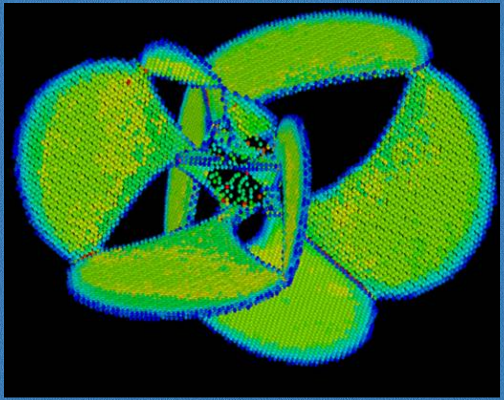
Simulaciones a gran escala en nanotecnología utilizando CPUs y GPUs



Eduardo M. Bringa

ebringa@yahoo.com

CONICET

FCEyN (Instituto de Ciencias Básicas), Universidad Nacional de Cuyo, Mendoza, Argentina

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

Fondos:

Agencia CyT, Argentina: PICT2008-1325

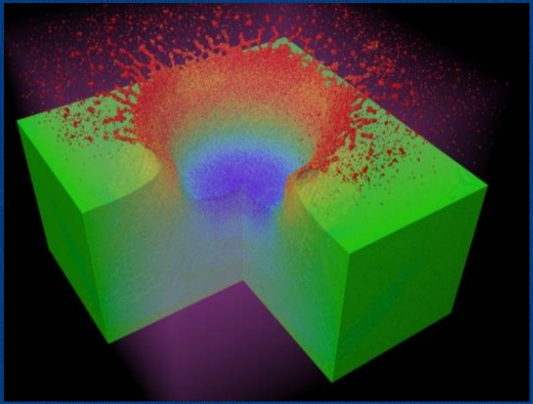
PICT2009-0092

SeCTyP, UN Cuyo

WHPC-2014

CORDOBA

Agosto 2014



COLLABORADORES: **D. Tramontina, C. Ruestes, E. Millan (U.N. Cuyo), J. Rodriguez-Nieva** (I. Balseiro,MIT), D. Farkas, J. Monk (VaTech), R. Ravelo, T. Germann, A. Caro, M. Caro, E. Fu, E. Martinez (LANL), N. Gunkelmann, C. Anders, H. Urbassek (TU Kaiserslautern), R.E. Johnson, T. Cassidy (U Virginia), 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. Hawreliak, R. Rudd (LLNL), M. Ruda, G. Bertolino (Instituto Balseiro, Argentina), A. Stukowski (TU Darmstadt, Germany), P. Erhart (Chalmers U., Sweden), N. Park (AWE, UK), A. Higginbotham, M. Suggit, J. Wark (University of Oxford, UK), R. Gonzales, A. Rivera, A. Prada (UP Madrid).

SiMAF

E.M. Bringa's group: Simulations in Materials Science, Astrophysics, and Physics

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

SiMAF

Simulaciones en Materiales Astrofísica y Física

Expertise in molecular dynamics (MD), granular mechanics, Monte Carlo (MC), and high performance computing (HPC) in general

1 postdoc, 3 Ph.D. students, 2 undergraduate students, several "visiting" students

Research activity in last 2 years:

Active collaborations & joint funding with groups in Argentina, USA, EU and LatAm

Nano-science (funding PICT-PRH-2010, SeCTyP UN Cuyo):
Mechanical and thermal properties of materials under extreme conditions

Materials at high pressures (funding PICT-2009, Royal Society,SeCyT-UNCuyo, DOE):
Strength, phase transformations

Radiation damage and astrophysics (funding PICT-PRH-2010, NASA, LANL, etc.):
Materials for GenIV and fusion reactors, cosmic rays, interstellar and solar grains

Ecosystem modeling (funding PICT, PICT-PRH-2012):
Arid ecosystems: nutrient cycles, interactions settlement/cattle/vegetation/water.

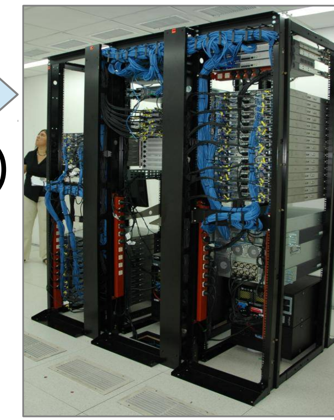
Computadoras son una herramienta esencial pero Argentina tiene clusters escala “nano”

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.

MD limitations in materials sciences

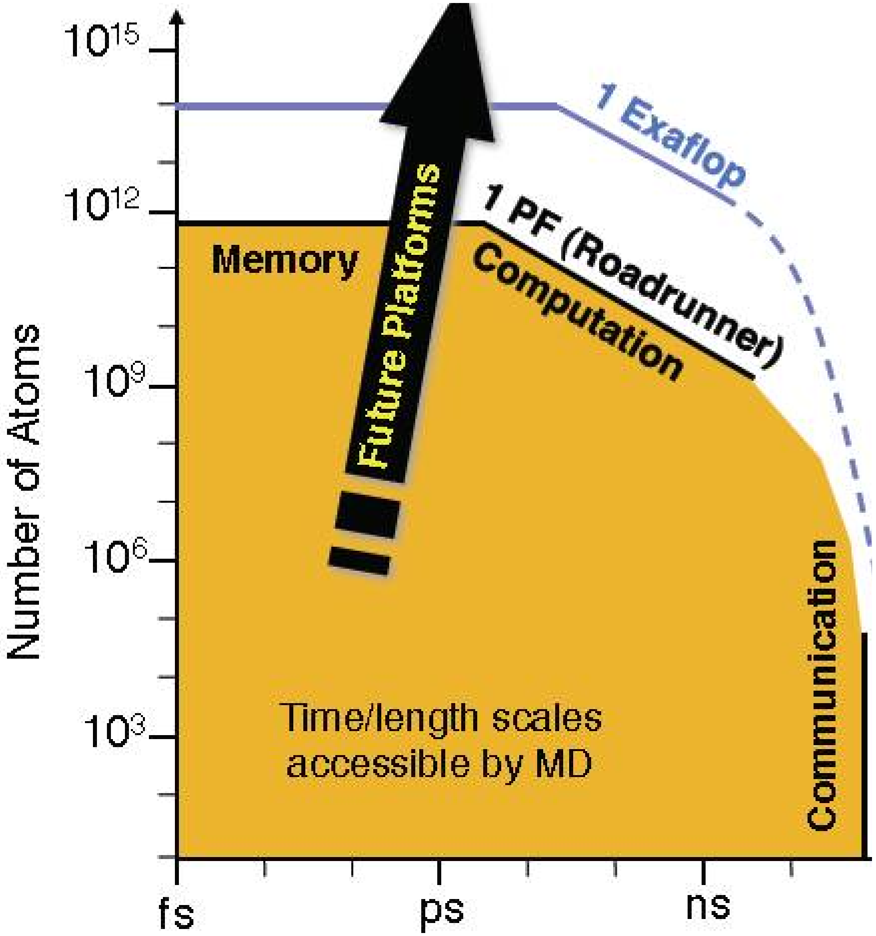


Figure by T. Germann for SPaSM (LANL)

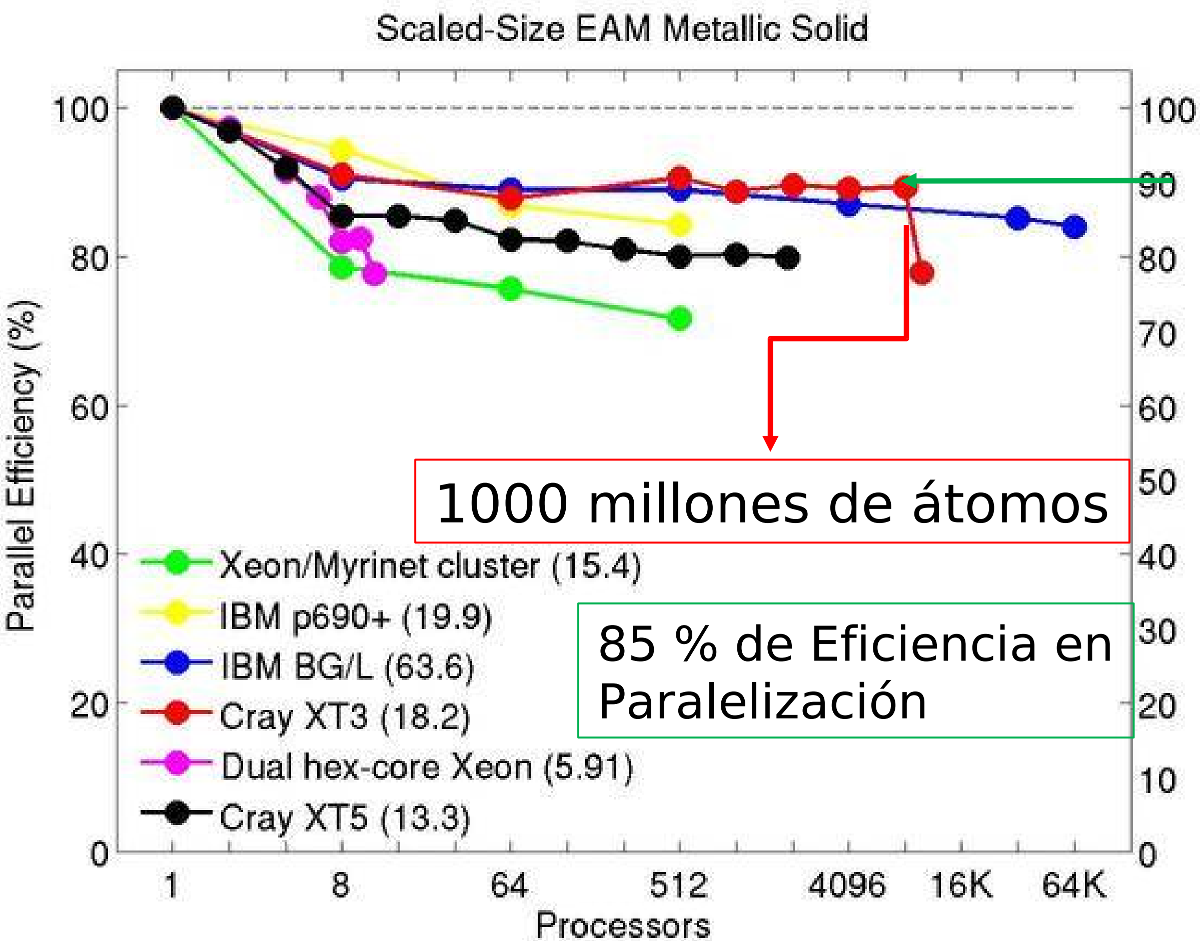
Main Challenges:
Memory limitations +
Communication limitations

Additional problems:
Short range vs. long range potentials (how to find neighbors?), increasing complexity of potentials, I/O (including checkpointing), on the fly analysis, etc.

Pushing boundaries has led to many Gordon-Bell awards

MD using "short-range" interactions has nearly perfect parallel scaling (fast connectivity, homogeneous clusters)

http://lammps.sandia.gov/bench.html#eam



LAMMPS

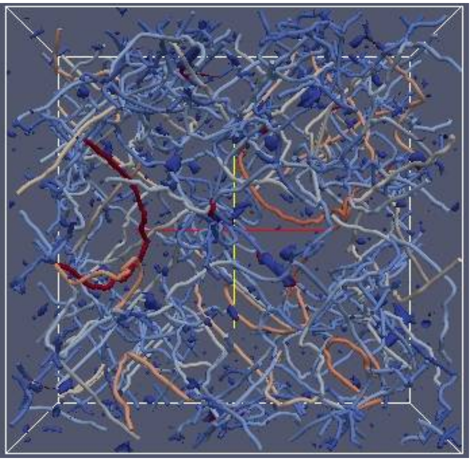
Large-scale Atomic/Molecular Massively Parallel Simulator

Freeware, open source. CPU-GPU

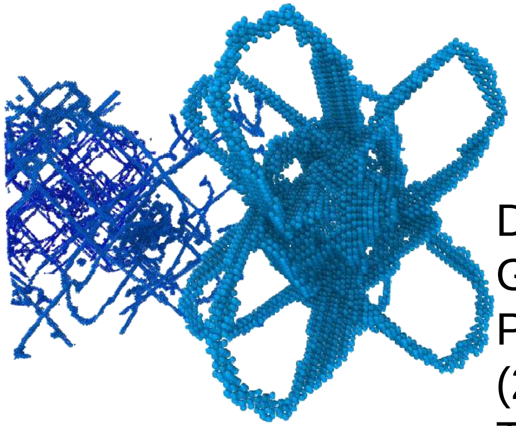
Use also other software as needed.

Big-data challenges!

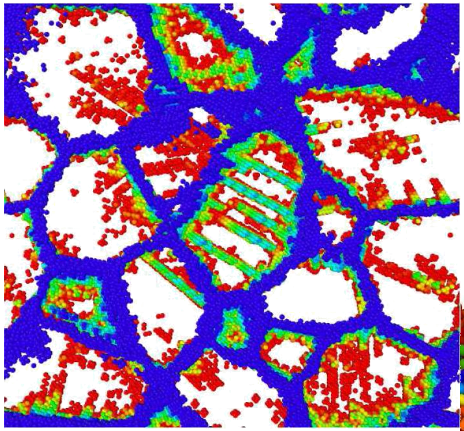
Ejemplos: Nuevos materiales gracias a estructuras con defectos: Utilizar dislocaciones, bordes de grano, porosidad, maclas, etc.



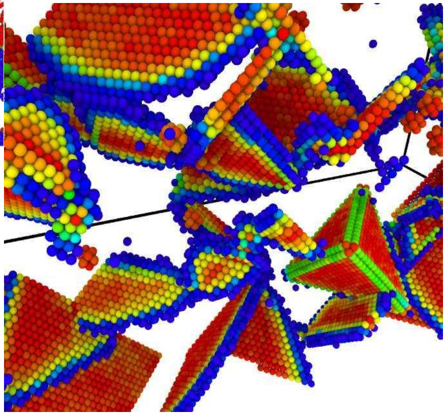
Dislocaciones en tantalio,
Ruestes *et al*.,
Comp. Mat. Sci. (2014)
ICB/UCSD



Plasticidad en tantalio,
Tramontina *et al*.,
HEDP (2013)
ICB/Oxford/LLNL/LANL



Dislocaciones en hierro
Gunkelmann *et al*.,
Phys. Rev. B. Rapid (2014)
TUK/ICB/Oxford

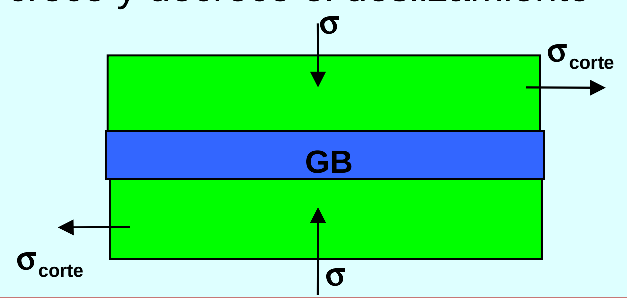


Fallas de apilamiento tetrahedricas en oro
Rodriguez-Nieva *et al*.,
en revision, Acta Mater. (2014)
ICB/MIT/JHU

Se puede controlar nano-estructura basado en velocidad de deformación y condiciones iniciales de defectos →
mejores propiedades mecanicas (dureza, resistencia a la friccion, etc.)

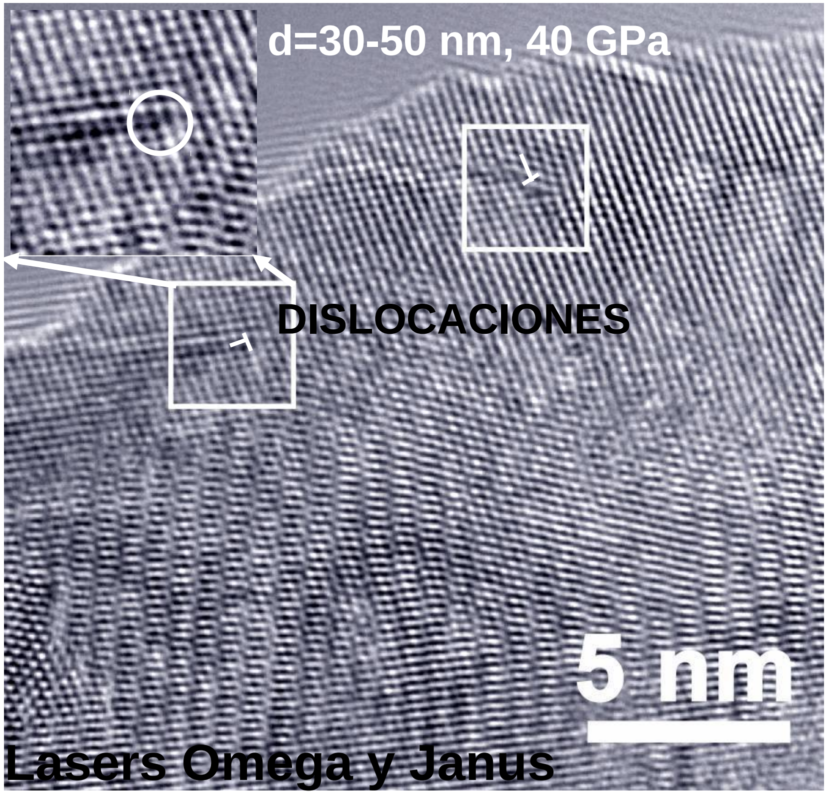
Simulaciones y experimentos muestran que es posible crear materiales ultra-duros utilizando ondas de choque

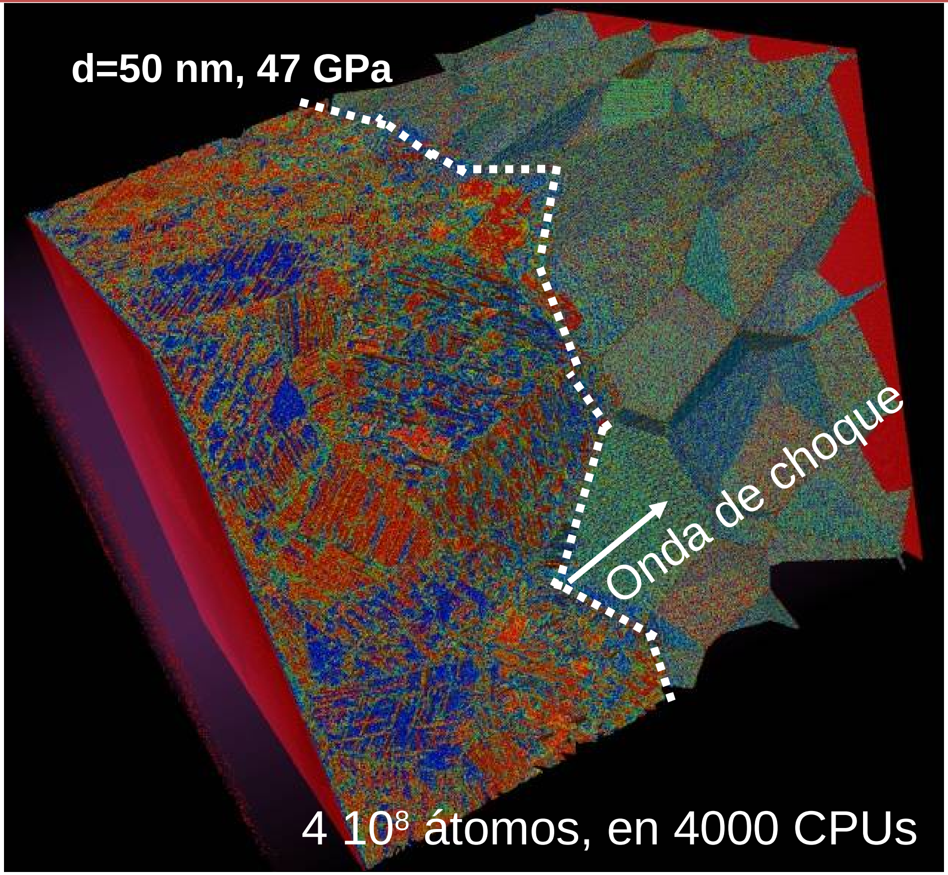
Fricción ~ fuerza normal **(σ)** ➔ σ crece y decrece el deslizamiento



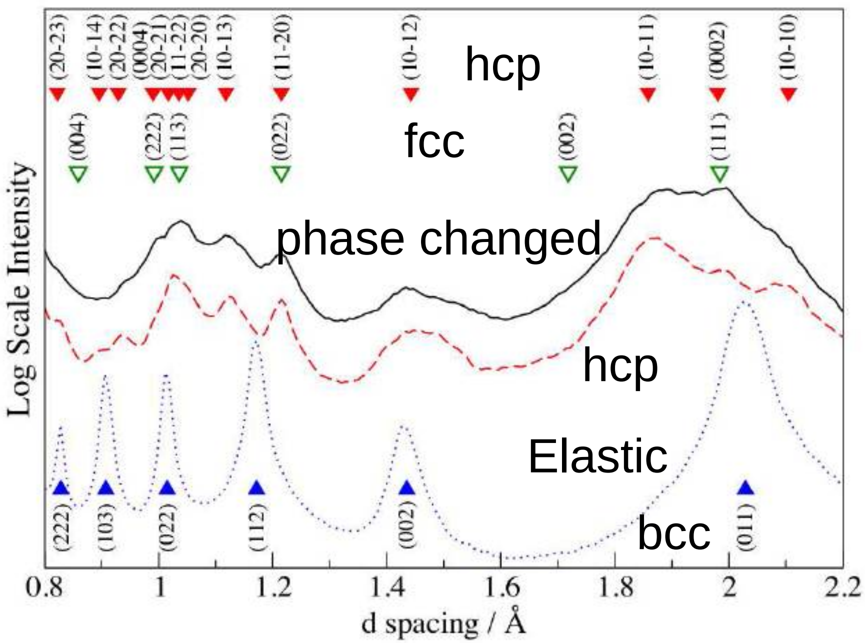
E. Bringa *et al*., *Science (2005), APL (2005 & 2006), etc.*

- **Presiones altas en la onda de choque decrecen deslizamiento de bordes de grano y producen dislocaciones.**
- **Alta densidad de dislocaciones lleva a una mayor dureza luego de la onda de choque (MD + exp.).**



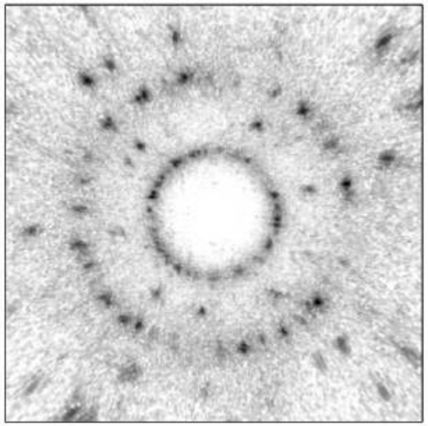


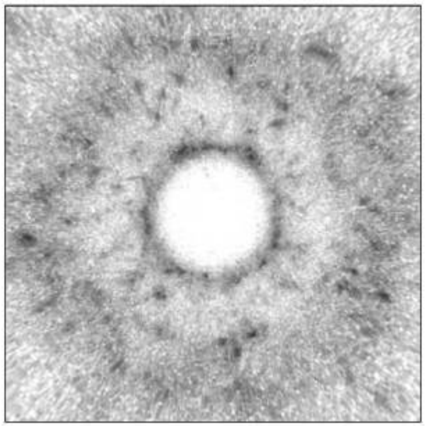
Novel simulated XRD processing for polycrystal simulations (J. Wark's group, Oxford, CPUs-GPUs) PRB-Rapid C. (2014)



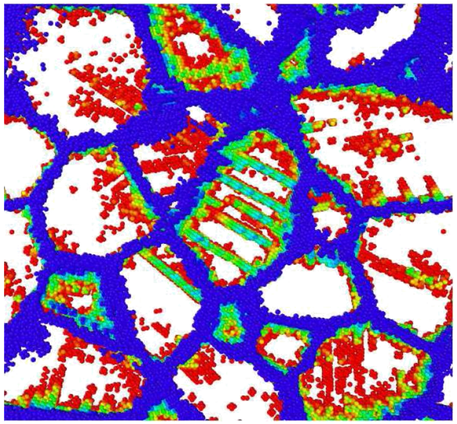
(a)

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


(b)
unshocked

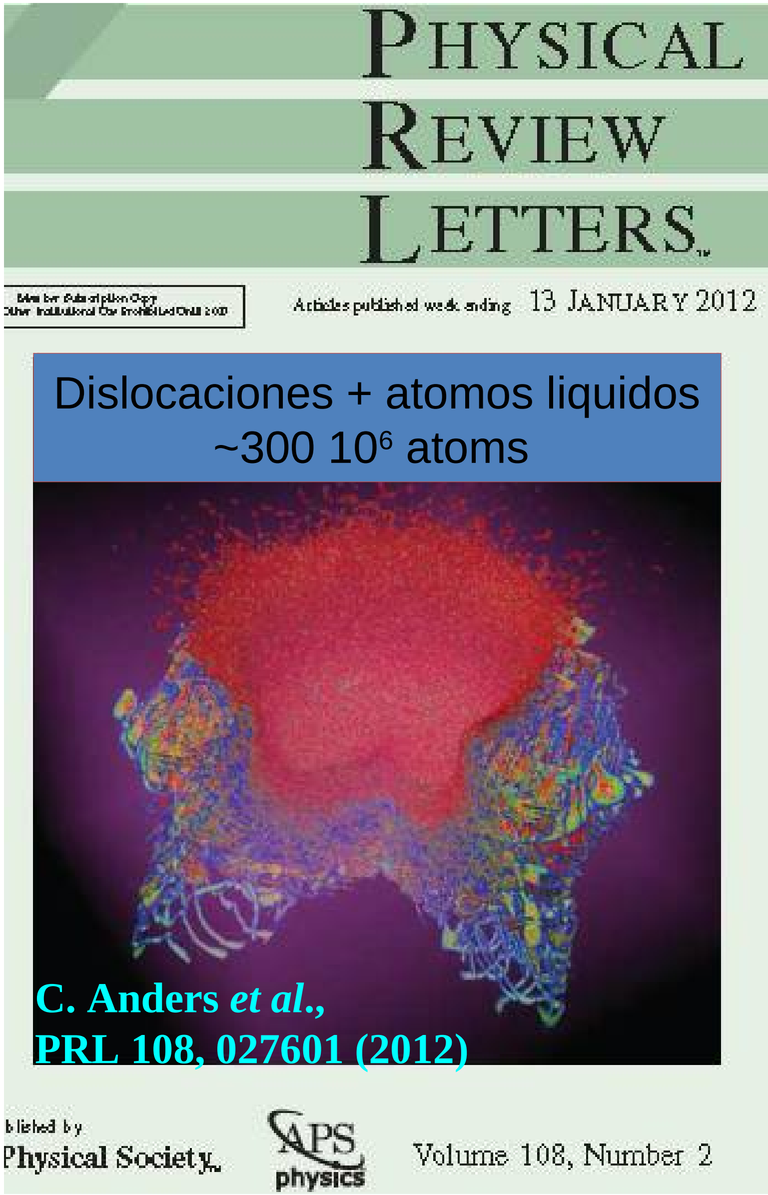

(c)
phase changed

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)?

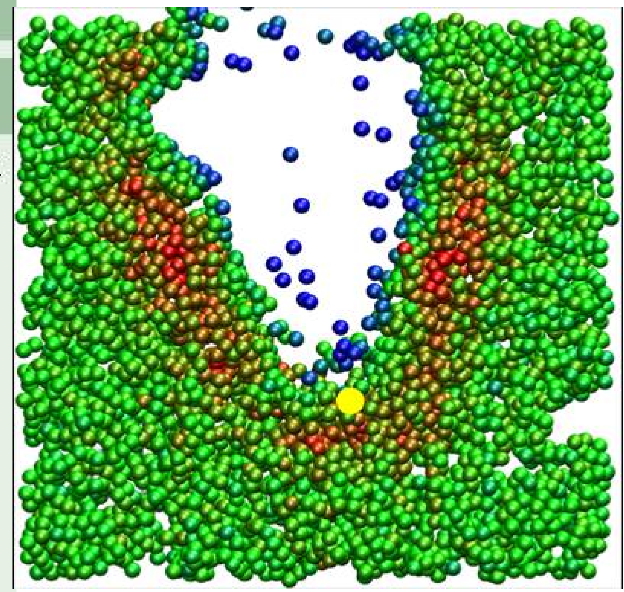
Simulaciones de impacto de nanoproyectiles:
(Micrometeoritos, nanoclusters para sintesis, etc.)



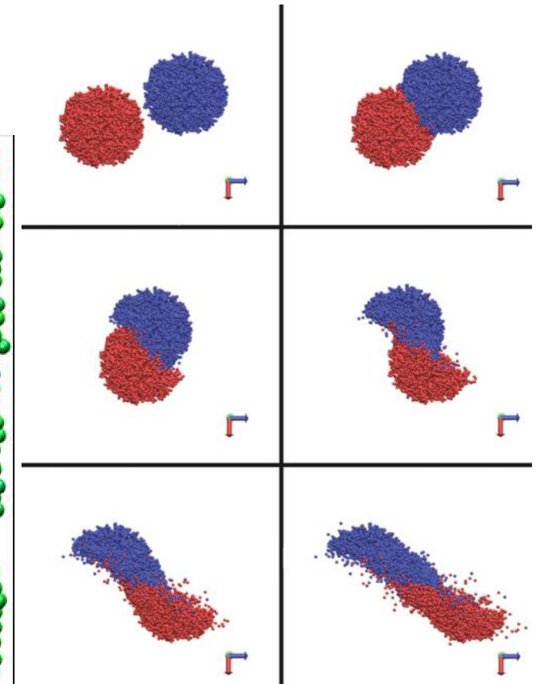
Dislocaciones + atomos liquidos
~300 10^6 atoms

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

1.2e9 atoms, 30 days in 1e4 cores

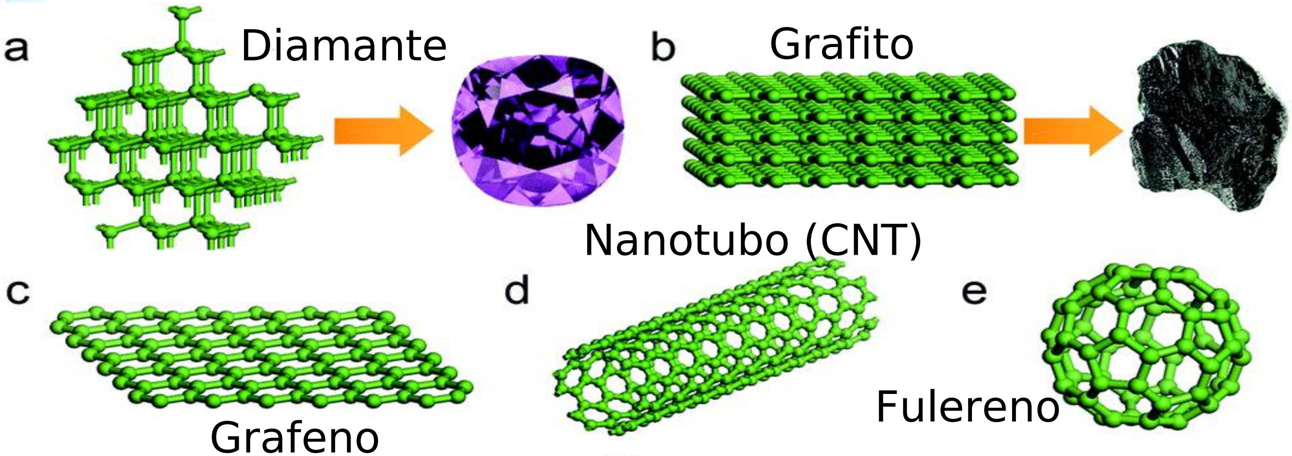


Colisiones proyectil-superficie em medios granulares
Ringl, Bringa, Urbassek,
PRE 86, 061313 (2012)
PRE KALEIDOSCOPE



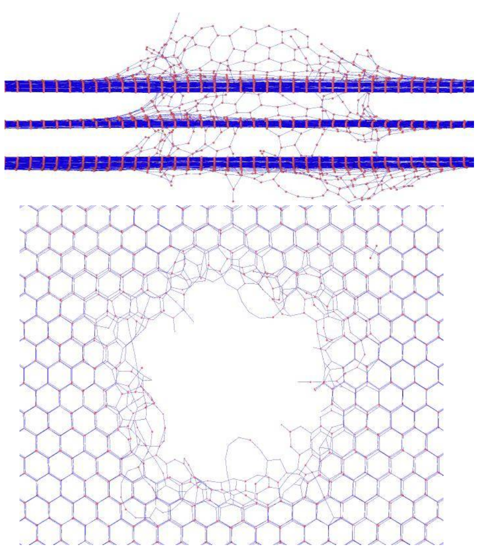
Colisiones de nano y micro granos
Ringl *et al.*, Ap.J. **752** (2012) 151
Nuevo esquema de friccion granular implementado en GPUs
Speedup: 6x-9x
(E. Millan *et al.* *Submitted to LAMMPS*)

Nanomateriales con C: numerosas aplicaciones actuales y futuras

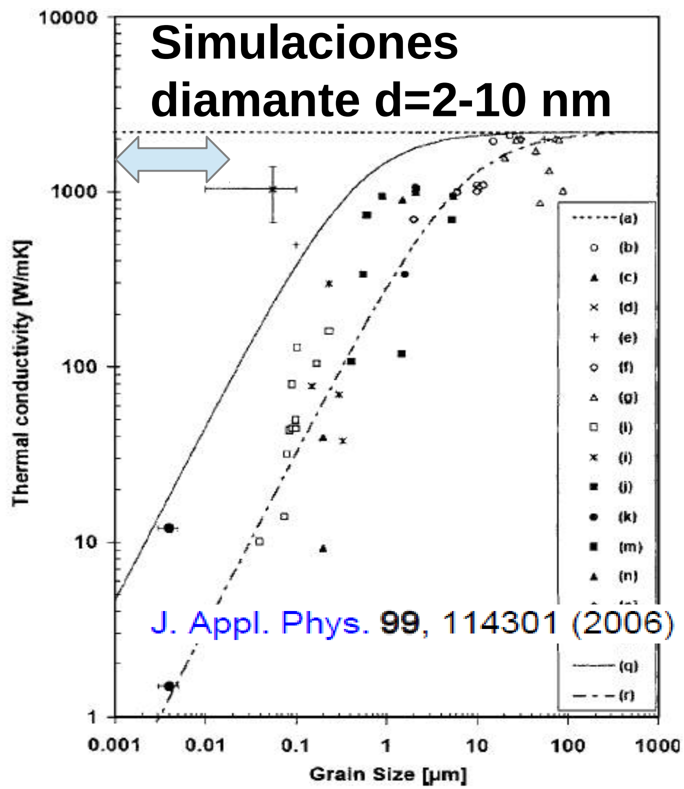


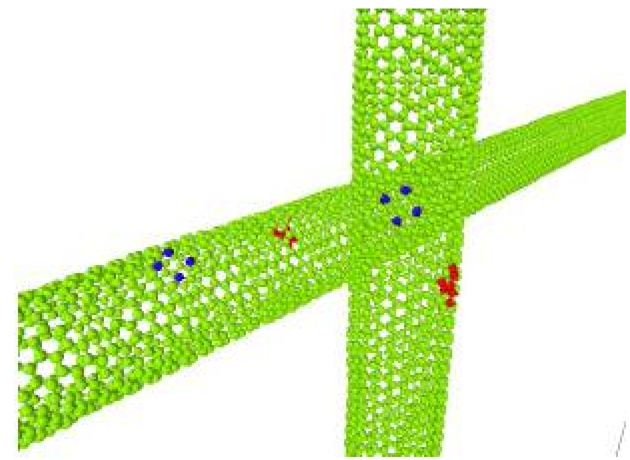
J. Mater.Chem. A 2,6266(2014)
DOI: 10.1039/C3TA14754A

Defectos controlan propiedades mecanicas y electronicas



Grafeno (3 capas): defectos creados por bombardeo de iones, con PUCRGS/UFRGS (Brasil)



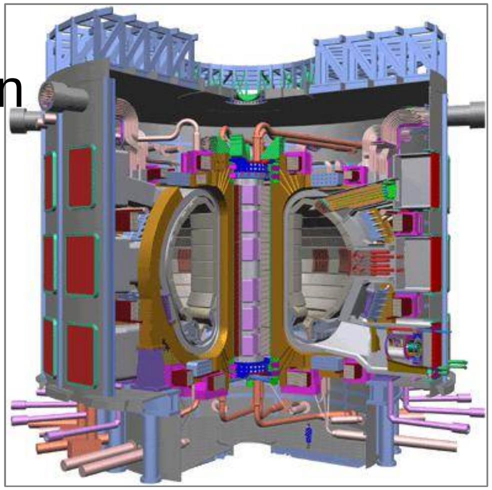


Conductividad entre CNT con defectos, con U.Va. (USA)

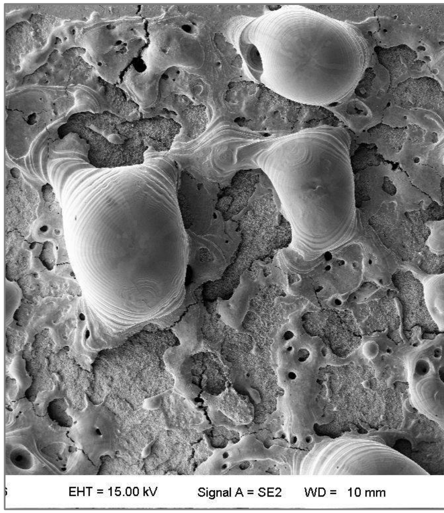
Materiales para reactores de fusión

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

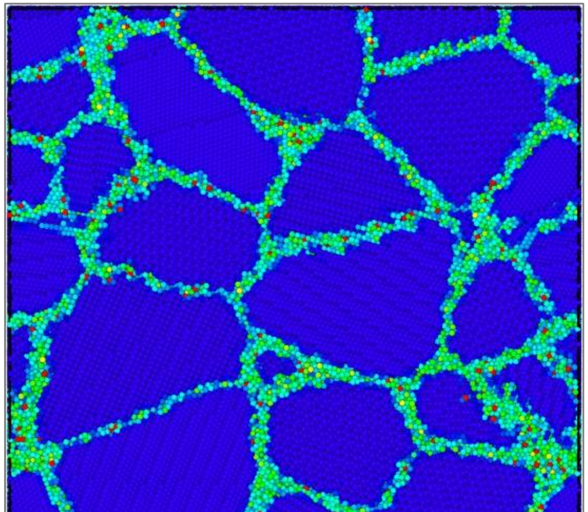
Los futuros reactores de fusión nuclear serán una fuente de energía sustentable y no contribuirán al calentamiento global.

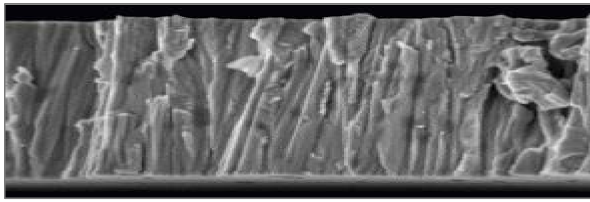


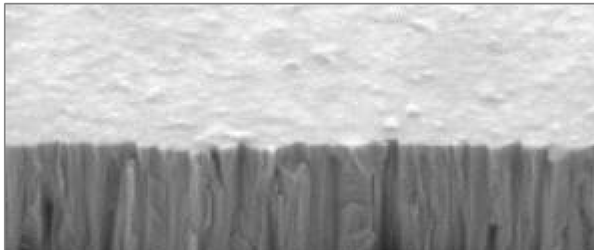
Entre los desafíos tecnológicos actuales se encuentra hallar materiales que toleren el ambiente severo del reactor.



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

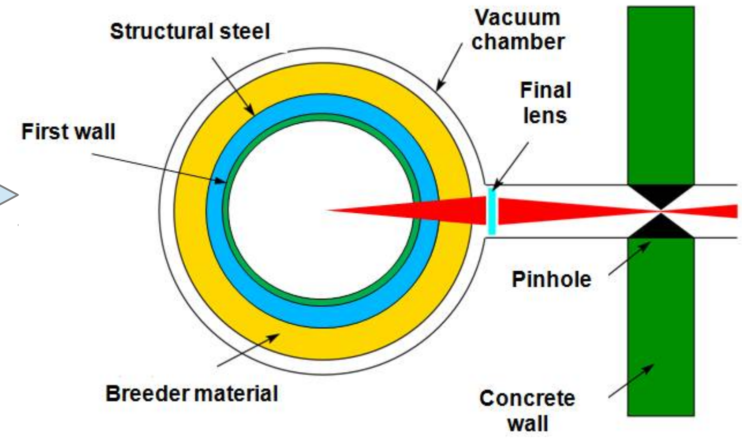




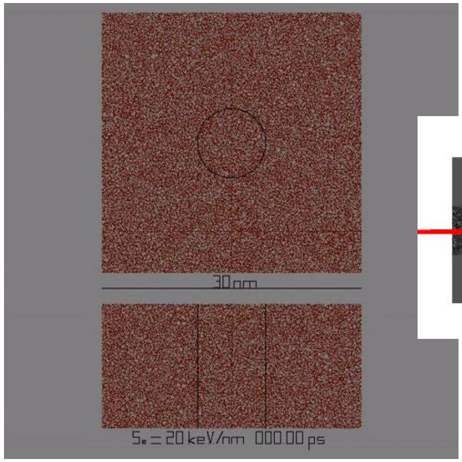


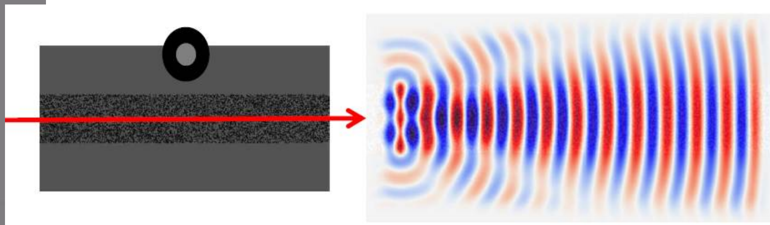
Materiales opticos con nanoestructuras

Industria energetica:
lentes para reactores de fusion



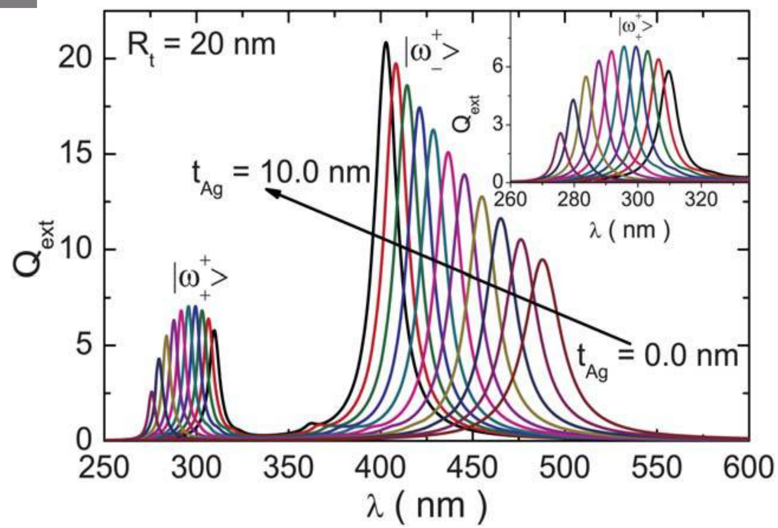
Industria electronica y optica:
irradiacion modifica propiedades opticas
(A. Prada-Valverde *et al.*, Enviado a PRL (2014))





(nano-guias)

Nanoparticulas (Au-Ag):
permiten "elegir" propiedades opticas
(O Pena *et al.*)



Colaboración con la UP Madrid
Maherit, 100-1000 cores

Motivacion para estudiar materiales nanoporosos

-Propiedades mecanicas novedosas

-Catalisis (Ag, Pd, etc.)

-Materiales para nuevos reactores de fision y fusion

Materiales nanoporosos pueden ser resistentes a la radiacion pero ...

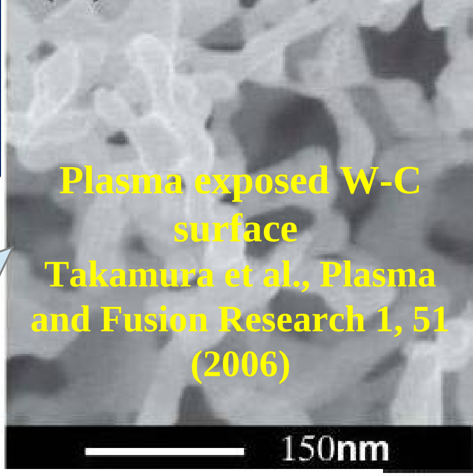
i) Irradiacion afecta propiedades mecanicas y durabilidad de reactores.

ii) Porosidad afecta transporte termico y de masa.

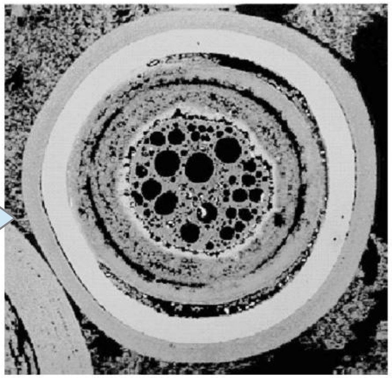
-Astrofisica:

i)Materiales en el espacio generalmente tienen porosidad nano: polvo interestelar, micrometeoritos, asteroides, cometas, superficie de satelites, ...

Irradiacion y porosidad importante para astroquimica.

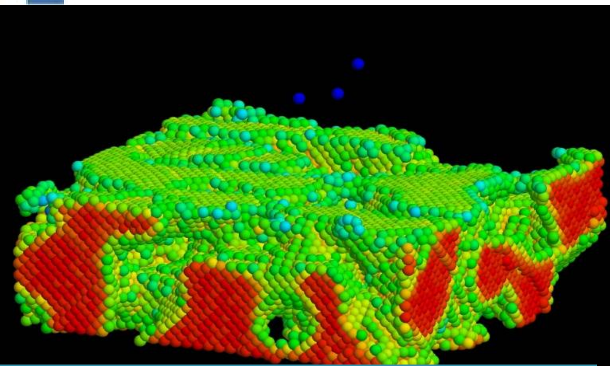


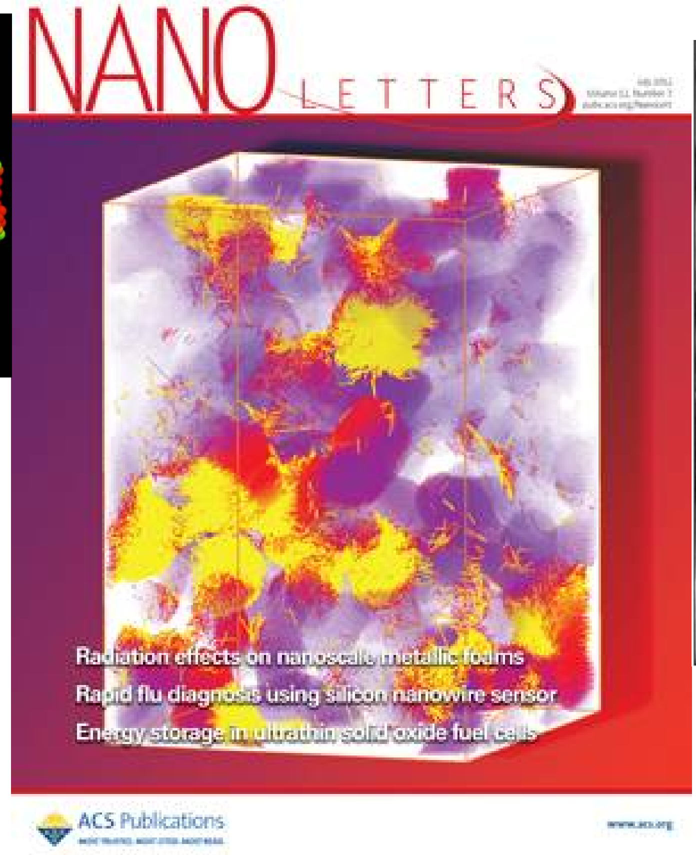
Pu Oxide ($PuO_{1.68}$)

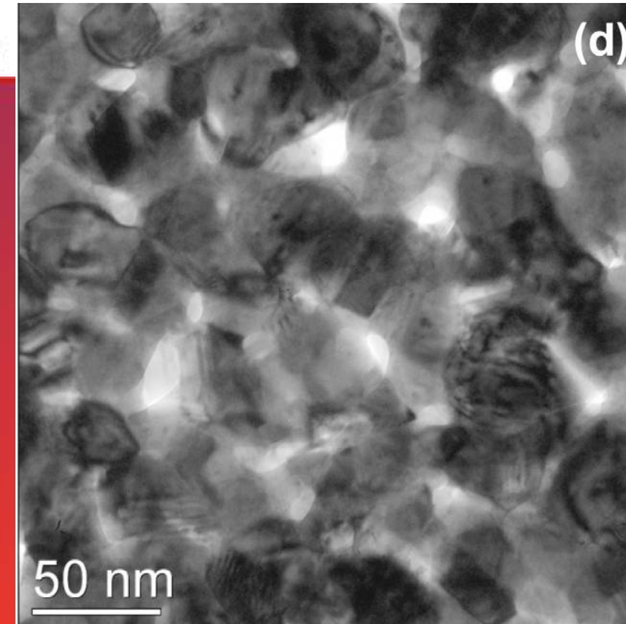


747,000 MW-days/tonne
>95% ^{239}Pu Transmuted at Peach Bottom I

Simulaciones/experimentos for nanoespumas







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

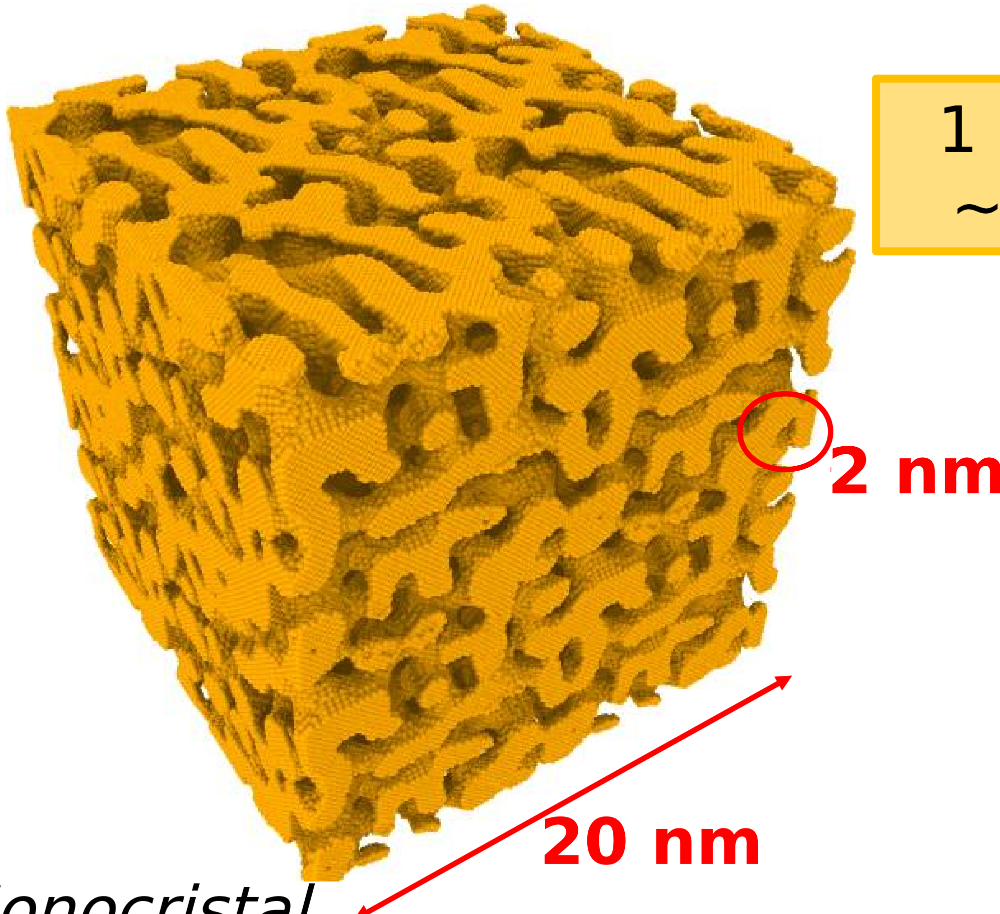
II) Modelo basado en geometria de nanoporos
Rodriguez-Nieva & Bringa, NIMB (2013).

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

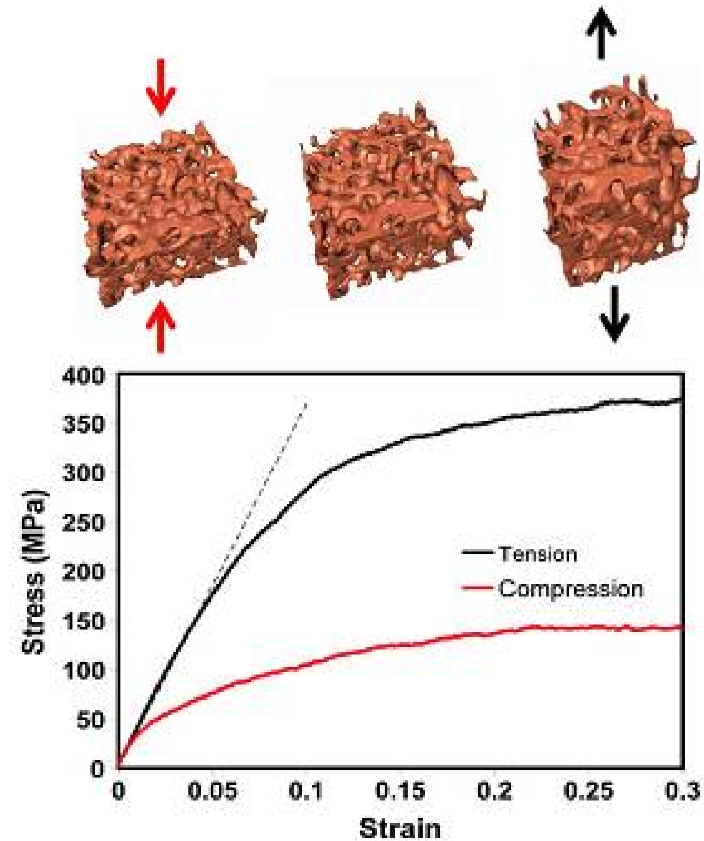
Espuma de Au. 5 bombardeos. Color: desplazamientos debidos al bombardeo (rojo= mas de 1.65 nm).
Bringa *et al*., Nano Letters (2012) ICB/LANL/VaTech

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

¿Donde estamos?
Nano-espumas “irreales”



1 millón de átomos x 1 ns
~12 horas en 10 núcleos



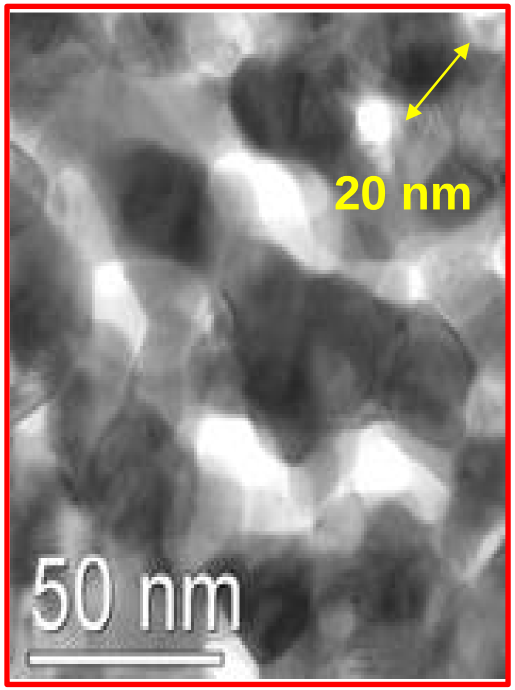
Monocristal
Sin defectos

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

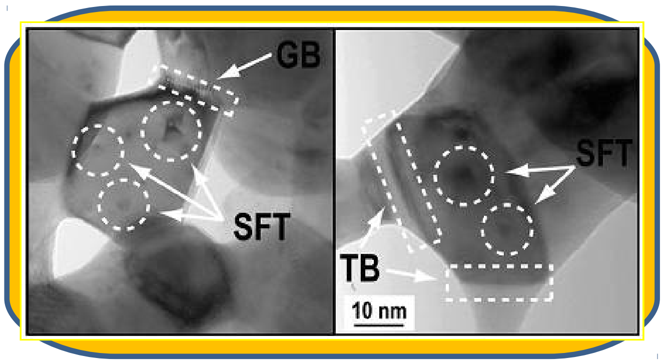
¿A qué apuntamos?
Nano-espumas a escala real

~15 horas en 10000 núcleos, ~50 TB

~200 nm



Nanoespuma policristalina con defectos reales

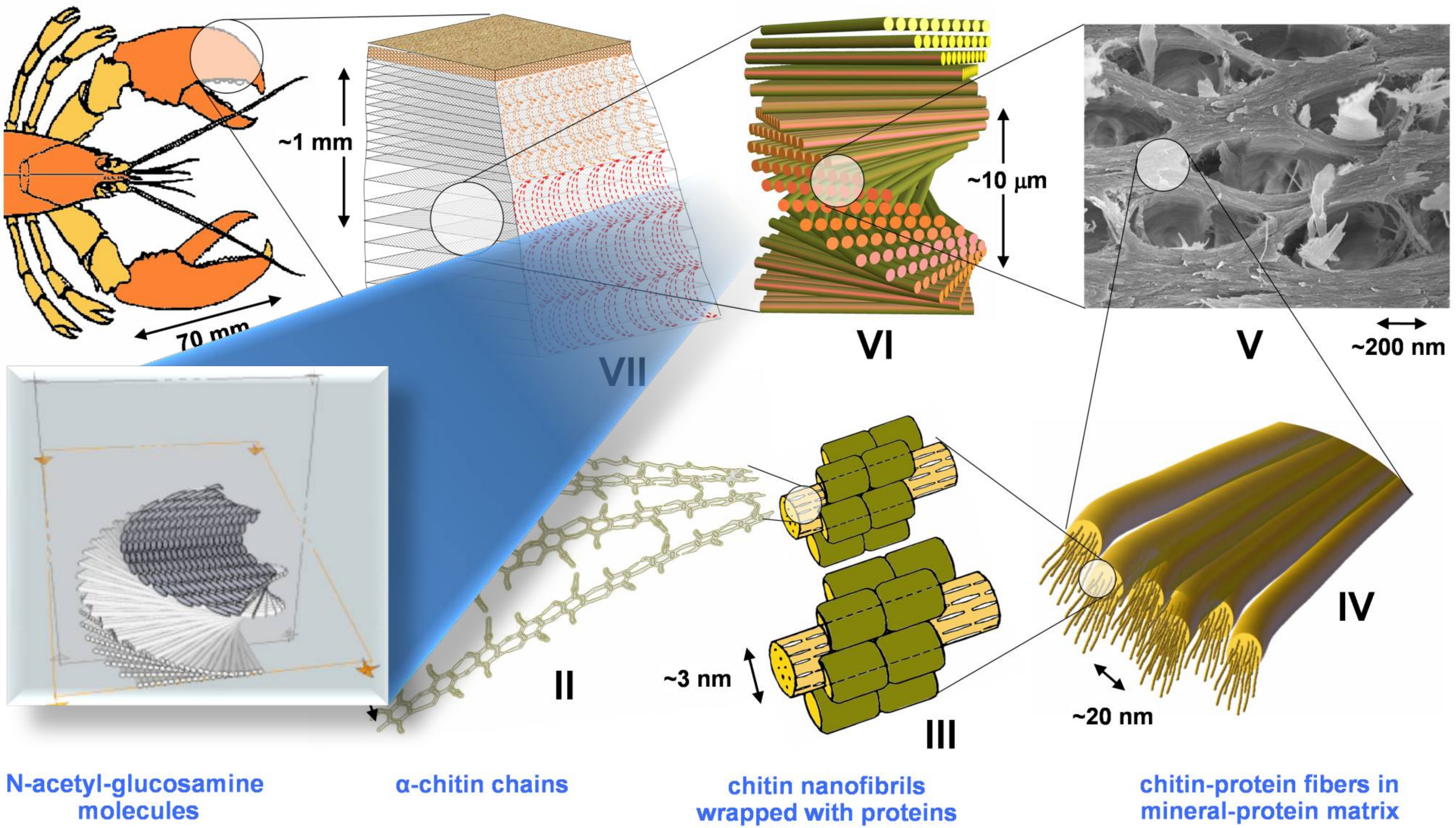


Ciencia interesante con aplicaciones tecnologicas!
Equipo internacional

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

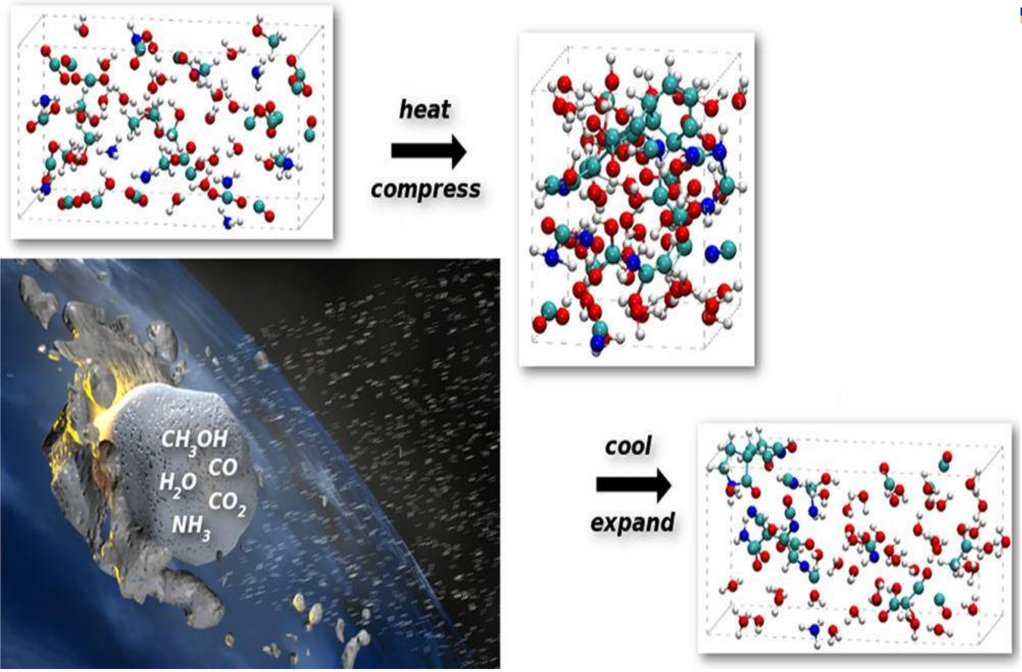
PICT-2014 enviado

FUTURO: Simulación de biomateriales
Escala "nano" controla comportamiento macro
Jerarquía estructural en artrópodos: la langosta marina



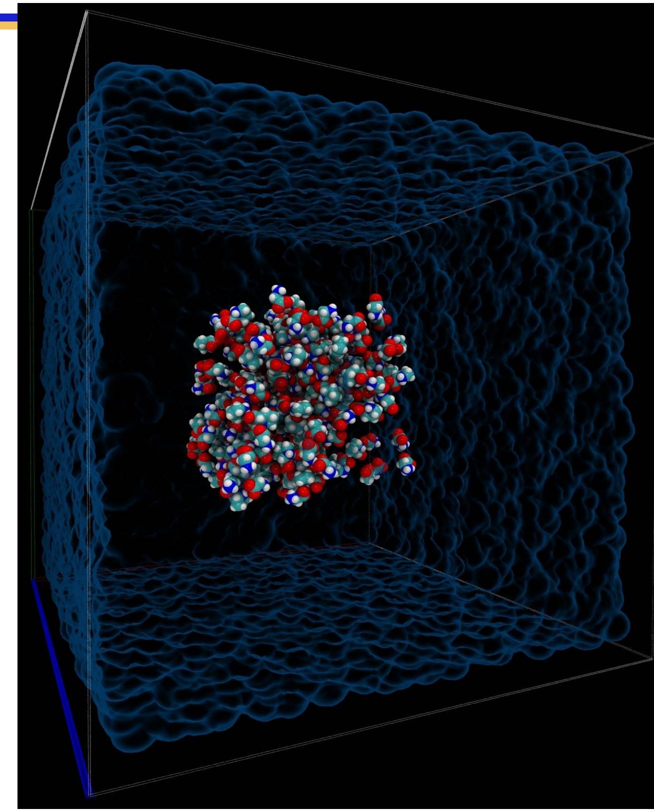
Al-Sawalmih, Li, Siegel, Fabritius, Yi, Raabe, Fratzl, Paris: Adv Funct Mater 18 (2008) 3307
Fabritius, Sachs, Romano, Raabe, Adv. Mater. 21 (2009) 391
Sachs, Fabritius, Raabe: Journal of Structural Biology 161 (2008) 120

Some recent research on collisions



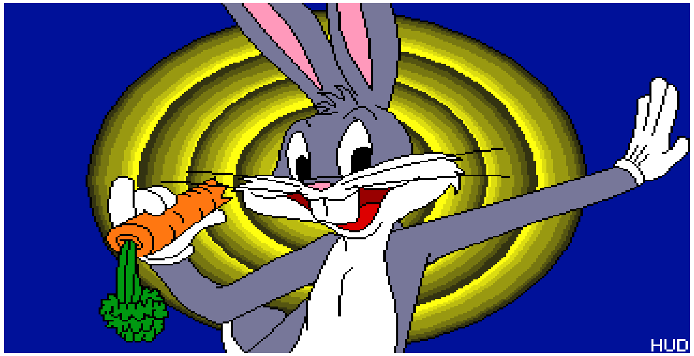
Prebiotic Chemistry within a Simple Impacting an Icy Mixture,
Goldman & Tamblyn, J. Phys. Chem. A. (2013)

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



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

That's all folks!!



SiMAF: Simulations in Materials Science, Astrophysics, and Physics

SiMAF
Simulaciones en Materiales Astrofísica y Física

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

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Ilusiones:

+10,000 CPUs,+ 1000 GPUs, Infiniband, 1000 TB de disco, soporte tecnico (hardware + soft, sysadmin 24/7). Colas: largas/chicas (<500 cores, 1 semana), grandes/cortas (>500 cores, 2 dias), debug (<1 h). Limite de trabajos simultaneos en base a costo computacional.