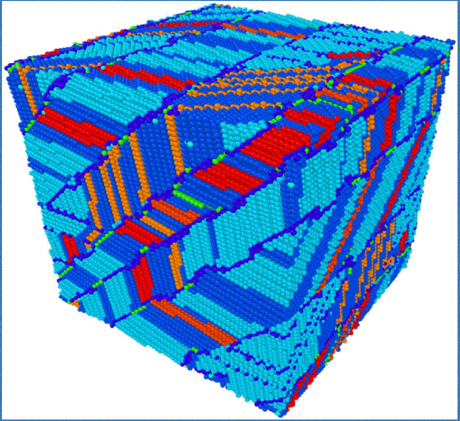
Simulaciones en Materiales, Astrofísica y Física (SiMAF)



Eduardo M. Bringa
ebringa@yahoo.com

CONICET
FCEN, UN Cuyo
Mendoza, Argentina

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

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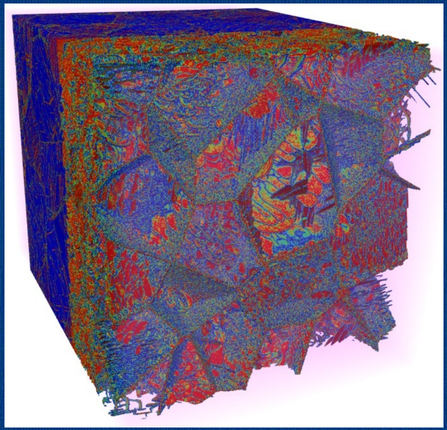
Mayo 2014



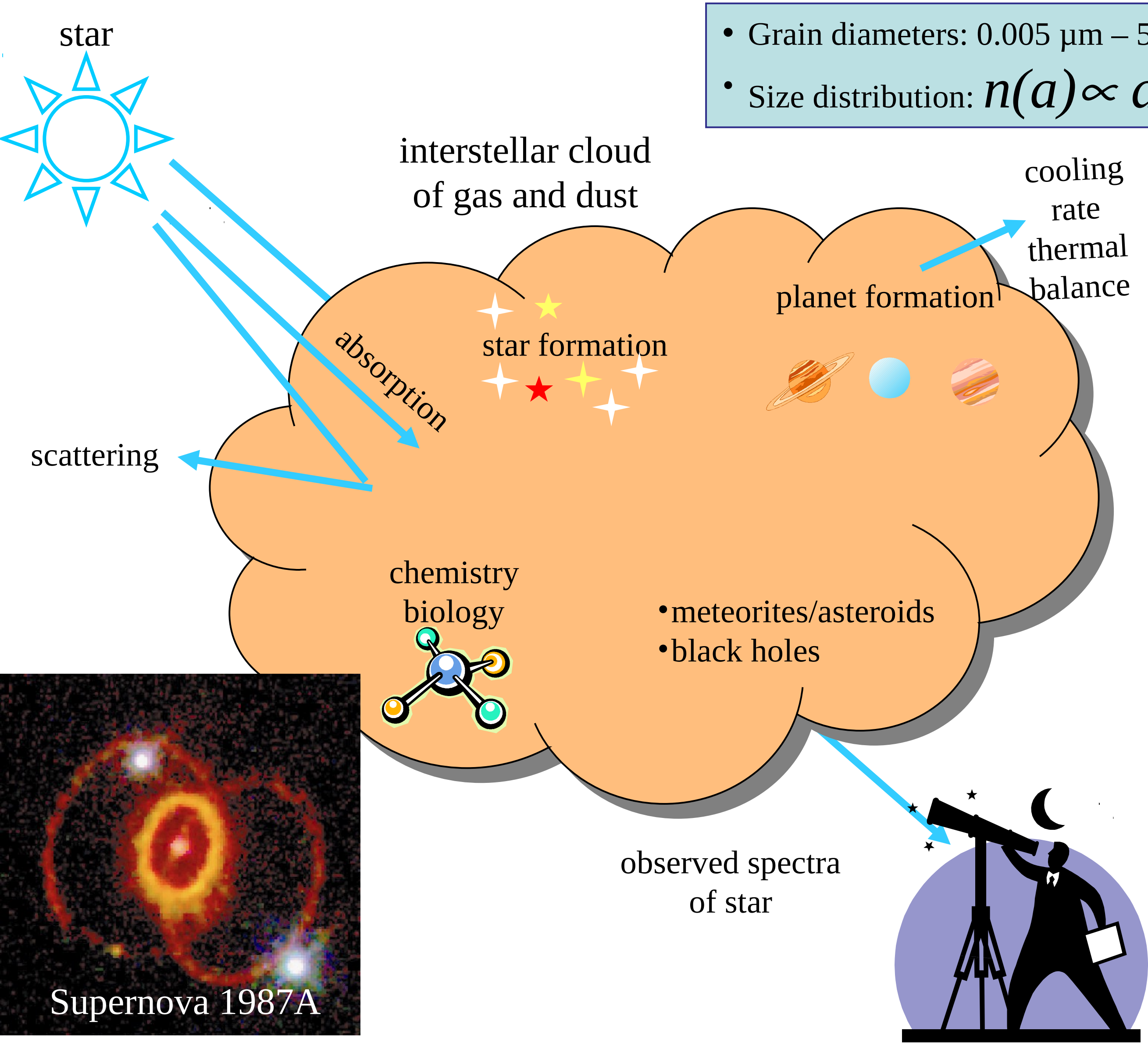
COLLABORATORS: **J. Rodriguez-Nieva** (I. Balseiro,MIT), N. Arista , M. Ruda, G. Bertolino (I. Balseiro), D. Farkas (VaTech), A. Caro, M. Caro, D. Schwen, R. Ravelo, T. Germann (LANL), M. Duchaineau, F. Abraham, R. Rudd, J. Hareliak, B. Remington (LLNL), R.E. Johnson, **R. Baragiola** (U Virginia), C. Anders, C. Ringl, N. Gunkelmann, H. Urbassek (TU Kaiserslautern), Y. Tang, E. Hahn, S. Zhao, K. Olney, D. Benson, M.A. Meyers (UCSD), G. Ackland (U. Edinburgh), S. Ramos, E. Crespo (UN Comahue), G. Graham, N. Park (AWE), A. Higginbotham, M. Suggit, J. Wark, E. Figueroa, G. Gutierrez (U Chile), **E. Millan, C. Ruestes, D. Tramontina, F. Fioretti** (U.N. Cuyo).

SiMAF

Interstellar dust plays an important role in astrophysical processes

Grain size matters for evolution, astro-chemistry, etc.

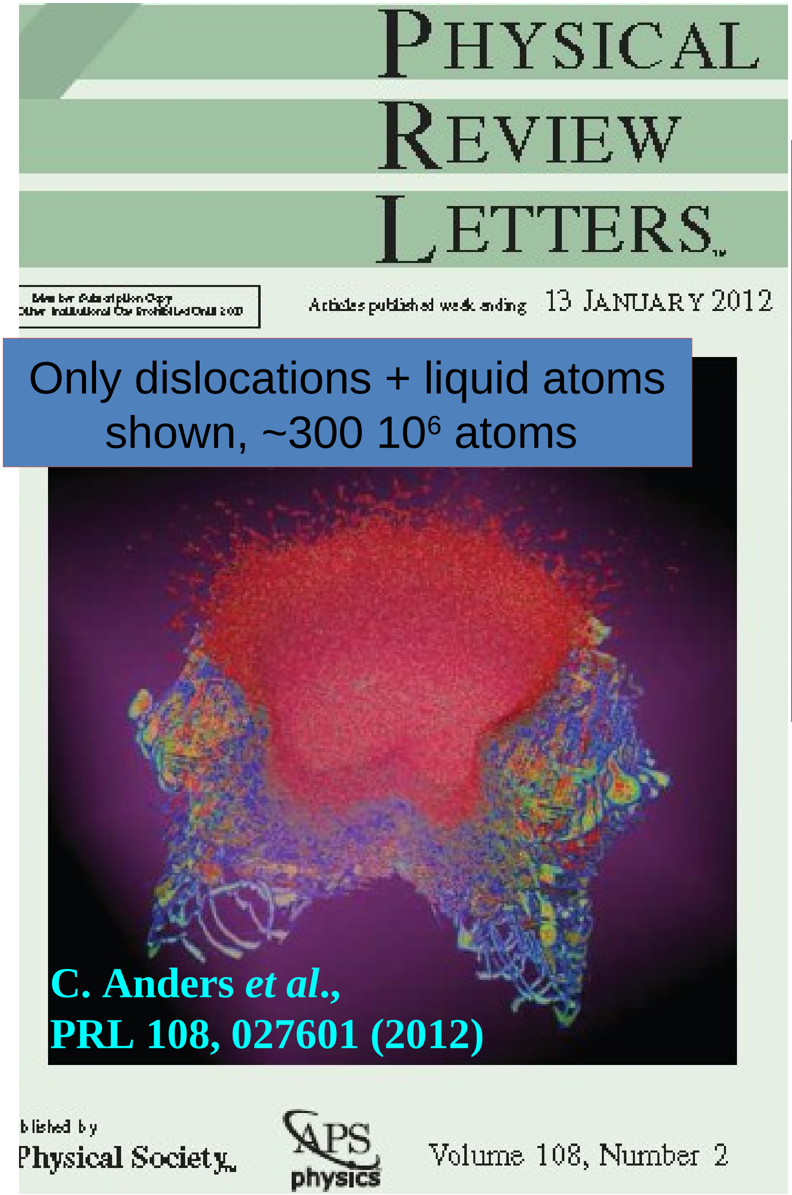
- Grain diameters: 0.005 µm – 5 µm
- Size distribution: $n(a) \propto a^{-3.5}$



Supernova 1987A

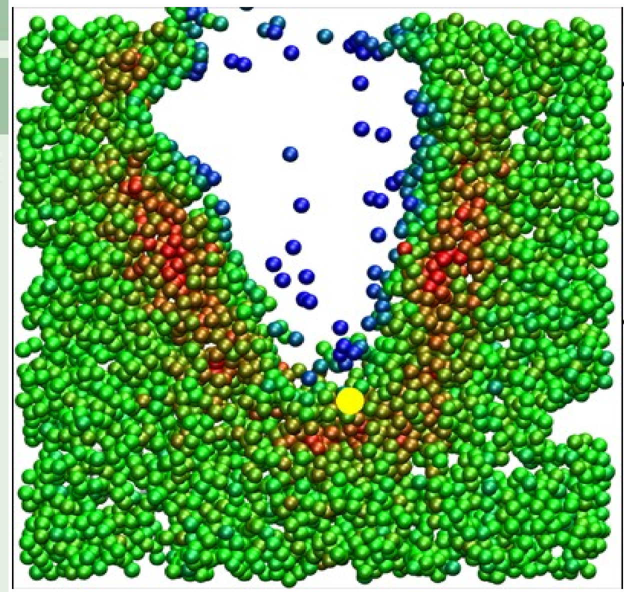
Modification of materials: phase transitions and damage to space hardware, and due to shrapnel (NIF)

Large-scale MD links nano and microscales in damage induced by nanoprojectiles

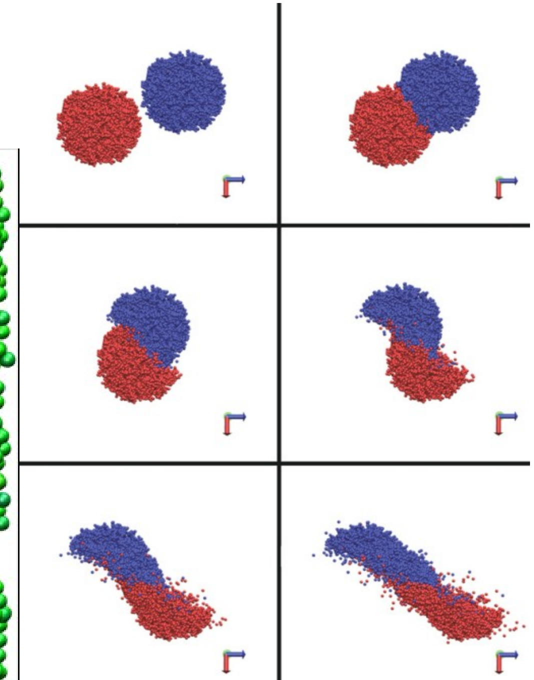


Only dislocations + liquid atoms shown, ~300 10^6 atoms

C. Anders *et al.*,
PRL 108, 027601 (2012)

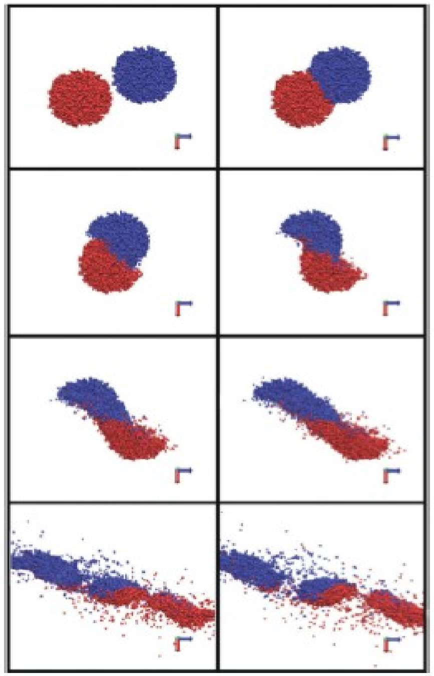


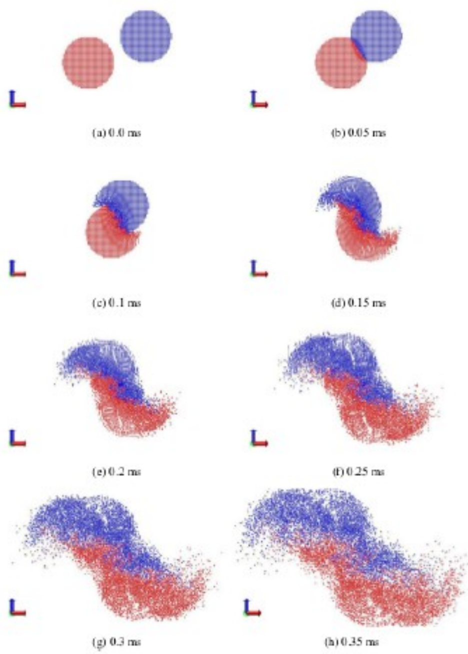
Granular mechanics of grain-surface collisions
Ringl *et al.*,
PRE 86, 061313 (2012)
PRE KALEIDOSCOPE



Granular mechanics of nano-grain collisions
Ringl *et al.*, Ap.J. **752** (2012) 151
New granular friction scheme implemented for GPUs by E. Millan

Cluster impact looks ~ the same at many scales

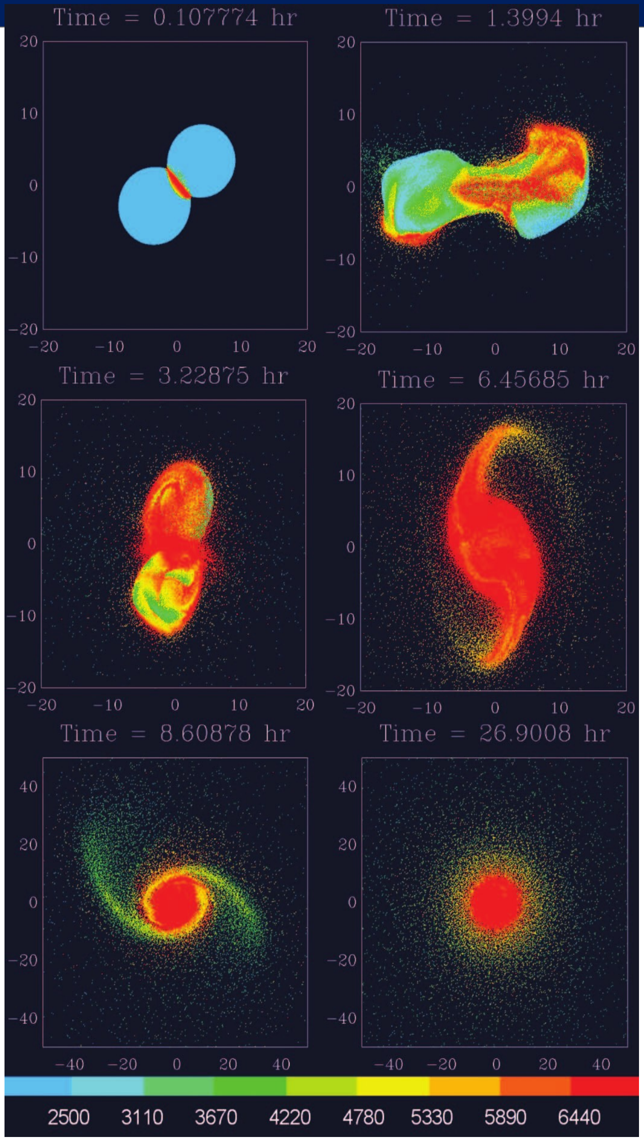




Granular
Ringl, Bringa, Bertoldi, & Urbaseek, Astrophysics J. (2011)

Peridynamics
Ruestes, Tramontina & Bringa, Anales MECOM (2012)

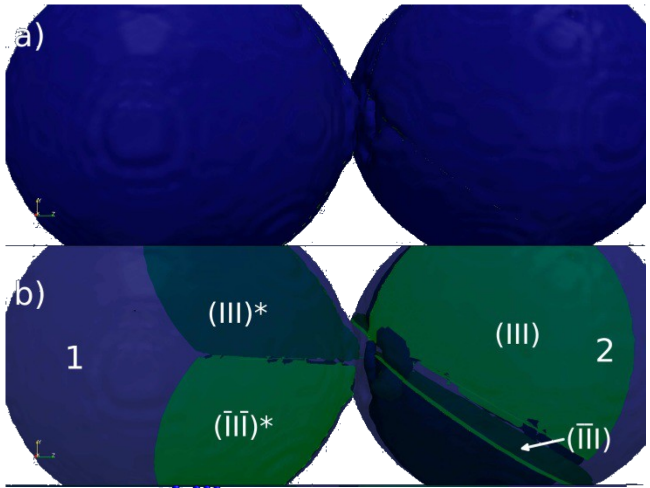
v = 5 m/s^{-1} b/R = 0.8, R~0.03 mm

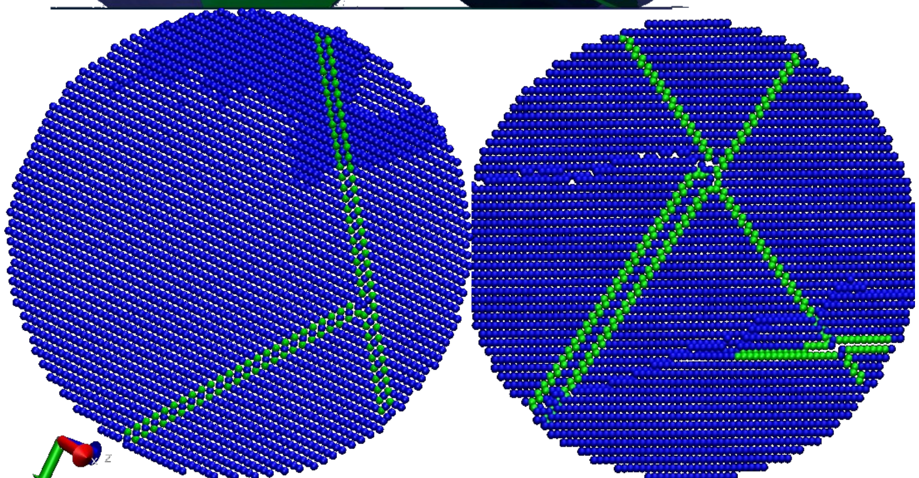


SPH (moon formation)
Canup, Science (2012). b/R=0.4; v= 4 km/s^{-1}

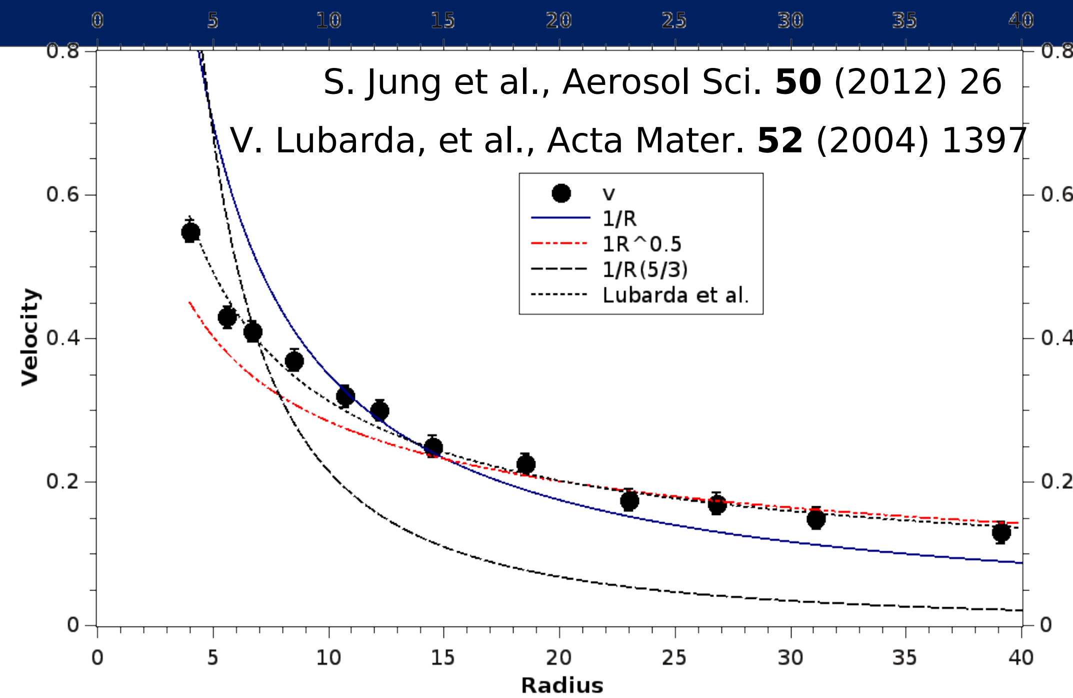
Plasticity threshold in grain-grain impacts

Granular models typically assume lack of plasticity





FCC → stacking faults and twins

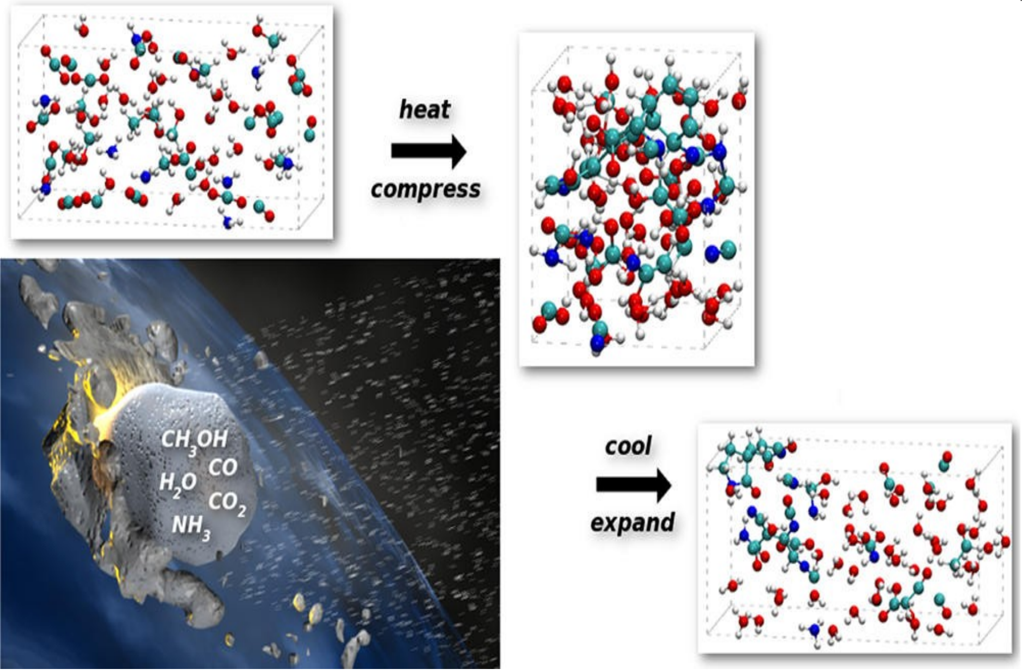


Dislocation-based model by Lubarda *et al*. agrees with MD. Millan, Tramontina, *et al*., to be submitted (2014)

GPUs + CPUs to run ~10000 independent MD simulations

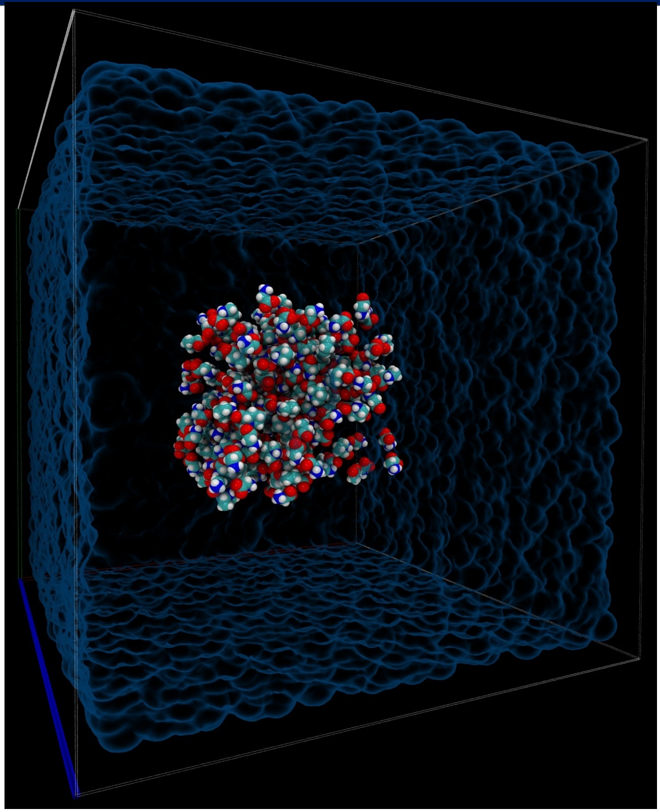
Millan, Tramontina, *et al*., Anales MACI (2013)

Some recent research on collisions



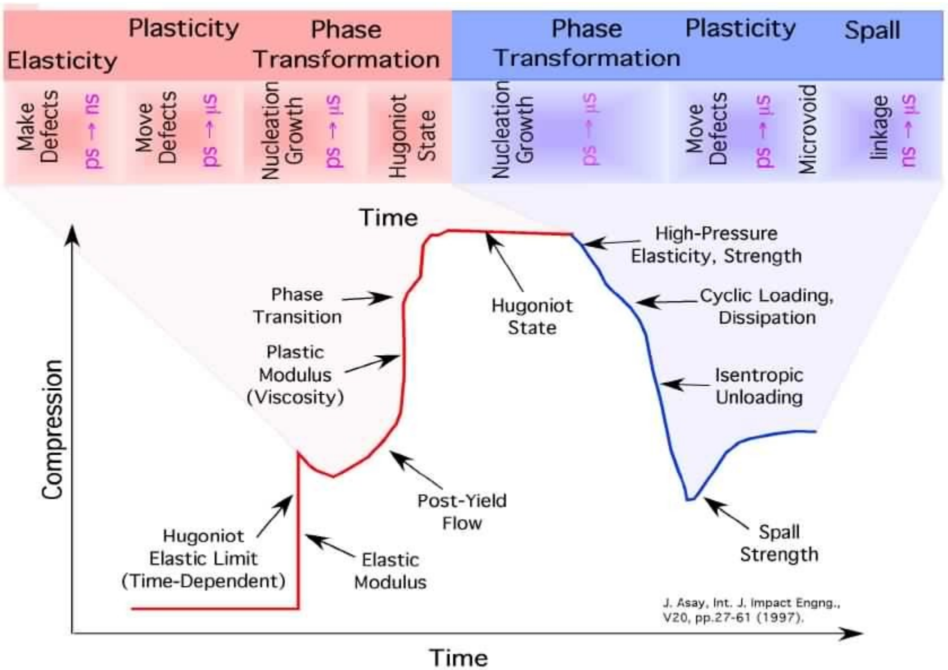
Prebiotic Chemistry within a Simple Impacting Icy Mixture,
Goldman & Tamblyn, J. Phys. Chem. A. (2013)

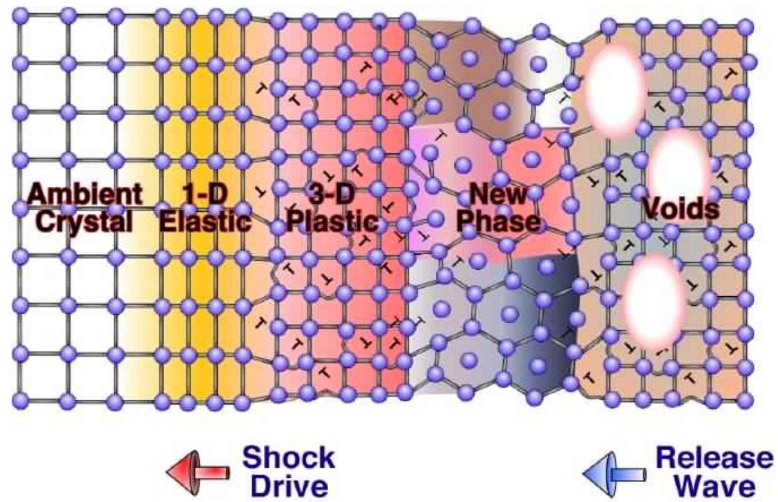
Shock synthesis of amino acids from impacting cometary and icy planet surface analogues
Martins *et al*., Nature Geo. (2013)



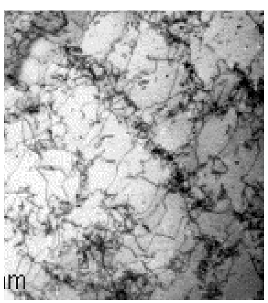
Anders *et al*.: using ReaxFF
100 gly + 100 pro + water →
No reactions for rapid compression
Need slower compression and better reactive potential.

Collision between two large objects: shock waves



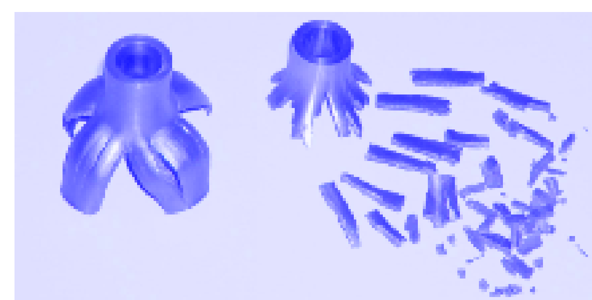


Initial state



Material response is history dependent, requiring an understanding at all time and length scales

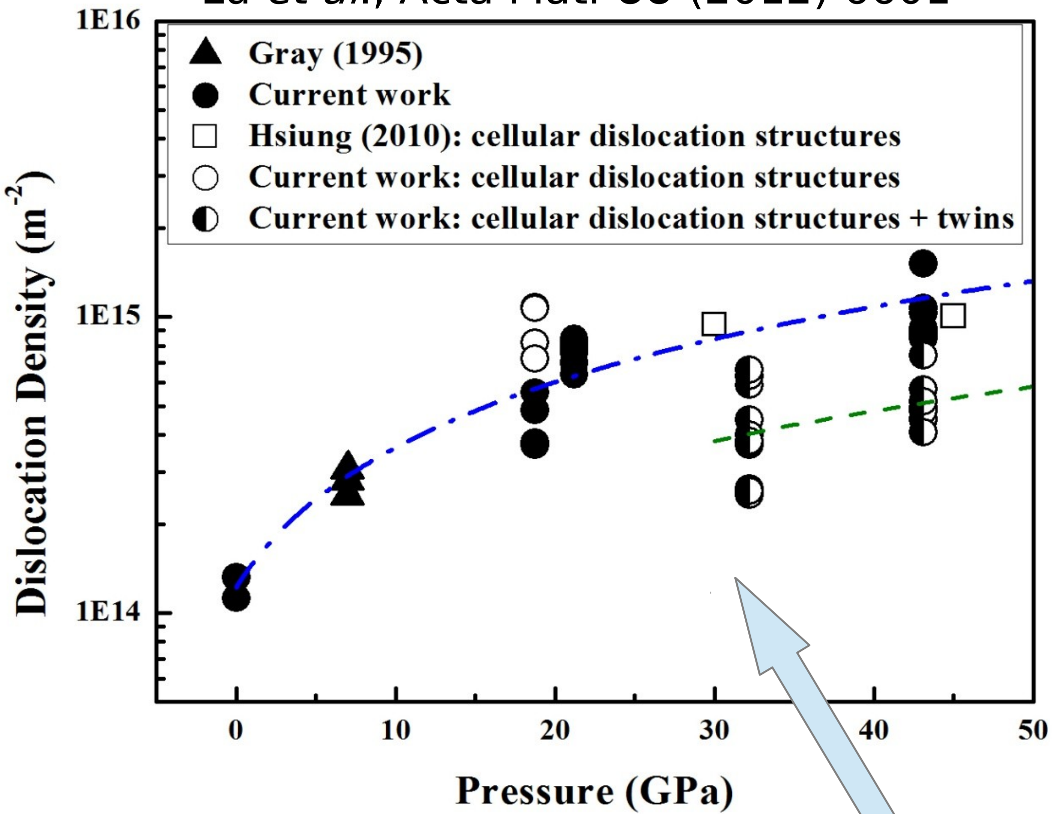
Recovered State



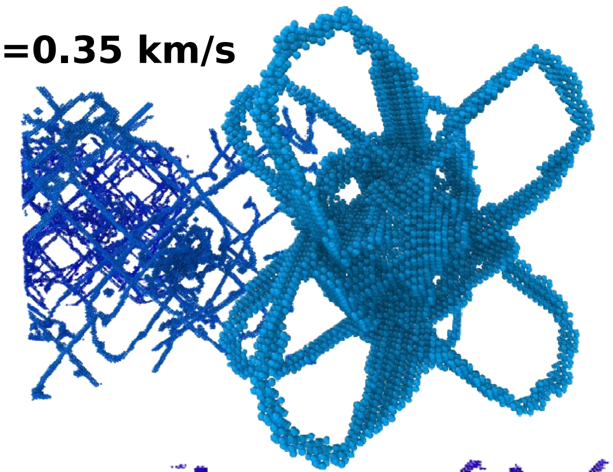
Slip-Twinning transition in Ta

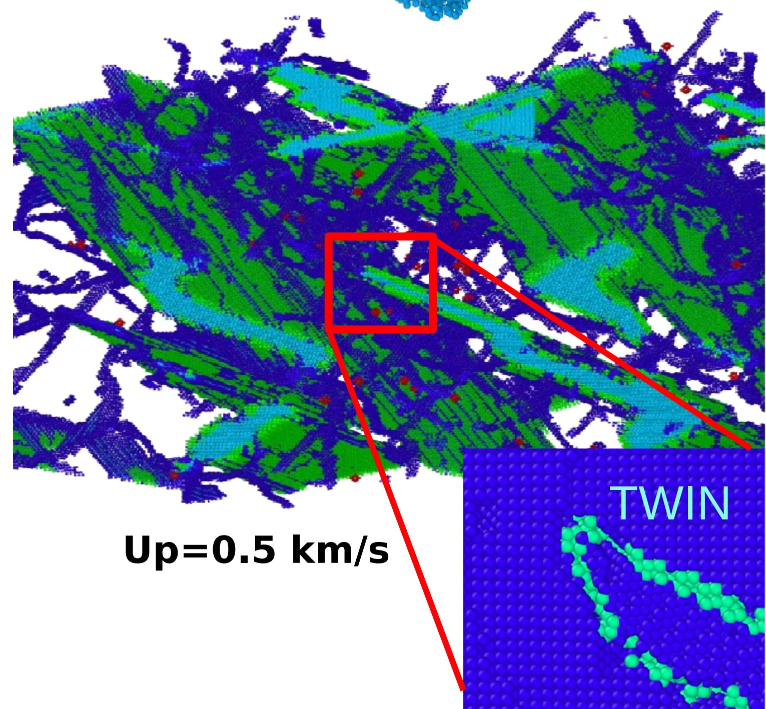
Need to include dislocation-twin interaction in constitutive model, as in Florando *et al*., JAP **113** (2013) 83522. Would also need twin nucleation model!

Lu *et al*., Acta Mat. **60** (2012) 6601



Up=0.35 km/s



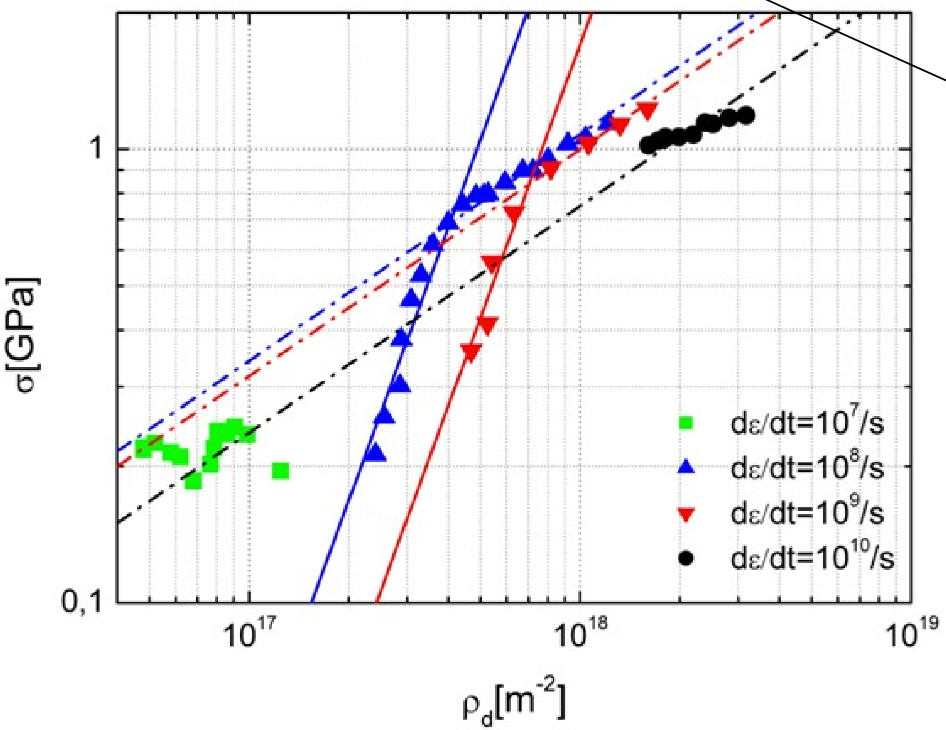


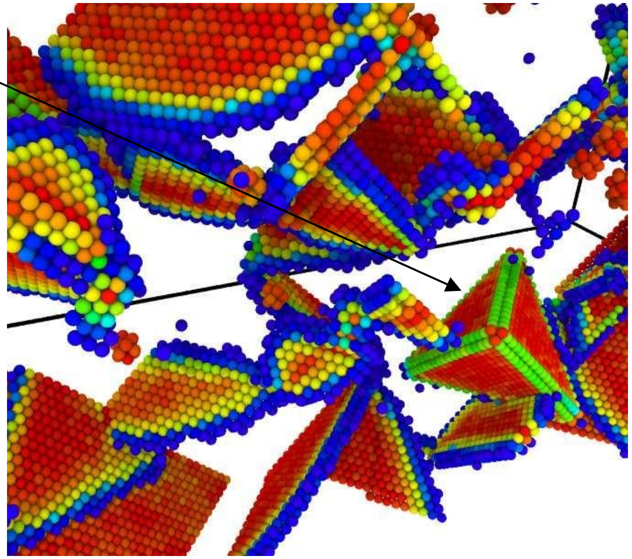
Up=0.5 km/s

Tramontina *et al*., HEDP (2013):
[001] shock loading→ slip-twinning transition at ~30 GPa
Twin nucleation: Suggit *et al*, PRB (2013)

Nanoporous "low" porosity fcc metals under pressure

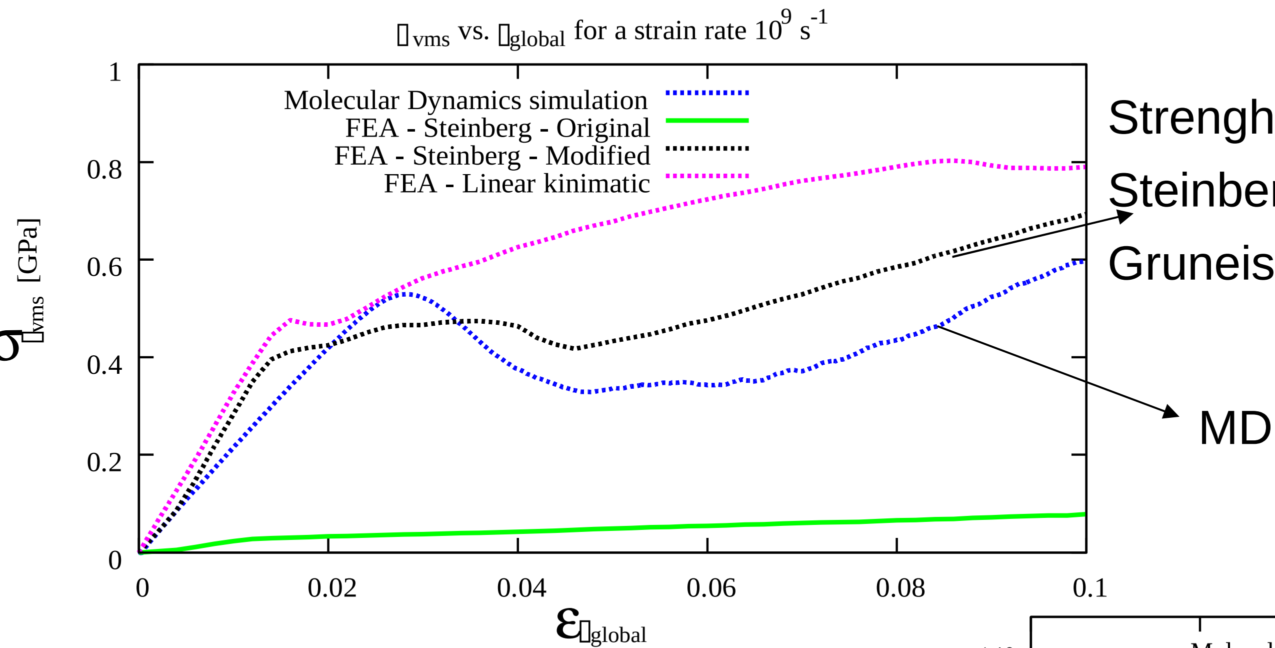
- Strong strain-rate effects. However, plastic yields for 10^7/s and 10^8/s are similar. Yield stresses lower than for single void simulations, due to void-void interactions, in agreement with Wu-Markenscoff model.
- Taylor-style hardenning only for well developed dislocation forest. ρ (MD)~ρ (Exp) at the same strain rates [Milithianakis, Science (2013)].
- Recovery leads to SFTs + vacancies → no "dislocation free" plasticity (Kiritani *et al.*)

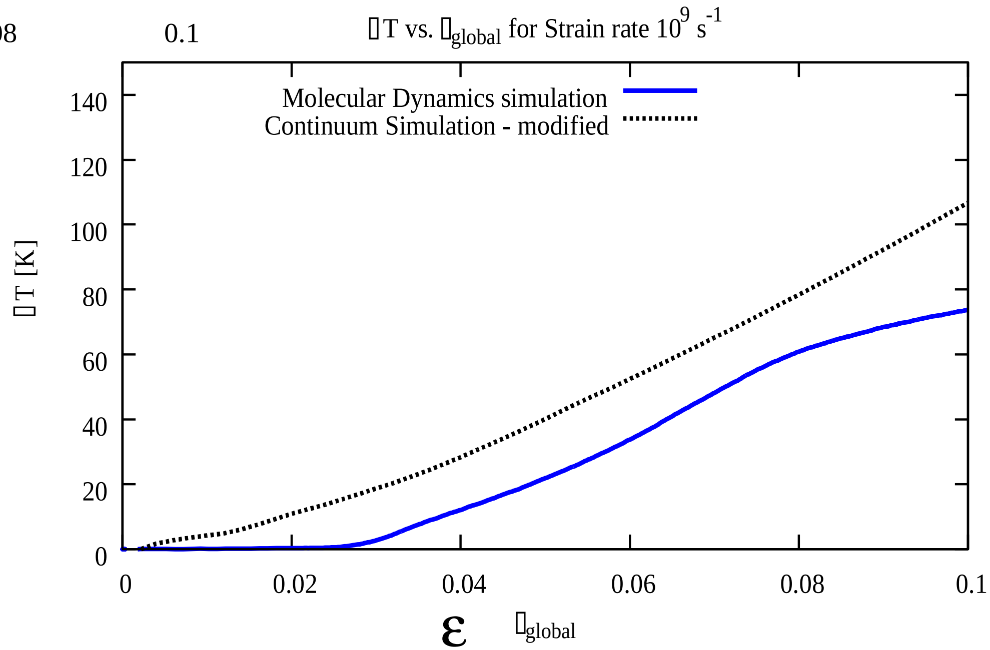




Rodriguez-Nieva *et al.*, submitted to Acta Mat. (2014)

Nanoporous "low" porosity metals: continuum modeling (K. Olney, D. Benson, UCSD). Submitted (2014).





1) Need to modify strenght: use MD result, similar to HP estimates for "filament" between voids.

3) Similar relaxation, hardenning and shear localization.

2) Plastic heating is difficult to describe properly.

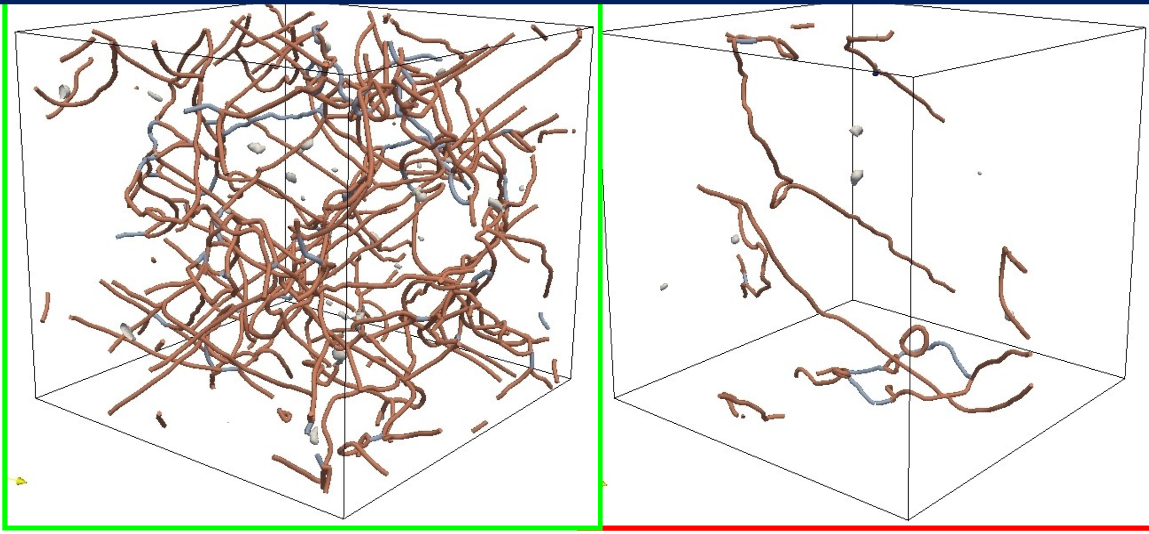
“Recovery” by unloading to zero stress

Can we compare our results with experiments?

Possibly, because long-term recovery of the microstructure in bcc samples should relatively minor effects on total density.

Absence of twins in the recovered sample, which can be checked with X-ray diffraction and agrees with results by Florando et al., JAP (2013).

Challenge: synthesis/fabrication of nanoporous bcc sample.
Could we use sample with incipient spall or radiation damage?



$\dot{\varepsilon} = 10^9 s^{-1}$

ρ ~ **5 10^{16}/m^2**

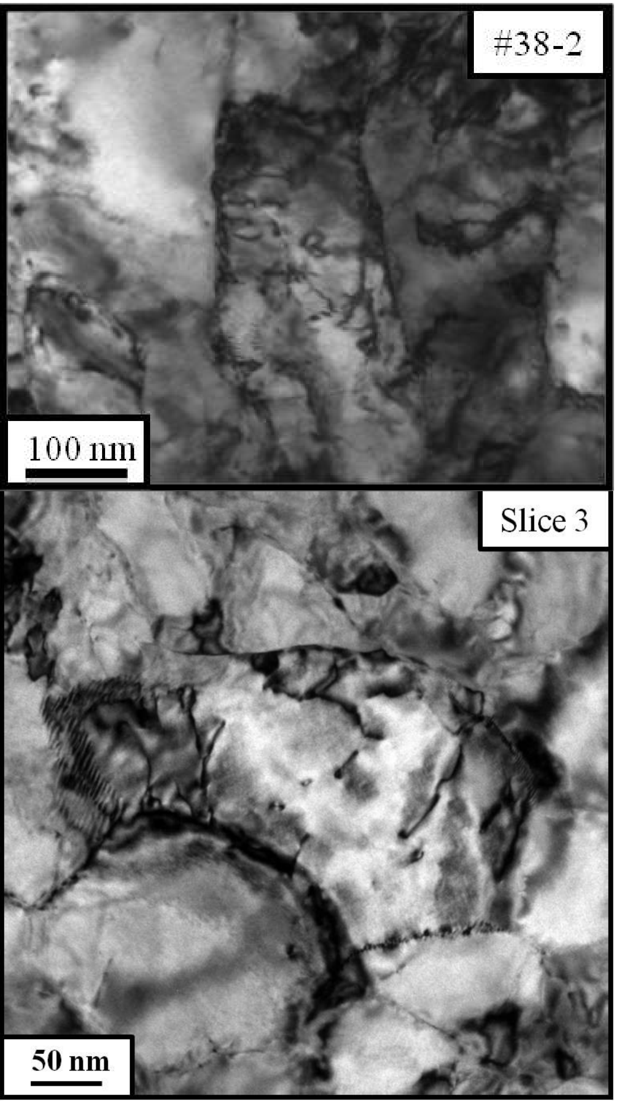
$\dot{\varepsilon} = 10^8 s^{-1}$

ρ~ **8 10^{15}/m^2**

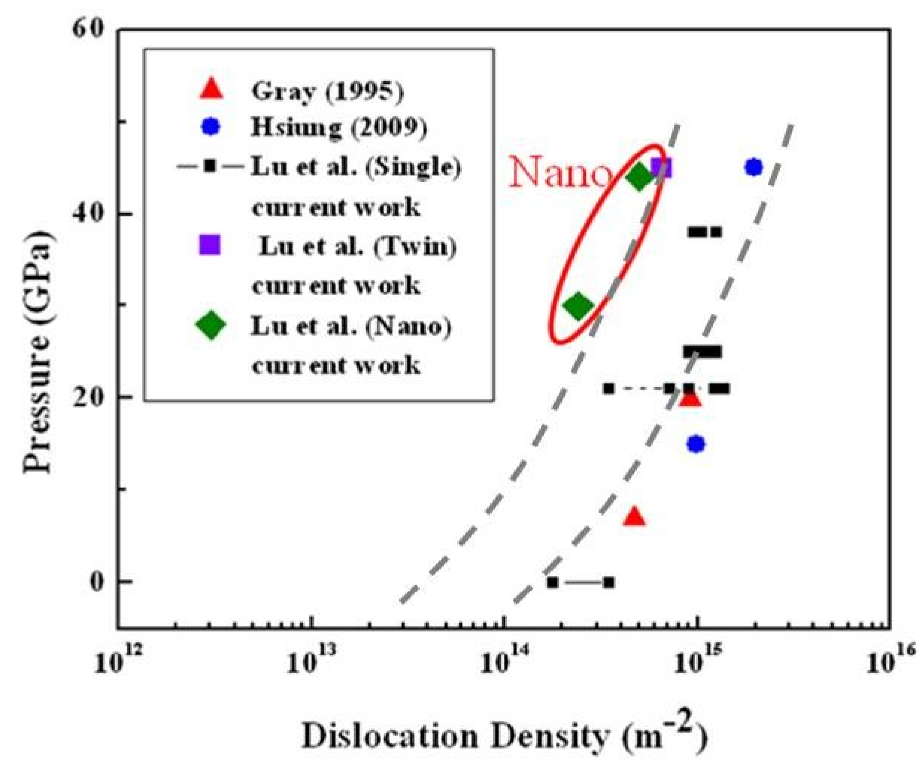
Density decreases by factor ~3.

In fcc metals decreases by factor 10-100

Nanocrystalline Tantalum: lower dislocation and twin densities

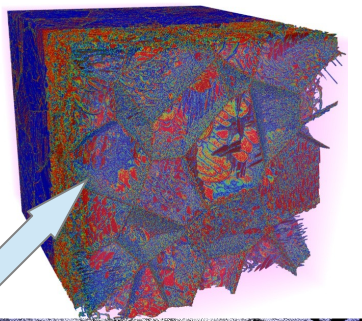


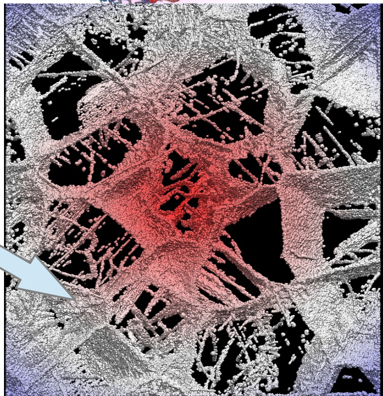
Lu *et al*. Acta Mat. (2013)



Nano is different!

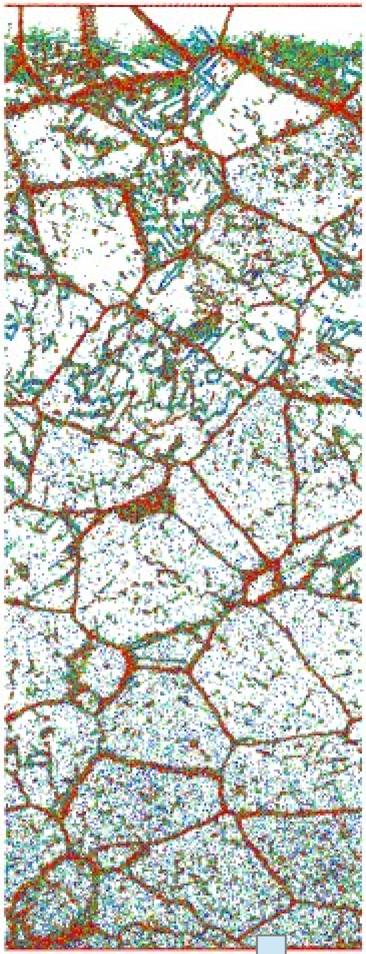
MD: lower dislocation density in nc FCC:
Bringa *et al*., Science **309** (2005) 1838.
Jarmakani *et al*. Acta Mat. 56 (2008) 5584
BCC:
Tang *et al*., MSE A **580** (2013) 414.
Tramontina *et al*., in preparation (2013).



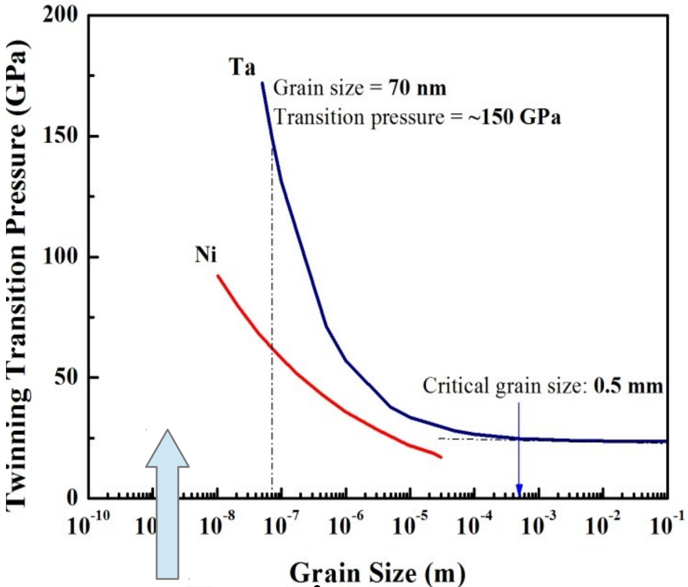


Nanocrystalline Ta: twinning and dislocations

E. Hanhn (UCSD), D. Tramontina (U.N. Cuyo), T. Germann (LANL)

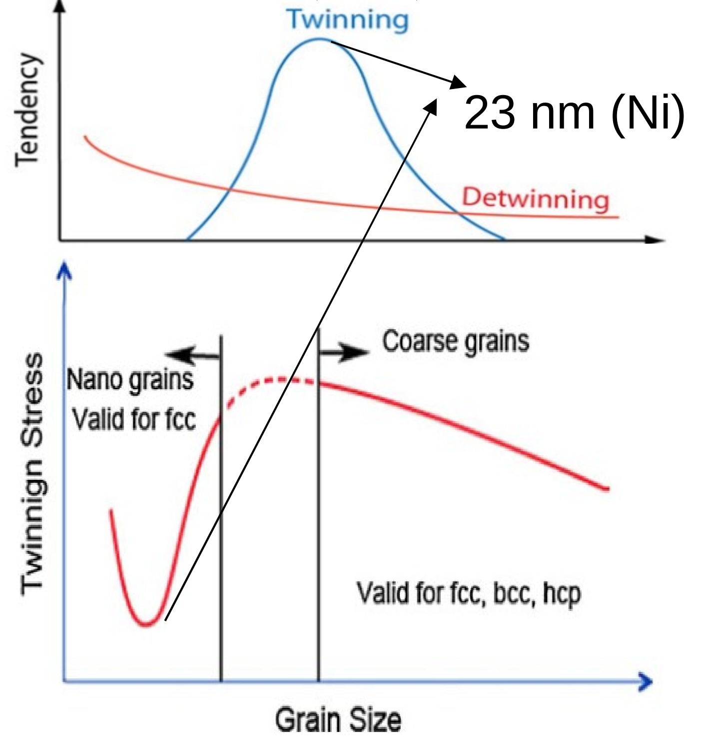


Hall-Petch for twinning



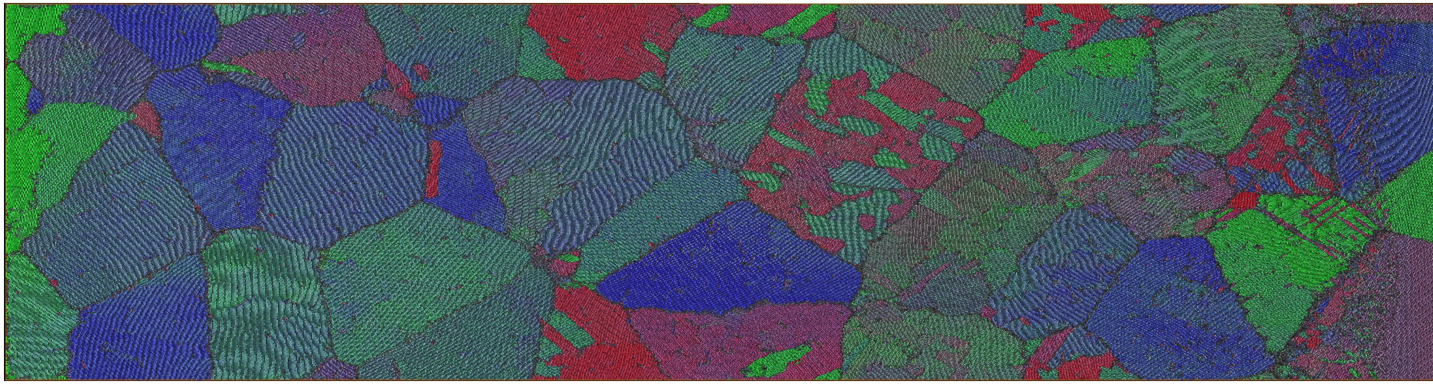
Experiment:
No twins for Ta d~70 nm
Lu *et al*. MSE A (2013)

FCC: exp + model by Zhu *et al*.
J. Mater Sci (2013) 48, 4467

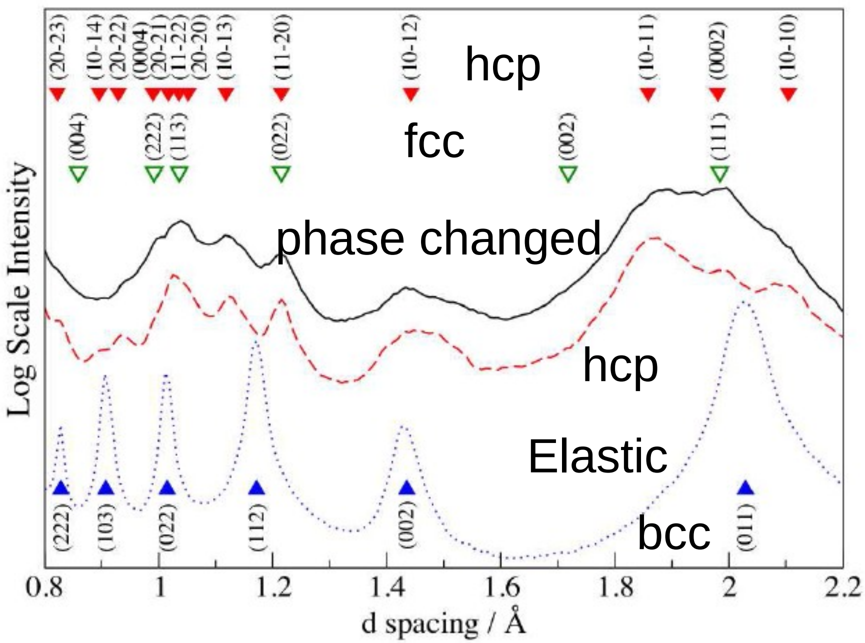


MD: d~5-30 nm

Inverse Hall-Petch for twinning

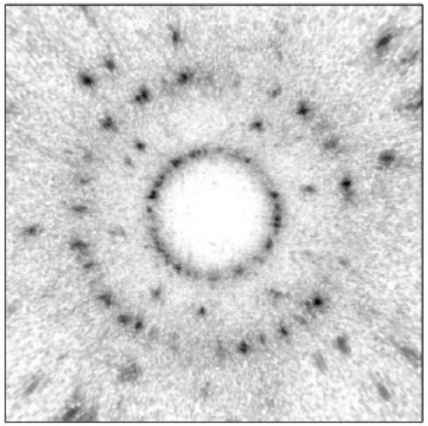


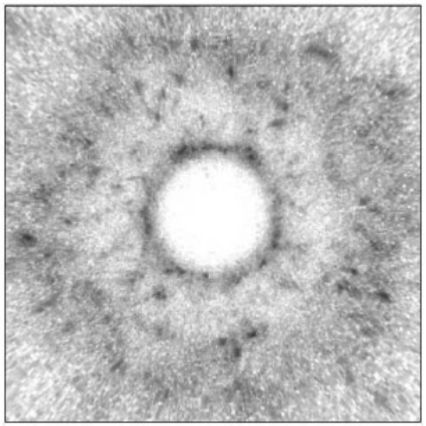
Novel simulated XRD processing for polycrystal simulations (J. Wark's group, University of Oxford) PRB (2014)



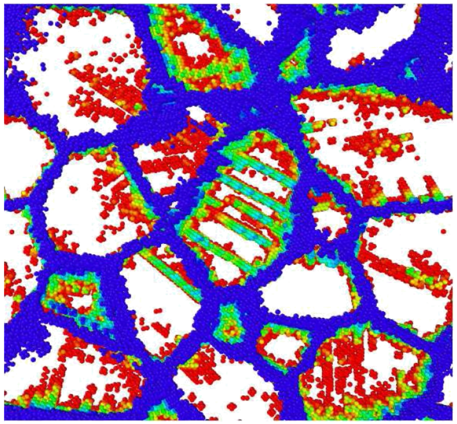
(a)

Experimental geometry: 50 × 50 mm film, placed 30 mm in transmission, 8.05 keV (Cu Kα) X-rays, perpendicular to the film.


(b)
unshocked


(c)
phase changed

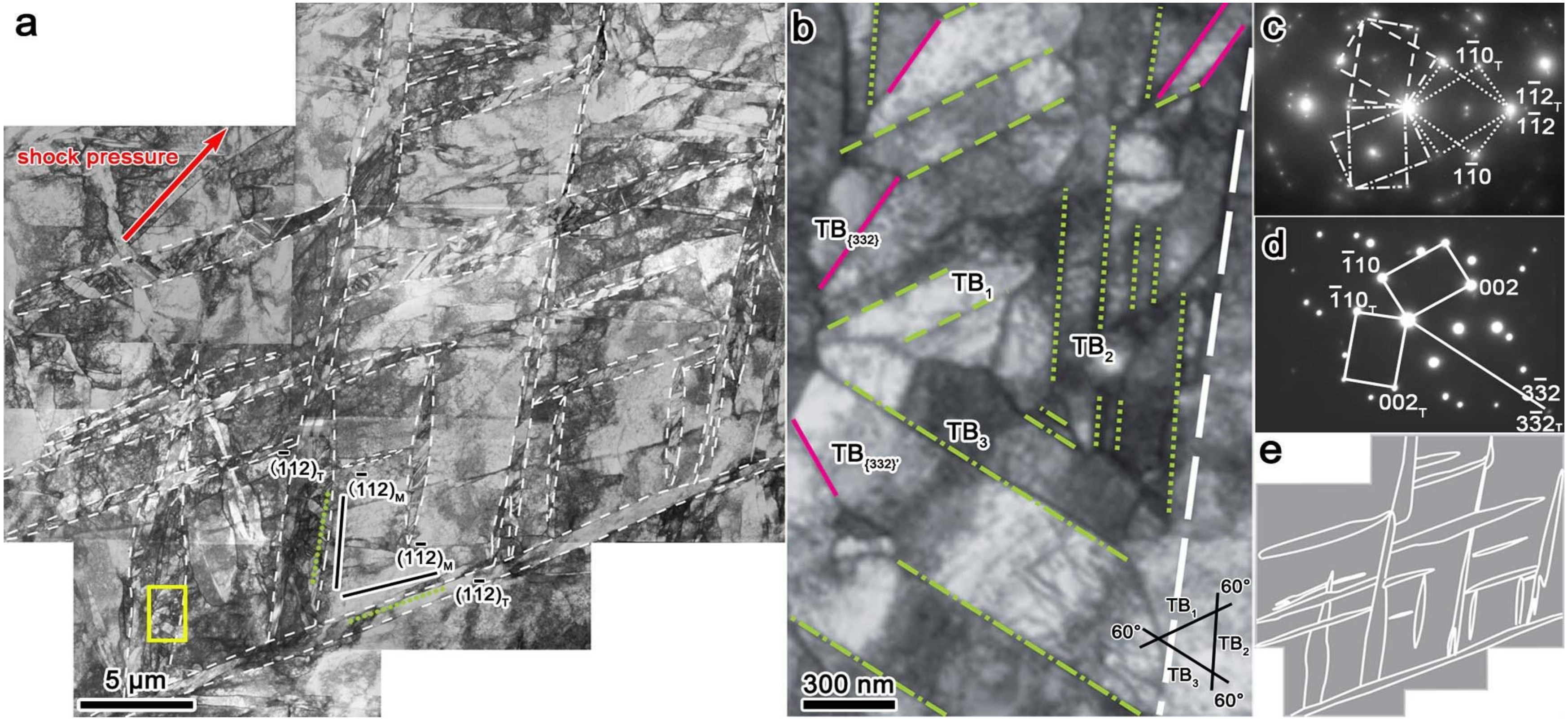
Simulated XRD agrees with existing experimental results for micron-sized polycrystals: there is almost no evidence for fcc phase in diffraction.



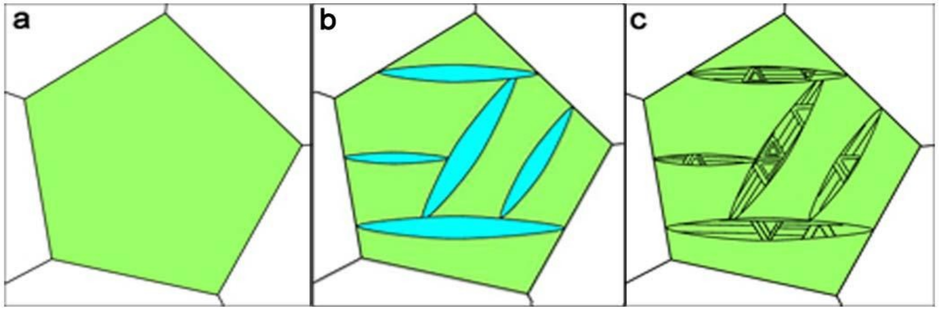
Time for phase change is extremely short (~50-100 ps). Could it be meassured in experiments similar to the one in Milithianaki *et al*, Science **342**, 220 (2013), for Cu 1D→3D relaxation (~100 ps)?

Twins in recovered samples

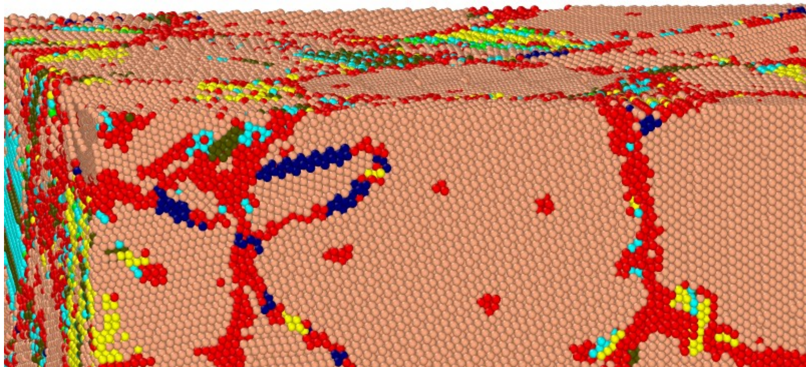
Wang *et al.*,
Sci. Rep. 3, 1086 (2013)



Schematic illustration of the α → ε → α transformations

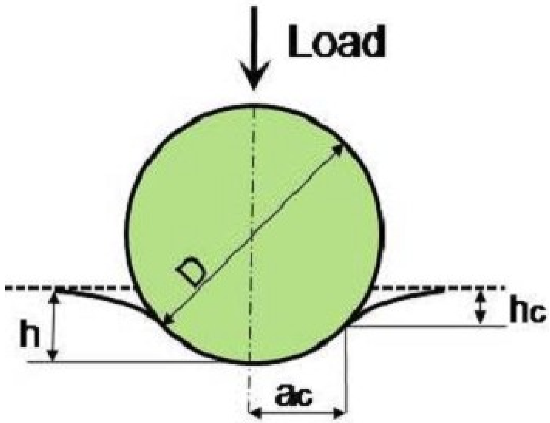


MD: Tramontina, Gunkelmann, *et al.*



Nanodureza: colisiones con una superficie a 3-30 m/s

SiMAF

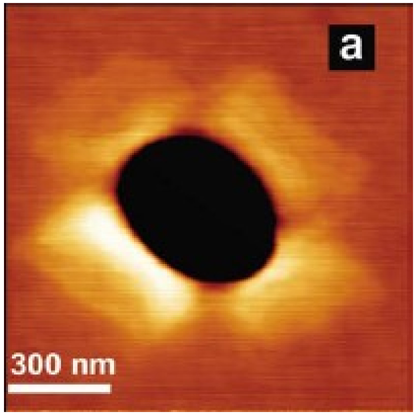


¿Qué es la dureza/nanodureza?
La *dureza* es la resistencia de un material a ser rayado o penetrado, por lo cual estamos midiendo la cohesión entre los átomos del material.

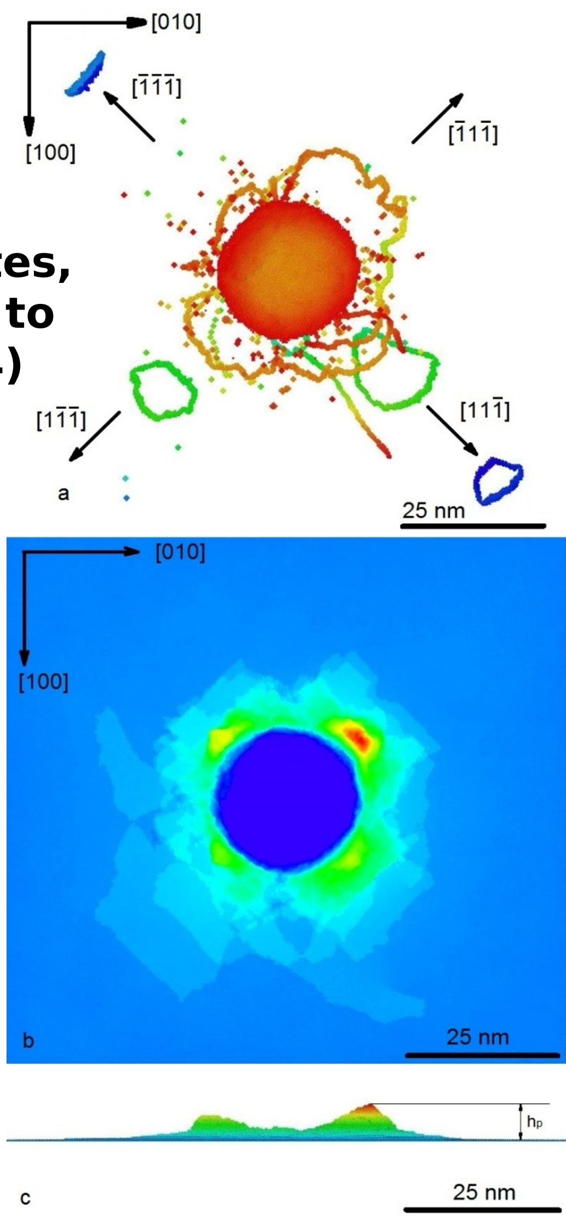
Simulaciones (ICB) & Exp. (UCSD)

Dislocaciones determinan promontorios

Remington, Ruestes, *et al*., submitted to Acta Mat. (2014)

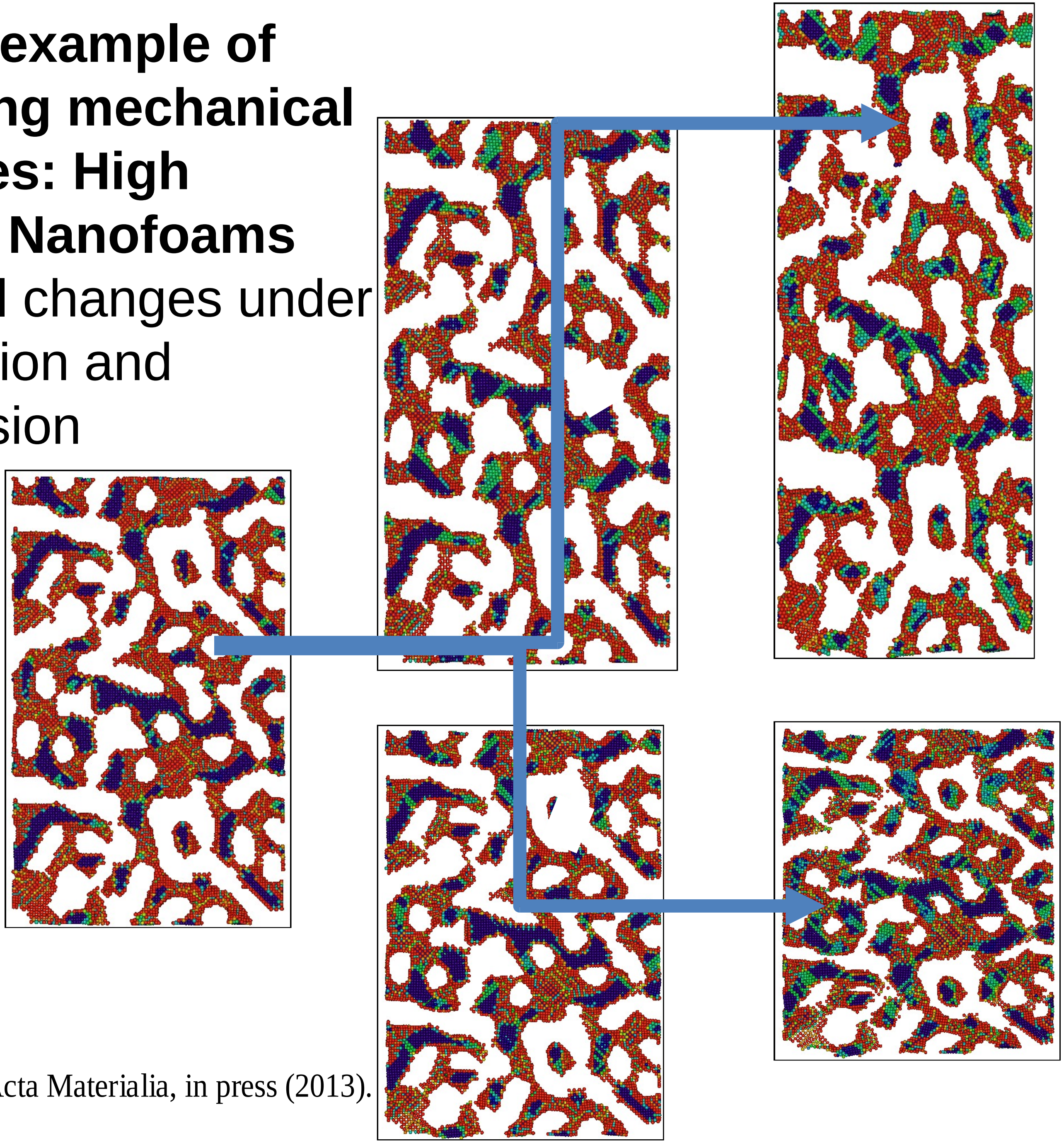


Biener *et al*. PRB 76 (2007) 165422



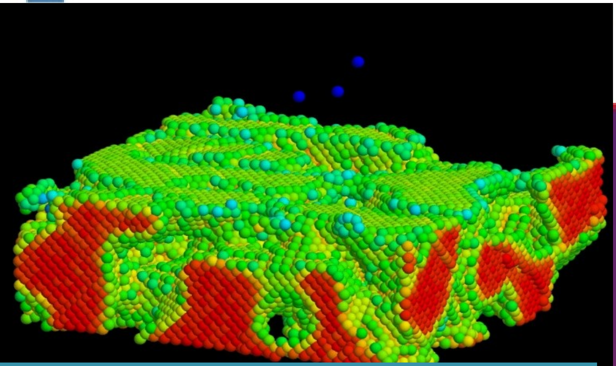
Another example of interesting mechanical properties: High Porosity Nanofoams

Structural changes under both tension and compression



D. Farkas *et al*., Acta Materialia, in press (2013).

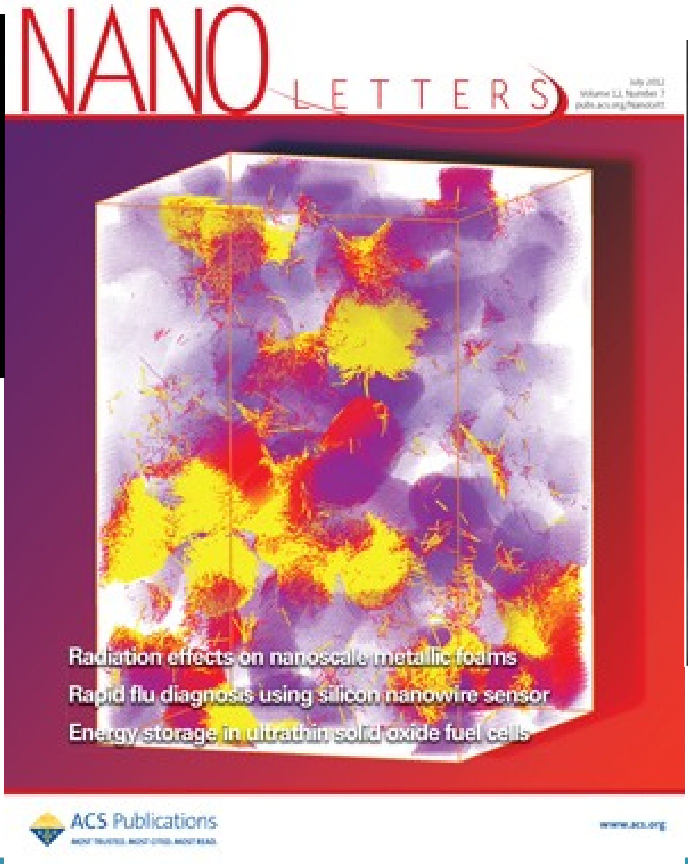
Simulaciones/experimentos for nanoespumas



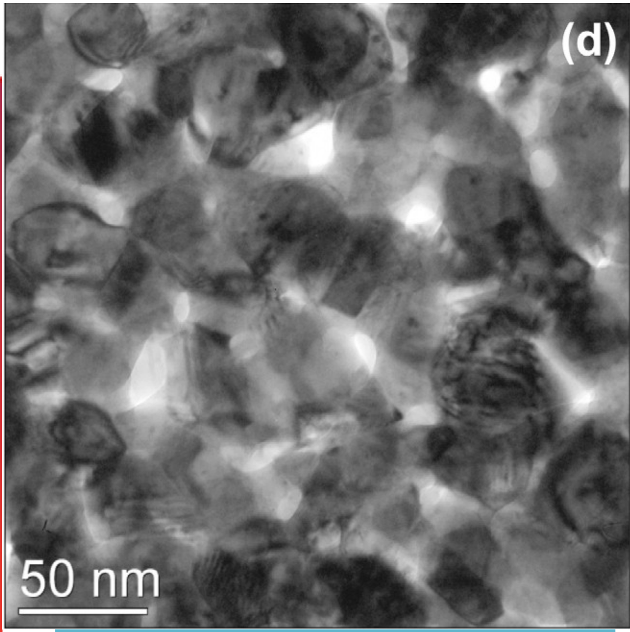
I) Bombardeo con iones rapidos.
Rodriguez-Nieva *et al*., Astrophysical J. Letters (2012). ICB/Uva/NASA/LANL

II) Modelo basado en geometria de nanoporos **Rodriguez-Nieva & Bringa, NIMB (2013).**

III) Bombardeo con iones de keV, Anders, Bringa & Urbassek, a enviarse (2014). ICB/TUK



Espuma de Au. 5 bombardeos. Color: desplazamientos debidos al bombardeo (rojo= mas de 1.65 nm).
Bringa *et al*., Nano Letters (2012) ICB/LANL/VaTech

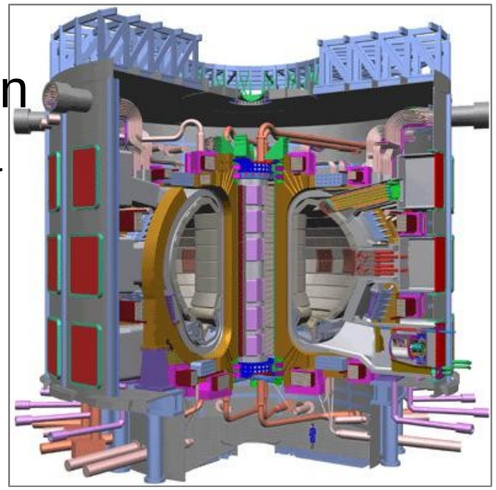


Espuma de Au
400 keV Ne (0.0035 dpa/s), mostrando bordes de grano, maclas y fallas de apilamiento tetrahedricas (SFT) debidas a irradiacion.
Fu *et al*., APL (2012). LANL/LLNL/ICB

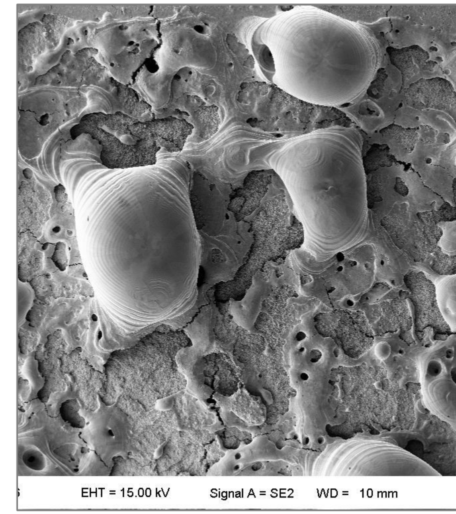
Materiales para reactores de fusión

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

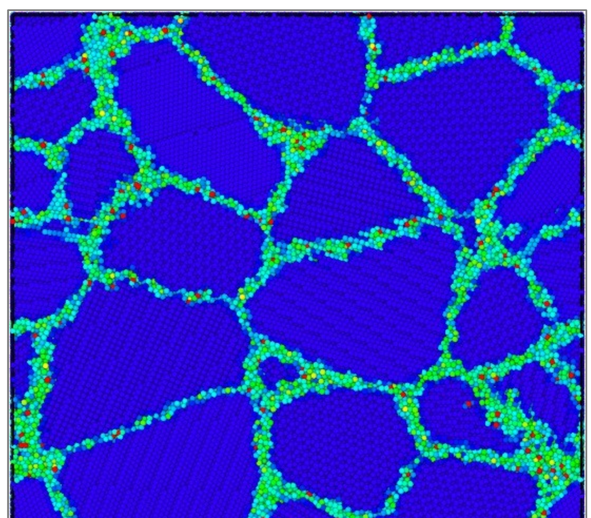
Los futuros reactores de fusión nuclear serán una fuente de energía sustentable y no contribuirán al calentamiento global.

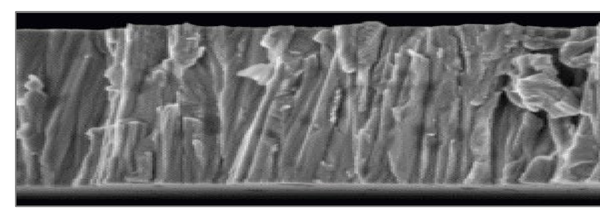


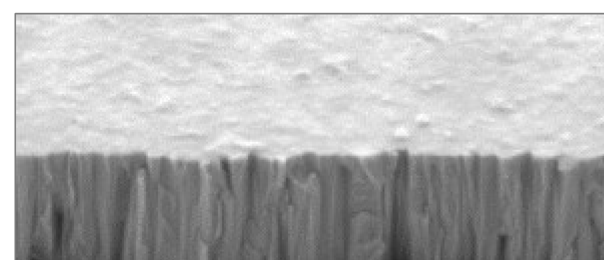
Entre los desafíos tecnológicos actuales se encuentra hallar materiales que toleren el ambiente severo del reactor.



Los nanomateriales presentan mayor dureza y resistencia a la radiación que sus contrapartes convencionales. Actualmente se está investigando el uso de tungsteno nanocristalino.







On going work in our group (MD+MC)

SiMAF
Simulaciones en Materiales Astrofísica y Física

- **High pressure (shocks and DAC)**: Cu, Ta, W, Zr, diamond, BMGs, organics, etc. (LLNL, LANL, UCSD, Oxford, T. U. Kaiserslautern, Florida St. U., Sweden, etc.).
- **Irradiation of materials with particles and lasers (reactors, astrophysics, etc.):** foams, nanowires, nanocrystals, etc. (LANL, T.U. Kaiserslautern, U. Helsinki, U. Chile, U. Pol. Madrid, MIT, U.Va, CAB).
- **Mechanical properties** (tension, compression, fracture, **nanoindentation**): nanocrystals (including impurities like H), porous materials, Bulk Metallic Glasses, granular materials, etc. (LANL, T.U. Kaiserslautern, Va. Tech, UCSD, CAB).
- **Thermodynamics of nanosystems**: nanoparticles, nanofilms, nanotubes, etc. (U. Catolica de Chile, U. Comahue, CAB).
- **Other lines:** (I) **Biology**: ecosystem modeling (CCT-Mendoza), (II) **Computer Science**: GPUs [data processing (Oxford), MD (T.U. Kaiserslautern), images (FUESMEN), CA and ABM (UNSL, UNC)].

New ICB-ITIC cluster (shared), affiliated to SNCAD, ~170 cores, 8 GPUs

Opportunities for Ph.D. students, postdocs. Escribir a ebringa@yahoo.com

Computadoras son una herramienta esencial pero Argentina tiene clusters escala “nano”

SiMAF

Nanotecnología: nuevos procesadores con nanocircuitos

Cluster: conjunto de computadoras interconectadas para cálculos en paralelo.

Argentina:1 de 2000? cores (Giol), 2 de 600 cores (UNC/CNEA), ~20 clusters con ~100-300 cores.“Cristina”, UNC 560 cores.

Cluster ICB-ITIC, 160 cores/7 GPUs; Admin: E. Millán (CONICET)

Titan, 300000 CPU cores, 20000 GPUs K20 (ORNL, USA).

Top 500 Mundial: entre 150000 y 3.2 millones de cores. http://www.top500.org/

GPUs: nueva manera de calcular, ecológicas y “económicas”

GPU (Graphics Processing Unit): placa de video para procesamiento de gráficos. Videojuegos/aplicaciones 3D. Calculo científico utiliza arquitectura optimizada para procesamiento paralelo.