure up to 20% strain.

Araguna, Ruestes, and Bringa, in preparation

NW d=10nm NI, Compression



Load a lot of Sfs and twins due the plasticity.

TTM improvements for thin wires

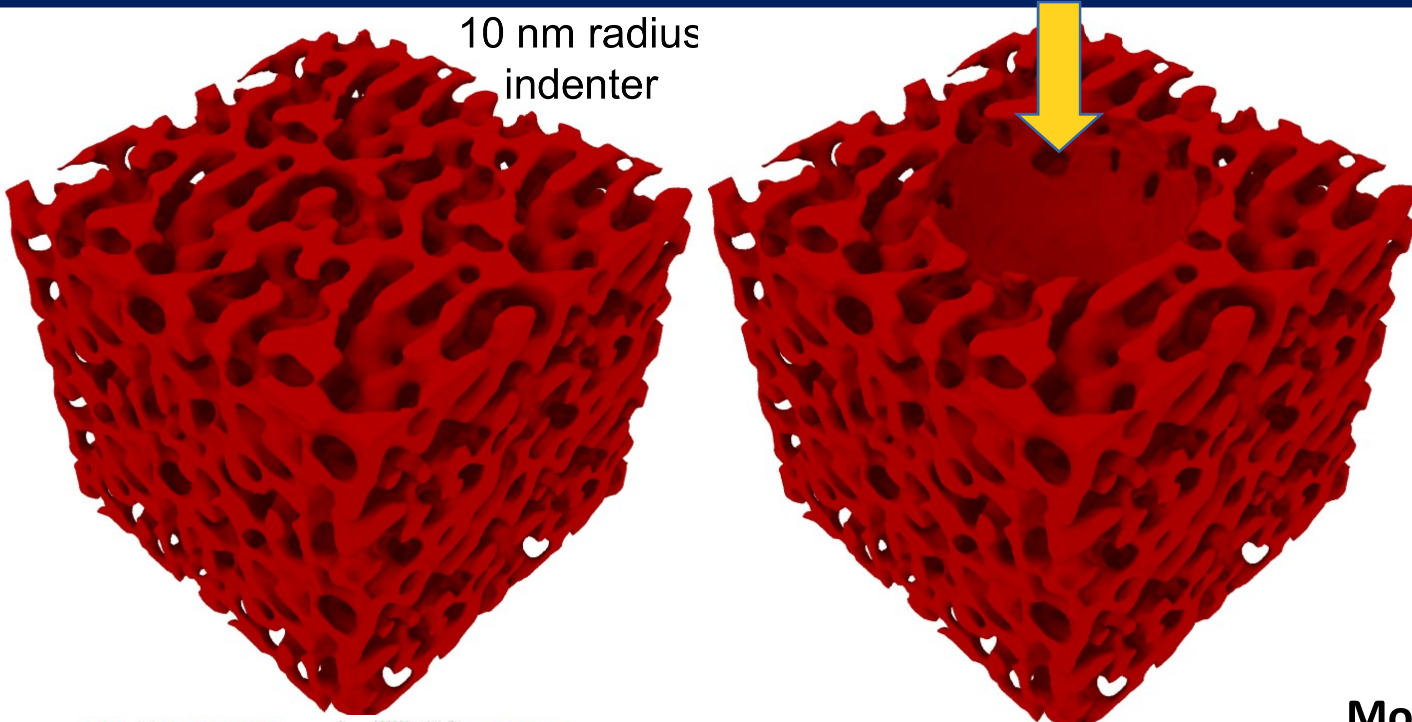
Joás Grossi, E. Atacho

- $C_e(T_e)$ is not linear for $T_e > 3000K$

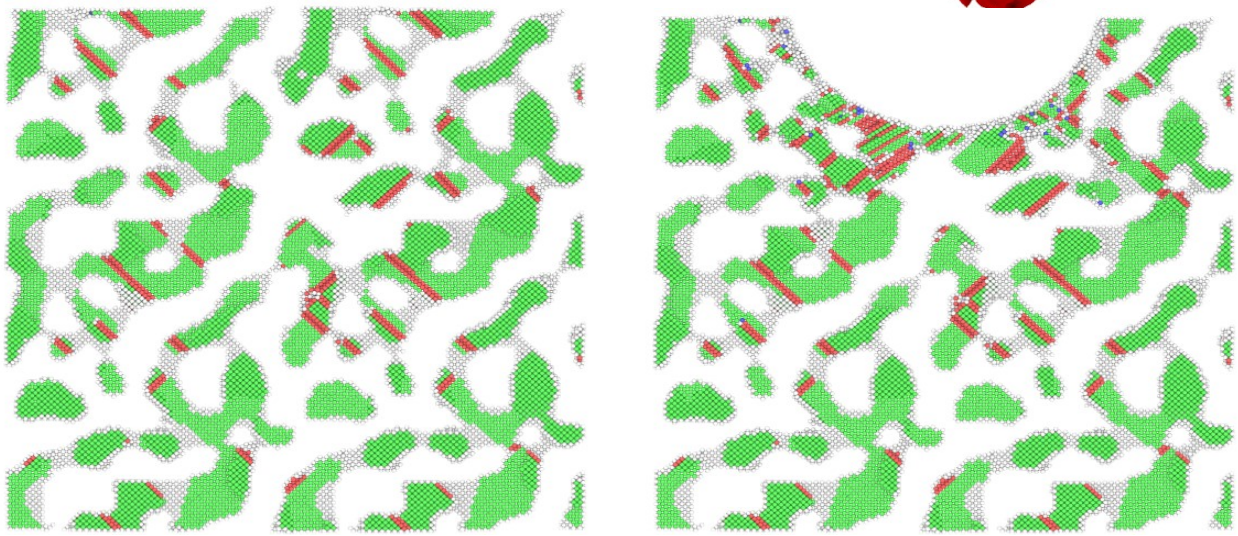
- $G_e(T_e)$ is not a constant for $T_e > 3000K$ and can increase by an order of magnitude close to 10000K

- K_e depends on the diameter of the wire and T_e and can decrease by an order of magnitude (compared to bulk) for Au at 300K

Irradiation and loading of high porosity ncAu foams
(2 nm filaments) C. Anders (TUK) and C Ruestes, UNCuyo

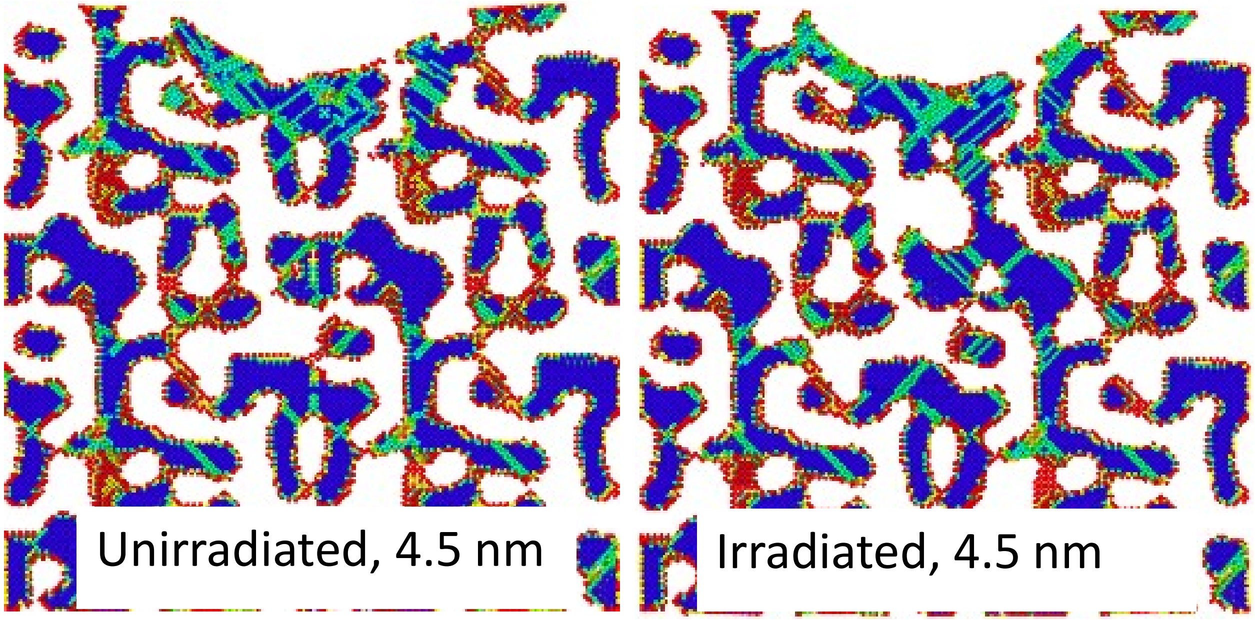


Loading: "realistic" foam includes full dislocations in addition to SFs and twins. New porosity evolution model.
Irradiation: 10 keV self-bombardment

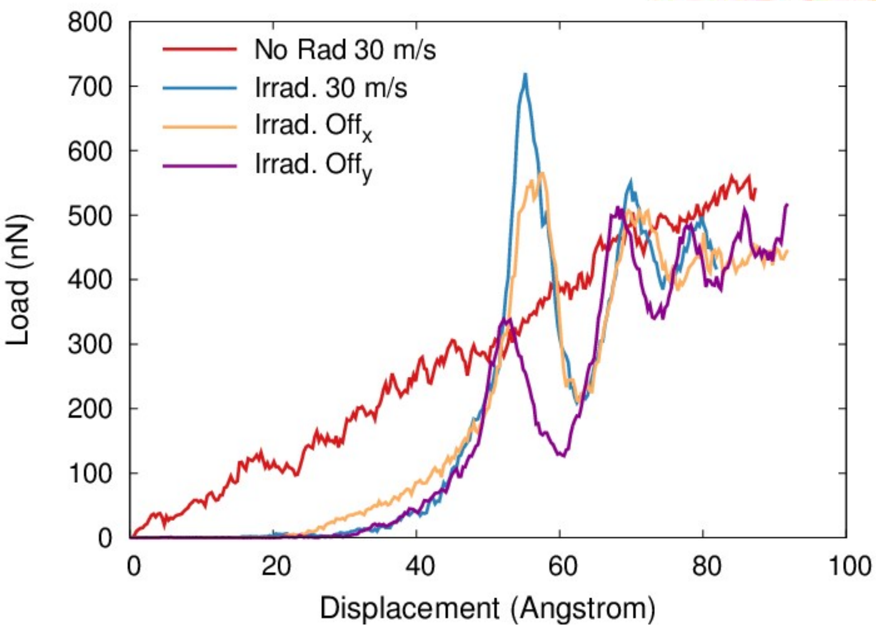


Motivation:
experimental work by Caro et al., *Appl. Phys. Lett.* (2014) reports foam hardenning under irradiation.

Irradiation and loading of high porosity ncAu foams (2 nm filaments) C. Anders (TUK) and C Ruestes, UNCuyo



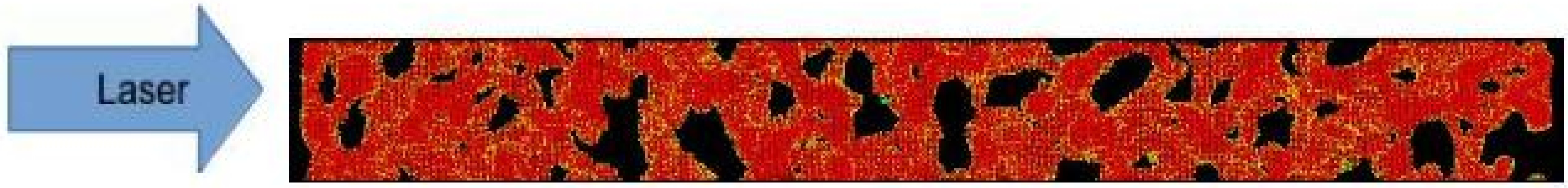
Both filament network topology and defect content (SFs and twins) are changed by irradiation.



What happens? Caro et al. [*Appl. Phys. Lett.* (2014)] present higher modulus, but only for 1dpa or larger.

Gold Nanofoam (laser ablation)

Joás Grossi



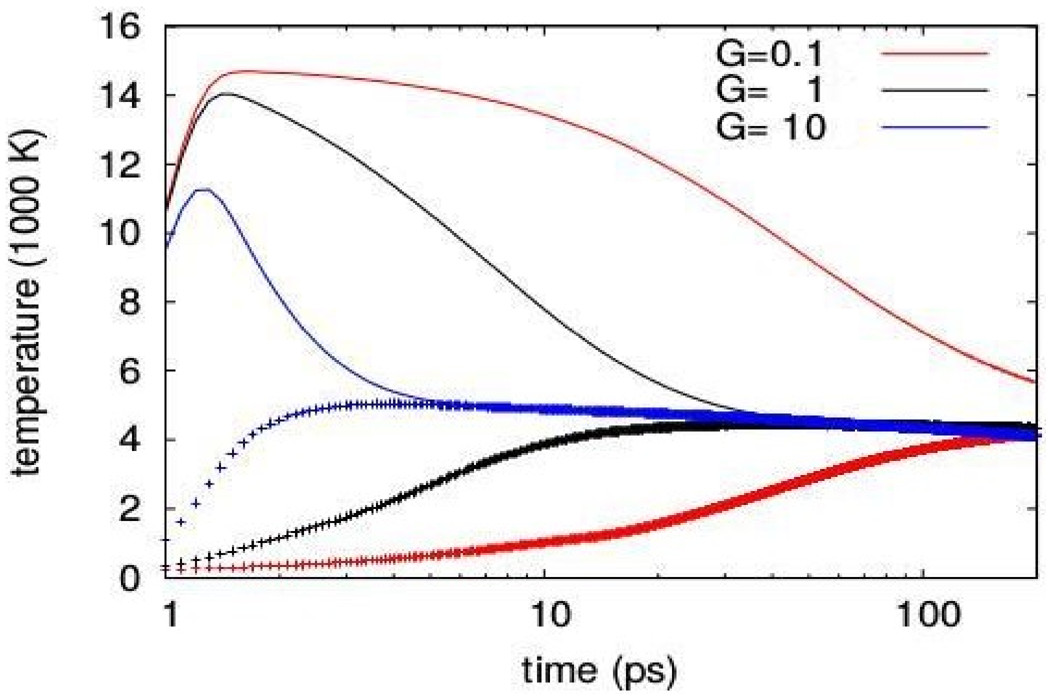
- Au foam of average porosity 79% and average filament diameter of 2.5nm

- G_e=0.1, 1 and 10
- K_e=0.1 and 1 for G_e=1

Numbers for G_e and K_e are scaling factors respect to bulk Au values for these parameters.

Gold Nanofoam - Results

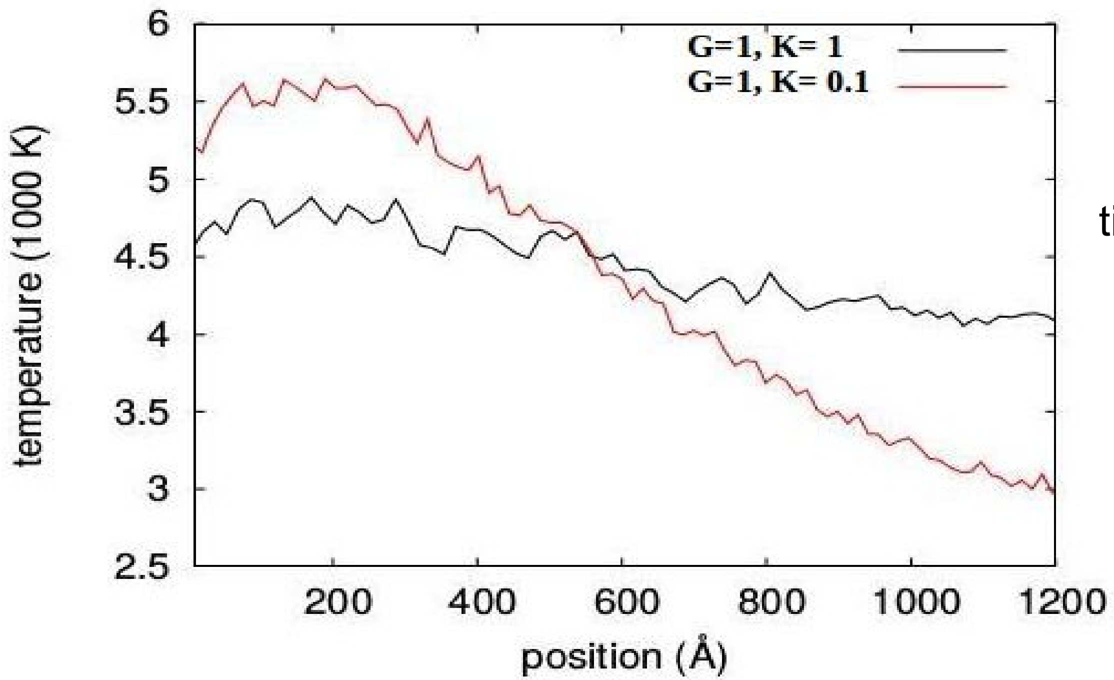
Joás Grossi



Magnitude of electron-phonon coupling is decisive for the time scale with which energy is transferred to the atomic system, and hence the speed of melting and evaporation processes.

Gold Nanofoam - Results

Joás Grossi

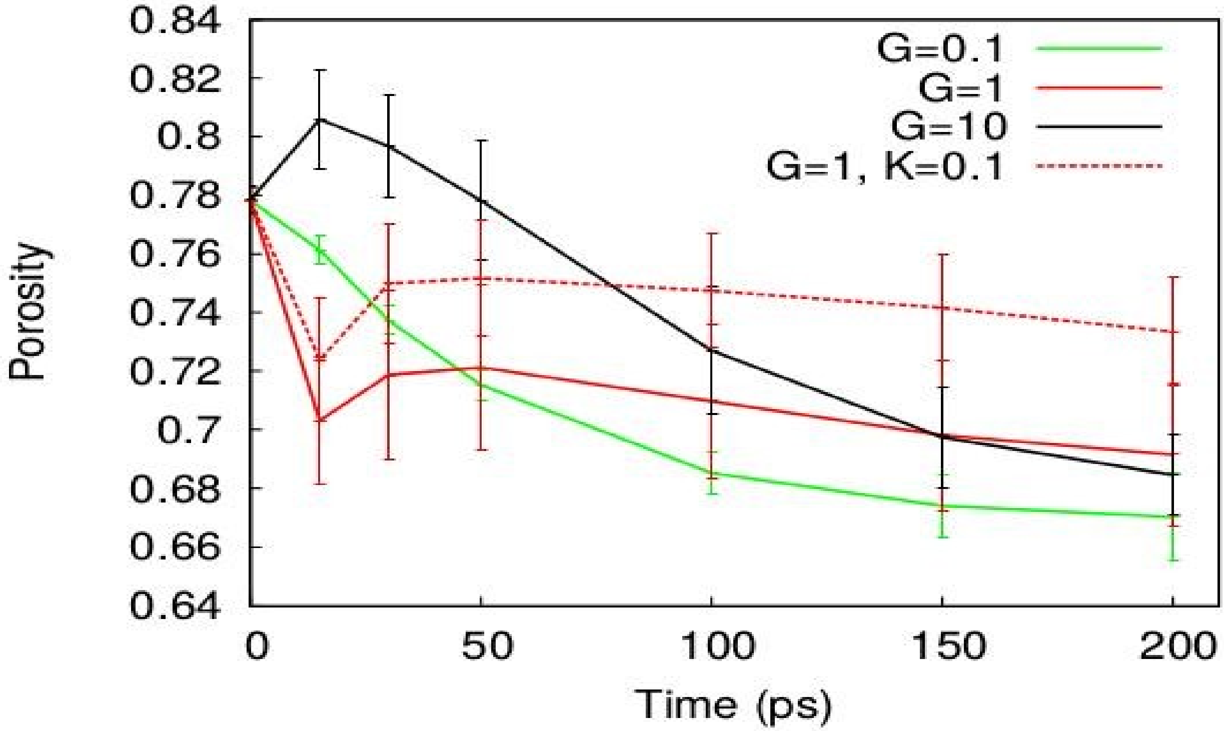


time=100ps

Thermal conductivity determines the homogeneity of the energy profile in the specimen. While a low heat diffusivity may localize the irradiated energy near the front surface and increase ablation there, a high value may transport energy quickly to the back side and enhance the processes there.

Gold Nanofoam - Results

Joás Grossi



The final porosity is nearly independent of the value of electron-phonon coupling; it depends, however, on the thermal conductivity in that low heat conductivities lead to smaller changes of the porosity.

Wish list

- **Need more experiments on ice, silica, carbon, metals, oxides, etc., including porous materials and nanostructured materials):** sputtering; compaction; defect production and evolution, chemistry, mechanical properties, etc.
  Use similarities in SHI/HCI/laser excitations.
- What is the long time evolution of defects/chemistry? Use accelerated dynamics or kMC methods?
- How much is the effective stopping in nanostructured and nanoporous materials? Possible changes in excitation spectra, electron-phonon coupling, confinement effects, etc.
- How can we connect QM-based calculations (10-100 atoms) to large-scale (1e6-1e9 atoms) classical calculations?