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Modelling advanced materials under high shock waves and foams for nuclear fusion engineering applications

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Modelling advanced materials under high shock waves and foams for nuclear fusion engineering applications

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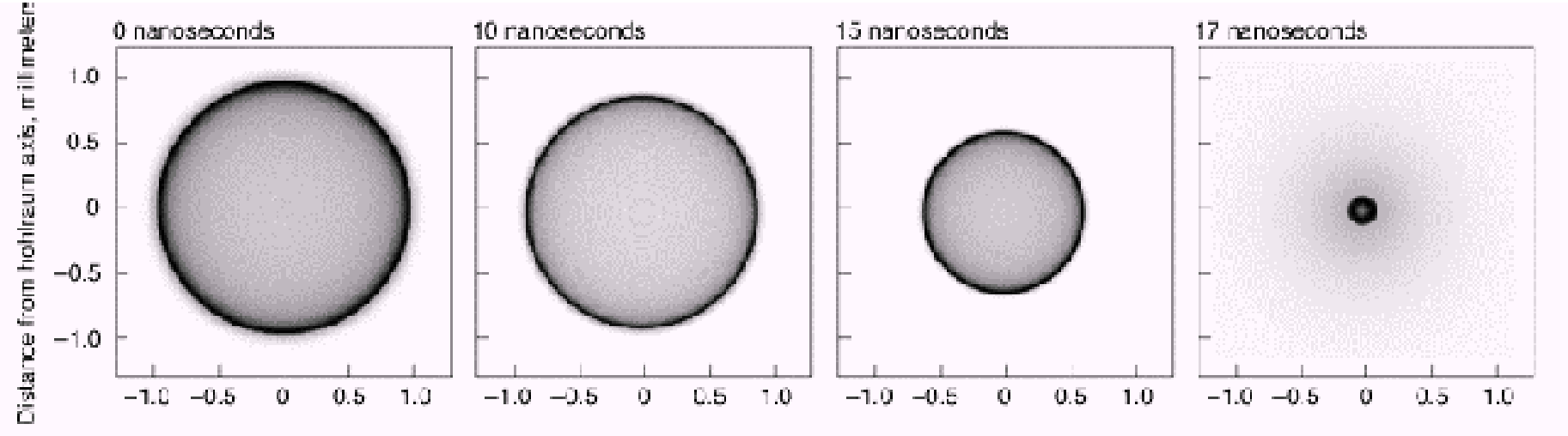
Main research lines:

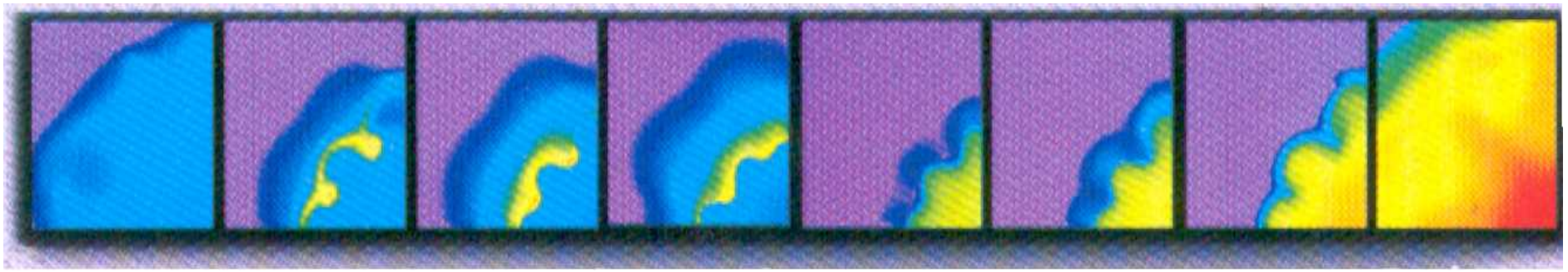
- We are modeling shock-wave generation and propagation in single crystal materials Fe, Au, Ta, W, and Al by means of different MD methodologies. Double layer conformations FeAl, AlCu are also being evaluated.

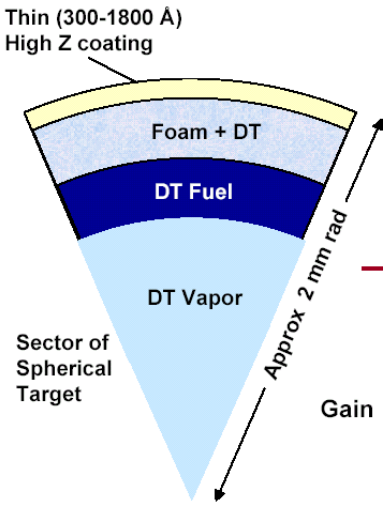
- New nanostructured materials, like nanocrystaline Fe, Cu, Ni are being tested under high pressure conditions.

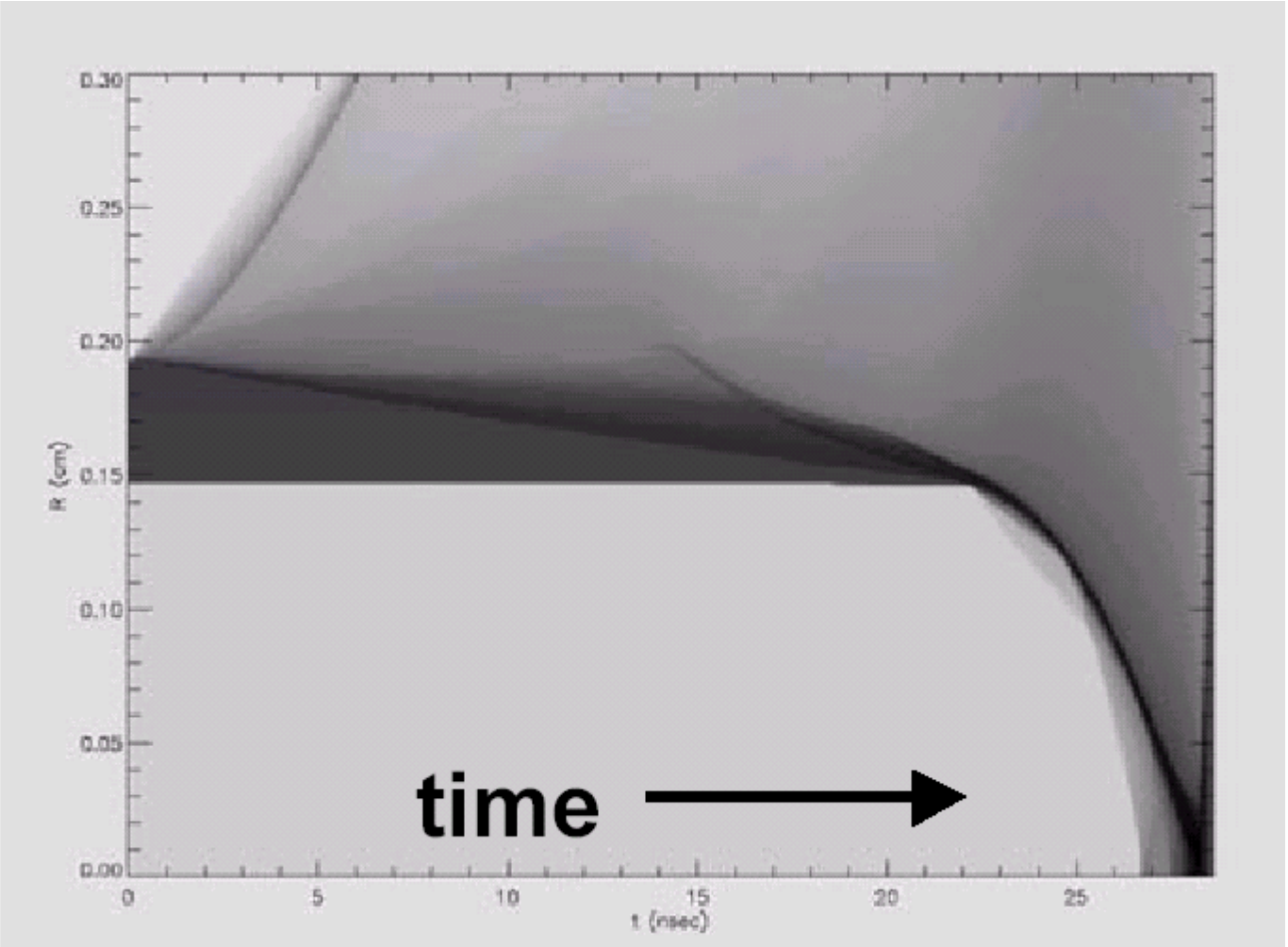
- We have developed a particular method to model nanoscale porous materials in an “ad hoc” target scenario.



Visualización de las fases de la Fusión por Confinamiento Inercial
***y su* ESCALA TEMPORAL**




Thin (300-1800 Å)
High Z coating
Foam + DT
DT Fuel
DT Vapor
Sector of
Spherical
Target
Approx 2 mm rad
Gain


0.30
0.25
0.20
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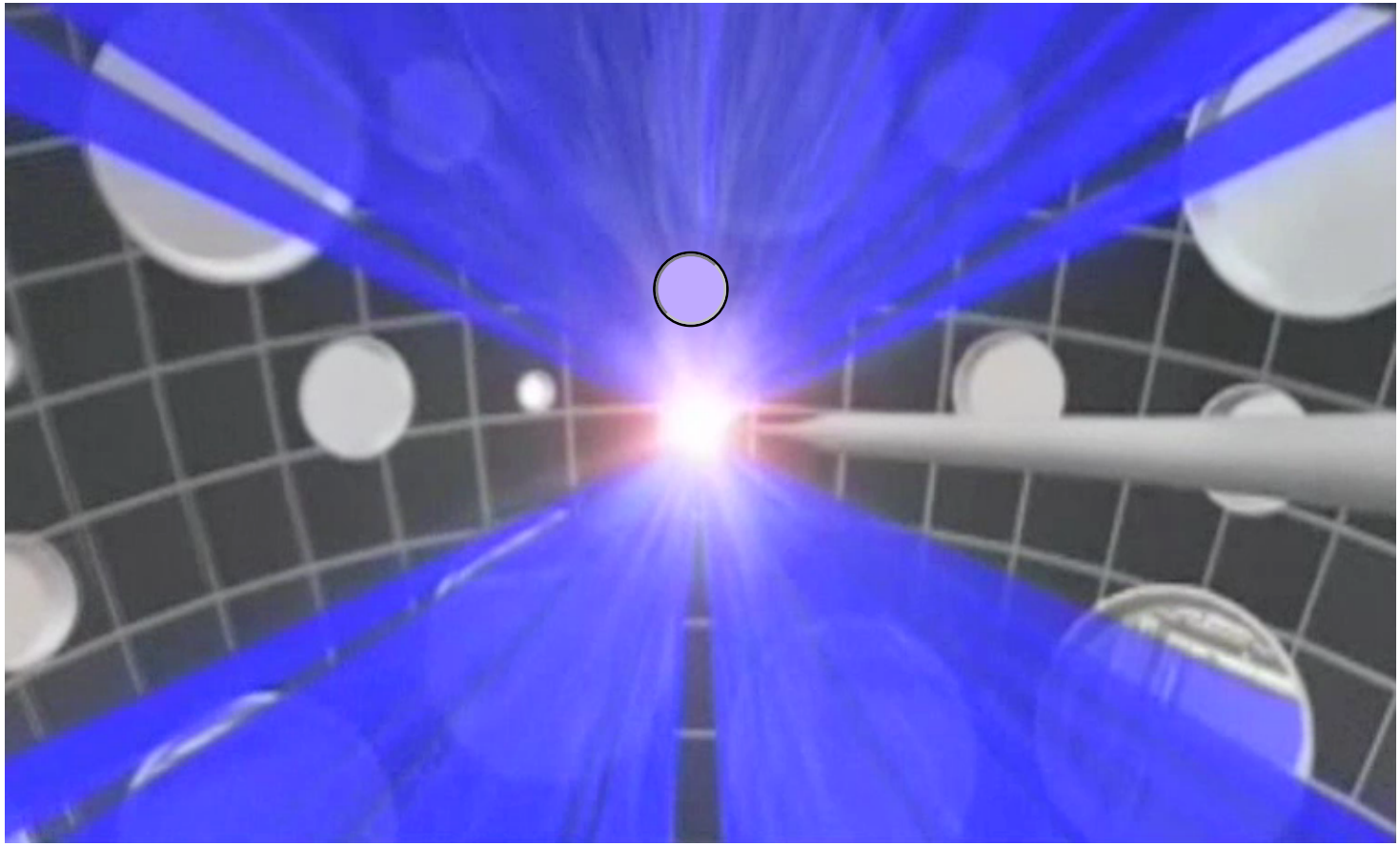
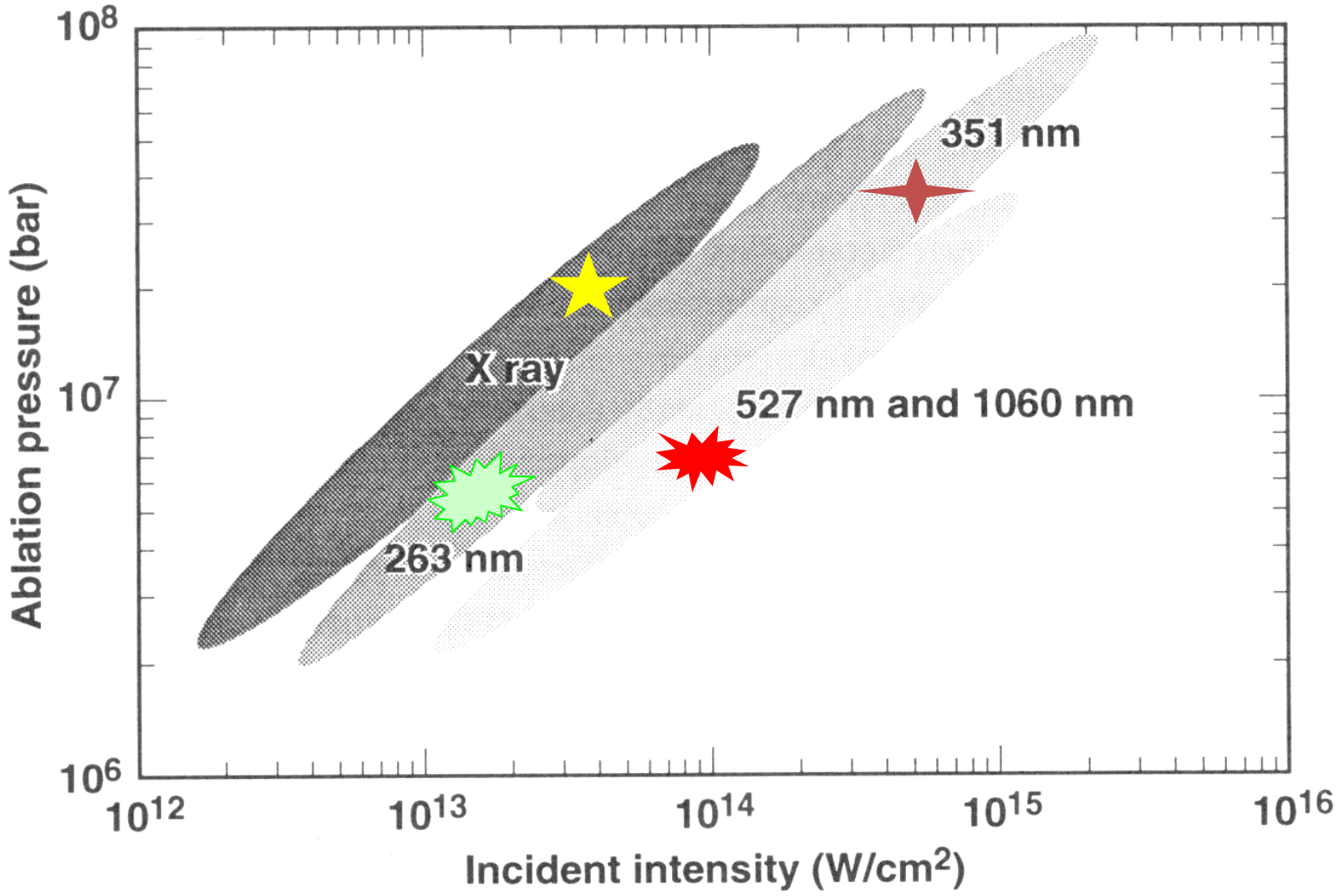
25
t (nsec)
time

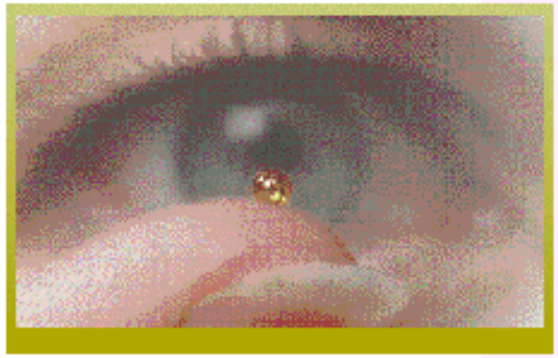
NIF VIDEO

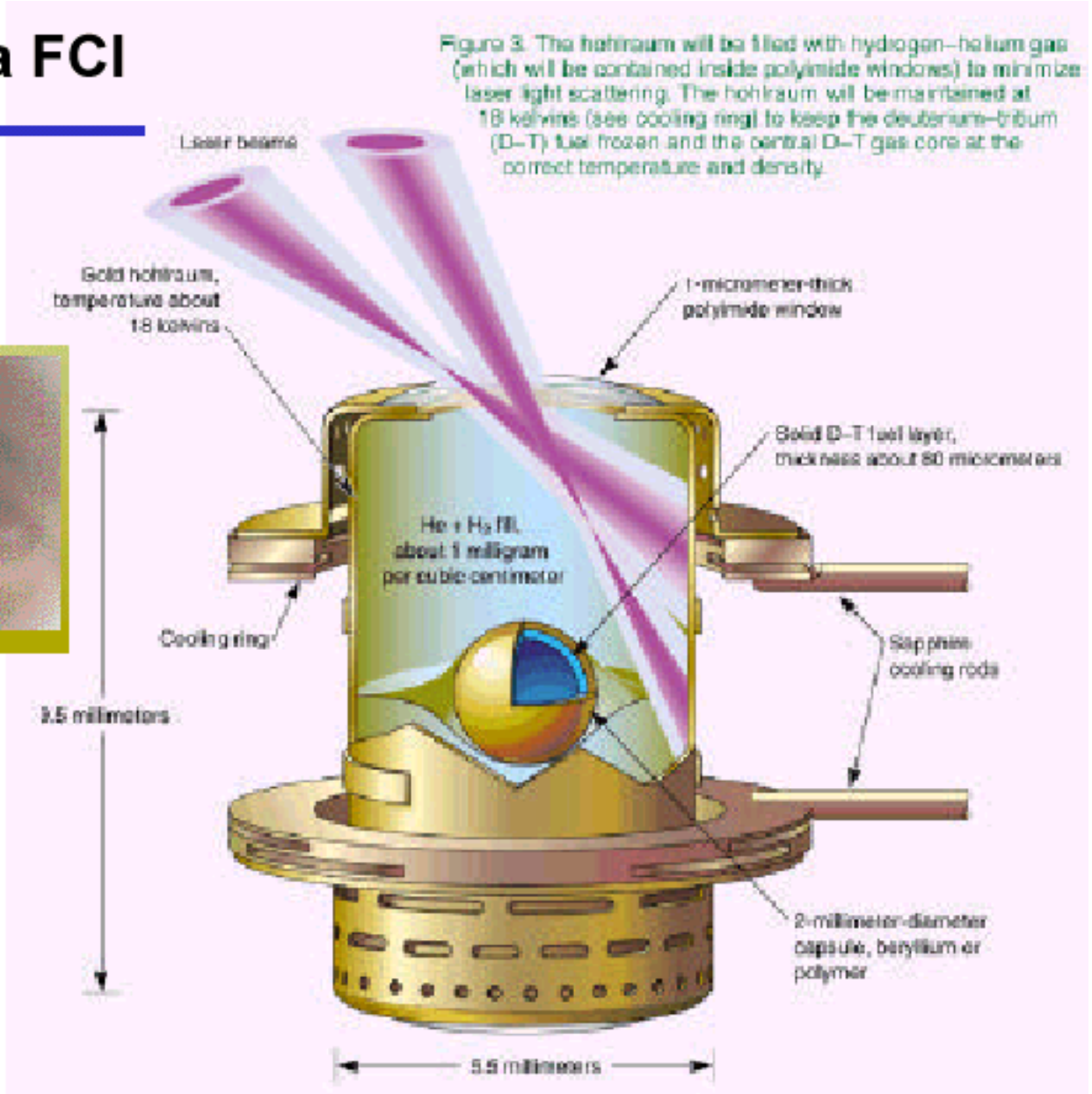




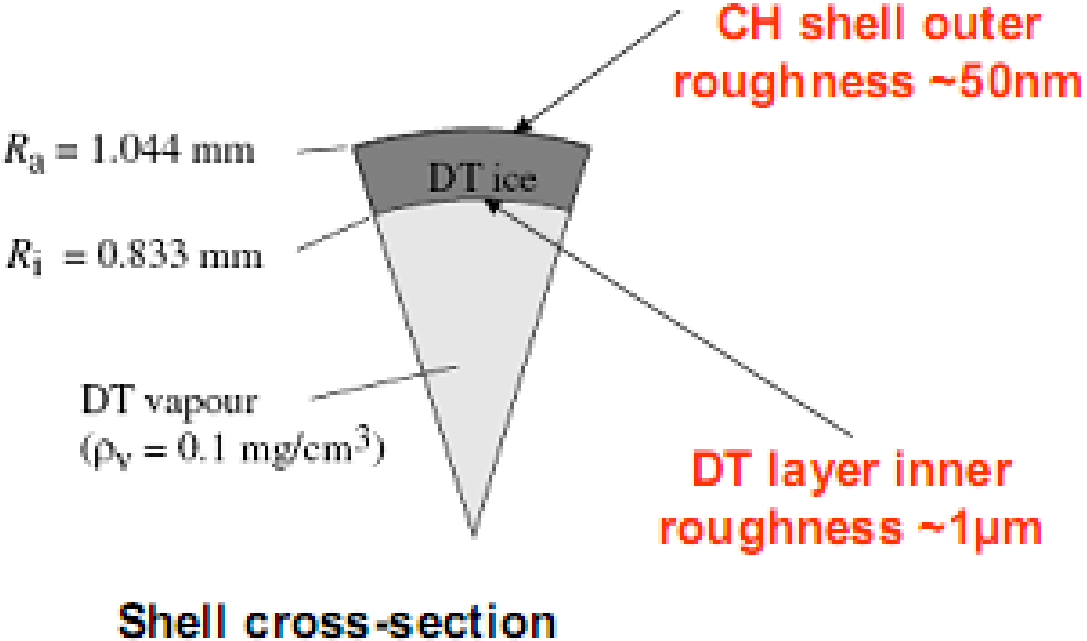
Implosion Velocity 2.4 x 10^7 cm.s^{-1}

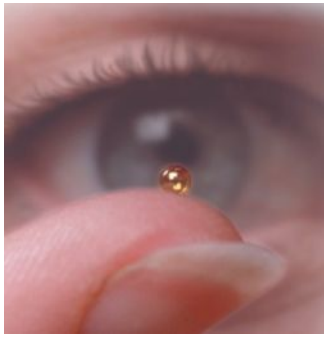
Blancos para FCI

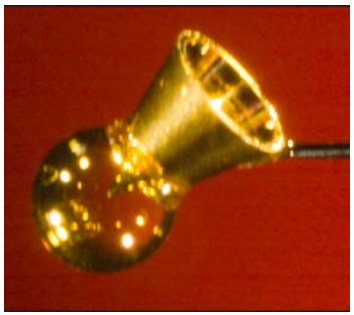




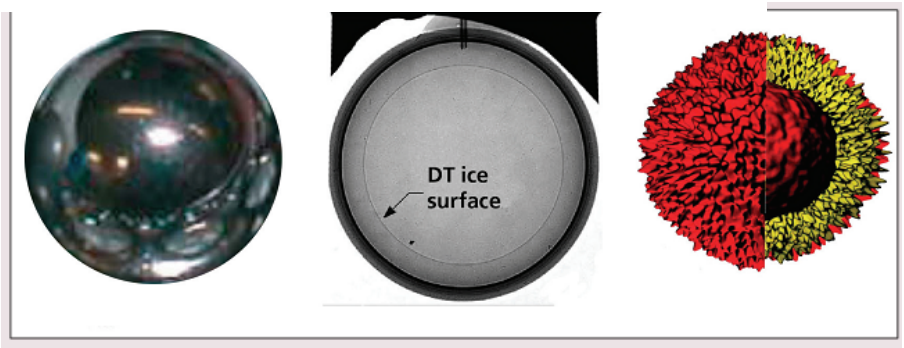
- **Shock wave propagation is the key process in the implosion of the fuel capsule and ignition :**



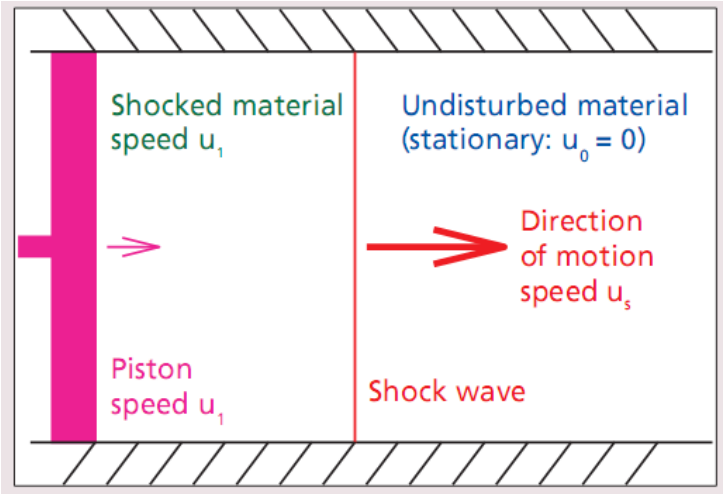




Shell cross-section



MODELING SHOCKWAVE PROPAGATION IN MATERIALS



- **Shock compression. The shock wave transmits information about the piston to the undisturbed material ahead.**

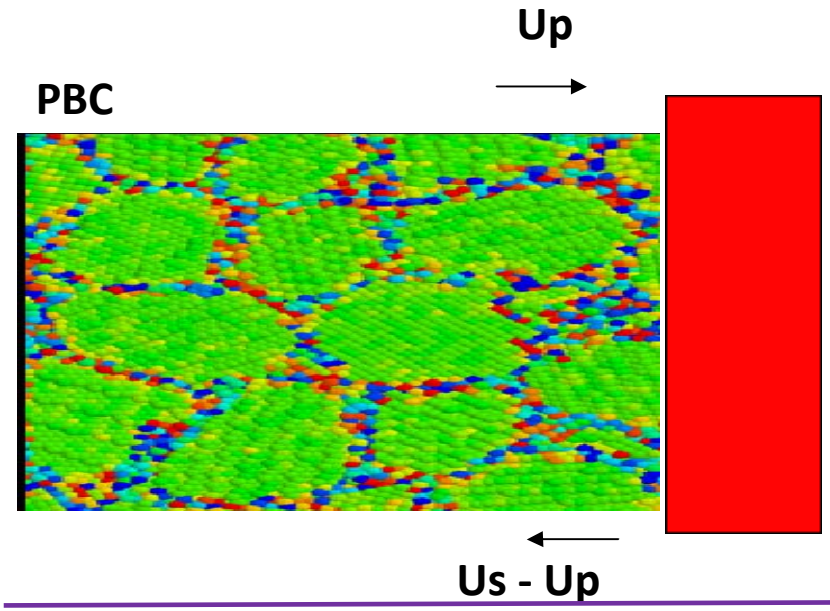
- **Rankine-Hugoniot equations, relating the speed of the shock wave to the driving pressure, are derived by considering the conservation of mass, momentum, and energy for material passing through the shock.**

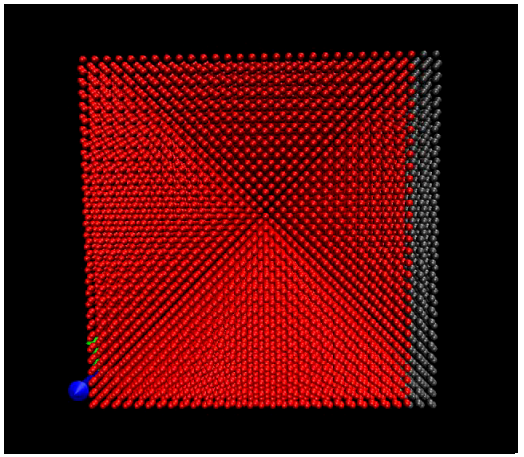
"In silico" shock generation:

- **We use EAM and MEAM potentials to describe atom interactions.**
- **High Performance Computing at the atomistic scale with own and public codes (LAMMPS).**
- **Momentum mirror method. Shock. Adiabatic NEMD:**

System is launched towards a static mirror that reflects every particle . In other words, the sample is slammed up against a specularly reflecting wall with velocity Up. As a result a shockwave is propagated in the other sense at velocity Us-Up.

Kai Kadau et al., Science, 296, 1681 (2002).
Brad Lee Holian et al., Science 280 2085 (1998).

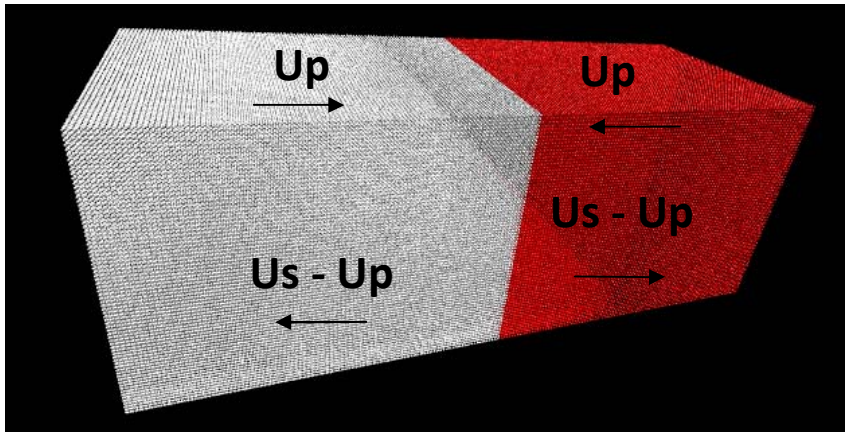




movie

• Double Impact Shock:

➡ Two blocks of material are launched towards each other with velocity Up. As a result a shockwave is propagated on each sense at velocity Us-Up.



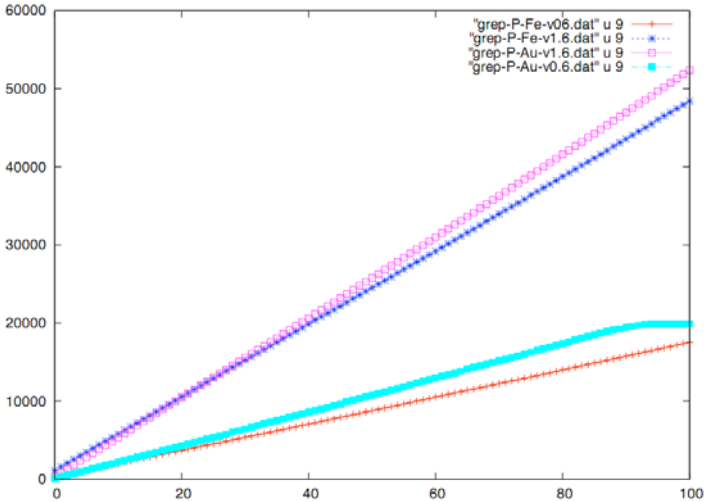
• We are applying this method to EAM potentials for Ta and Be (under test) .

• In depth comparison of bcc and fcc materials. Full simulations with W, Au, Ni, Cu and Fe .

First results on shockwave generation and propagation on different materials lattices (5-10 millions of atoms)

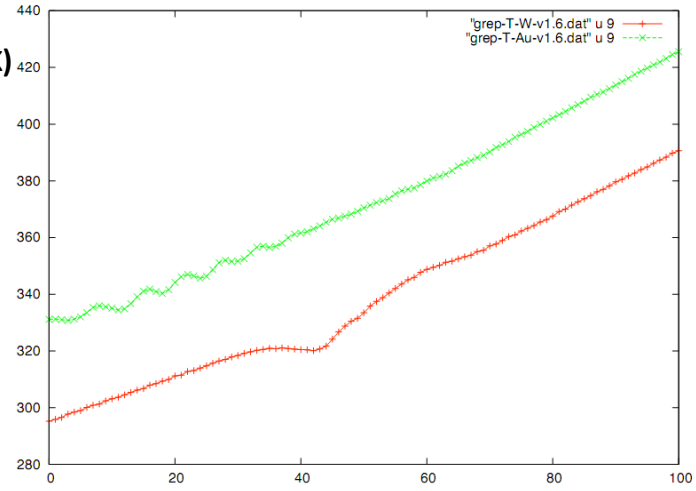
Lattices	Potential	MD method	Piston velocities (A/ps)	Sample sizes (M atoms)
Au	eam	2impact/mirror	0.1-2.0	1-5
W	eam/eamfs	2impact/mirror	0.1-2.0	1-5
Fe	eam	2impact/mirror	0.1-5.0	5-10
Ni	meam,eam	2impact	0.1-5.0	1-5
Al	meam,eam	2impact	0.1-2.0	5-7

Pressure (bars)



MD time (1/100 ps)

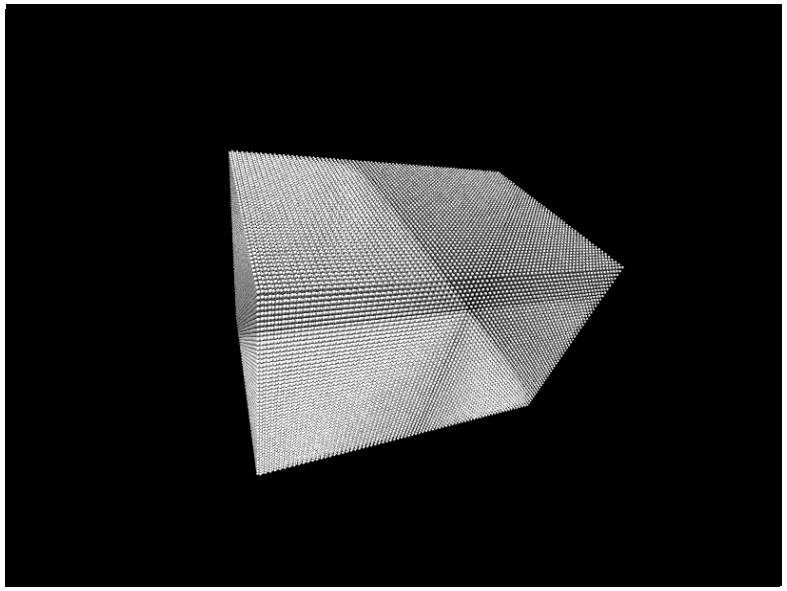
Average Temperature (K)

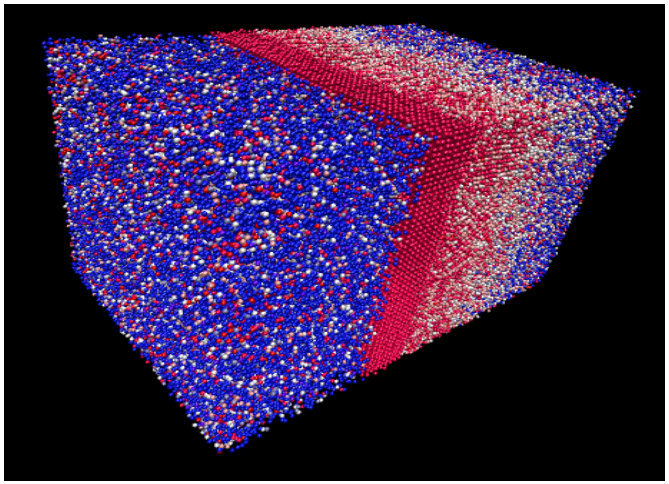


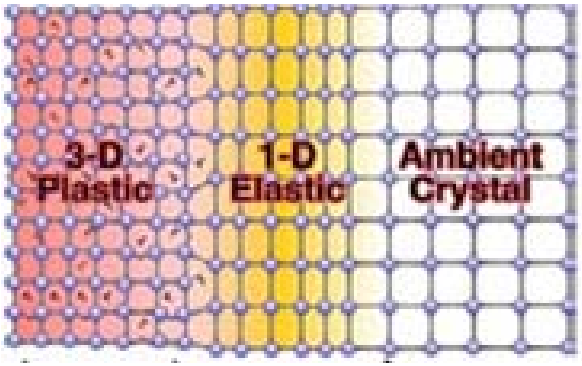
MD time (1/100 ps)

First results on shockwave generation and propagation on Ta: Pictures show the resulting crystal structure (5 millions of atoms) after 5ps MD. Shock propagates in direction [100].

All our samples have been perfectly equilibrated and relaxed to working temperature, previously to shock generation.







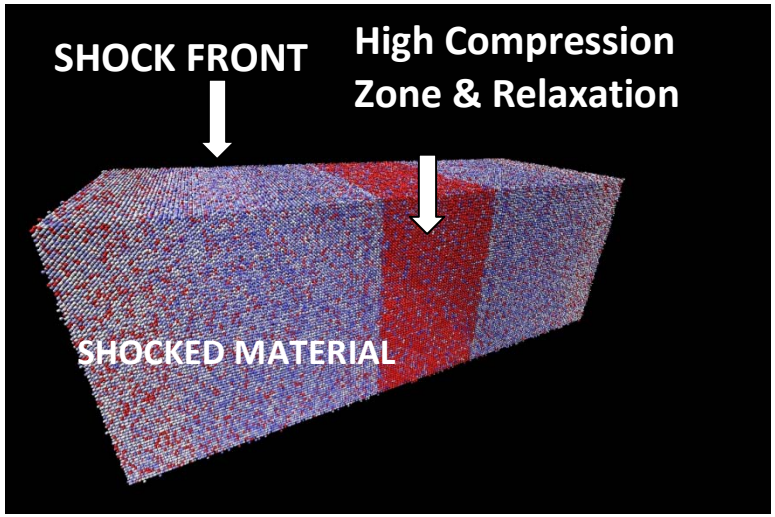
Atoms are colored by centro symmetry parameter study to favor the inspection of dislocations and defects..

$$P = \sum_{i=1}^{6} |\vec{R}_i + \vec{R}_{i+6}|^2$$

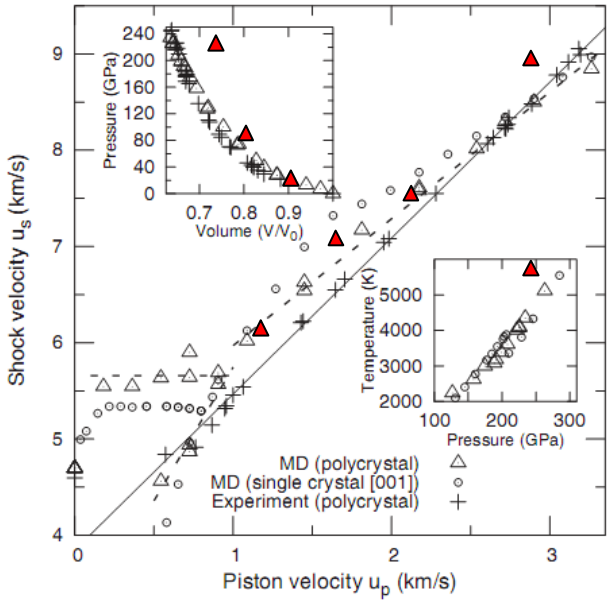
"Piston" velocities were in the range from 0.5 A/ps to 7 A/ps. Sample compression reaches on average $10^{5\text{-}7}$ bars.

movie

Shock Simulation by double impact method of single crystal bcc pure Fe Mendelev type #2

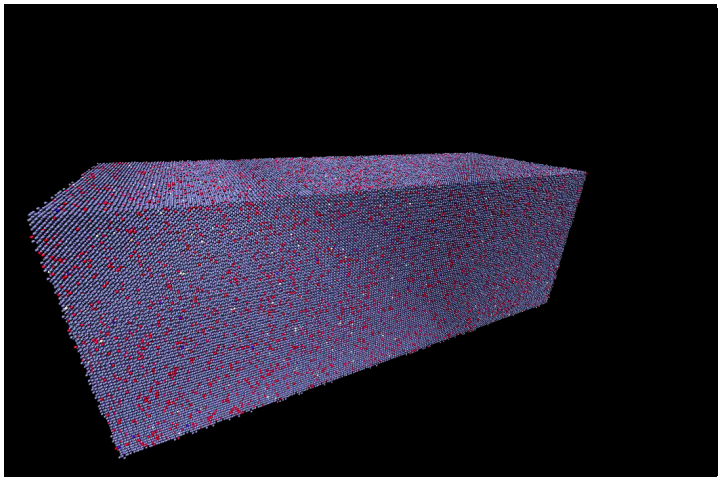


UPM RESULTS



TOTAL MD Time

t= 100 ps



Playing with the PBC in the shock propagation direction we are also studying shock wave instabilities & interferences.

movie

NEW ADVANCED MATERIALS:
Design and suitability for inertial fusion targets.

ATOMISTIC VIEW OF NANOCRYSTALS UNDER HIGH PRESSURE & SHOCK LOADING:

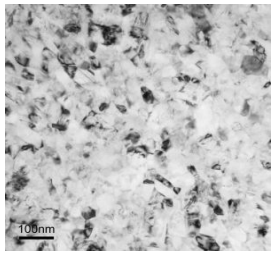
- Nanocrystals have revealed as materials with extraordinary mechanical properties.

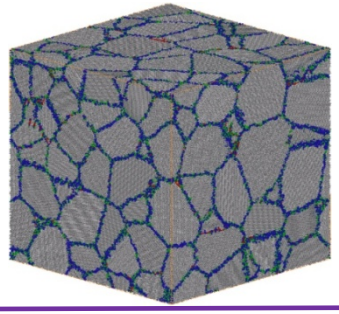
- Molecular dynamics simulations of nanocrystalline (nc) copper under shock loading show an unexpected ultra-high strength behind the shock front. (*E.Bringa et al Science Vol. 309. no. 5742, pp. 1838. 2005*).

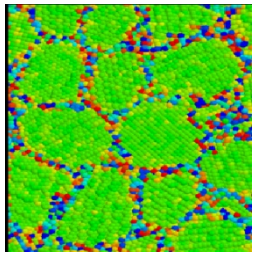
- These novel and promising simulations, together with new shock experiments on nc nickel, raise the possibility of achieving ultra-hard materials during and after shock loading. Therefore, it raises the possibility of considering nanocrystals in the design of inertial fusion targets.

- The use of large-scale atomistic simulations in the study of structural and mechanical properties of nanocrystalline metals can provide a level of atomic detail that still remains inaccessible to experiments.

- It enables the structure of the grain boundaries and triple junctions to be addressed and to relate their equilibrium-state directly to the deformation mechanism.







- We have implemented advanced MD techniques in parallel codes suitable for supercomputer machines. Modified EAM potentials for Cu and Au have been tested. Quenched MD to characterize snapshots equilibrium states. MREMD possible option to explore phase space. We need to simulate up to 25 million atoms !!

- We have developed a software to compute Voronoi cells and Volumes generating Nanocrystal samples.

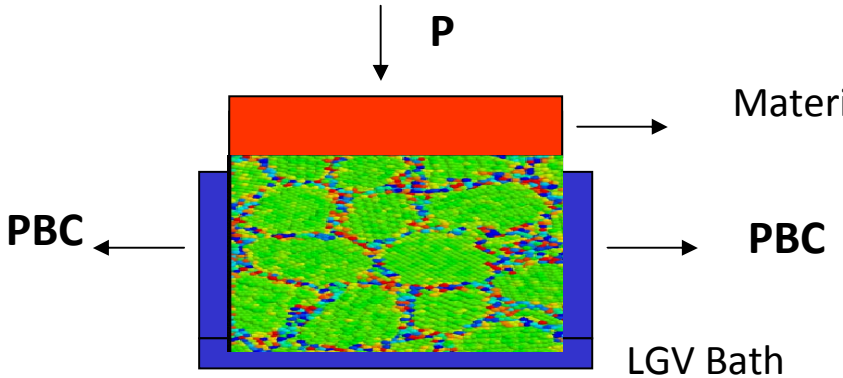
  Basic and preliminary stage to **generate samples**. The first Fe (Mendelev potential types #2,4) Ta, Be Nanocrystals have been already generated. A complex relaxation process prior to shock application have been developed.

- We have initiated trials and different simulation procedures in Cu based nanocrystalline cells in order to reproduce the unique existing results (*E.Bringa et al Vol. 309. no. 5742, pp. 1838. 2005*) testing in that way our methodology.

  We point out in the next future to W & Au as goal materials.

- Note that were are working Out of equilibrium MD. The shock-wave formalism and treatment in MD simulations should be revisited and improved. We are starting a parallel research line in that sense.

• NEMD coupled to Dissipative Brownian Dynamics:

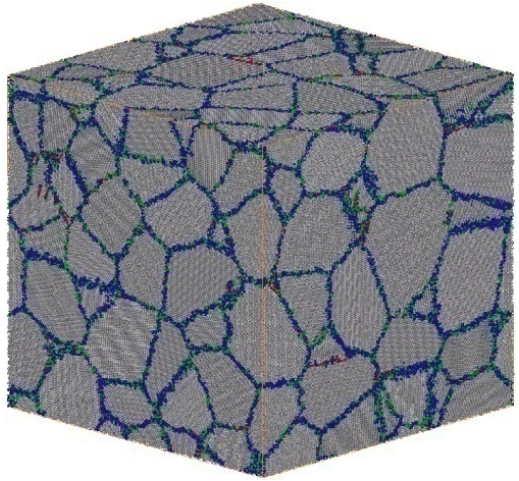


Material Layer acting as piston

P: Either NPT or out of equilibrium (shock wave)

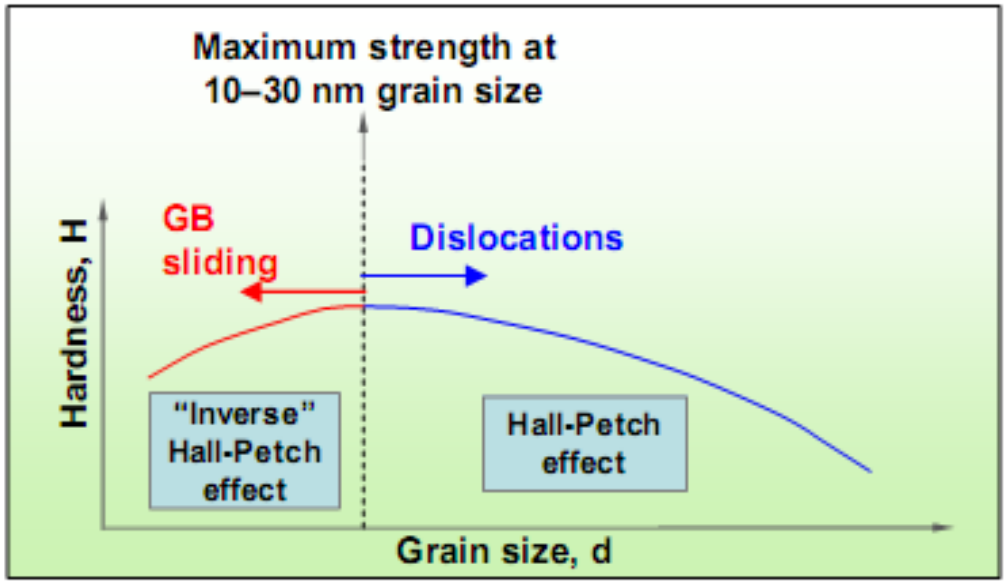
• Few atomic planes ("piston") are moved at desired velocity along desired shock direction
➔ supersonic wave created, $U_s > U_p$

•Mass, momentum and energy conservation➔ Hugoniot equations, i.e. ($P_1 - P_o = \rho_o U_s U_p$), etc.



OUR GOAL:

- **Create new very strong materials suitable for multiple applications in addition to Inertial Fusion targets.**
- **As *E. Bringa et al* have already demonstrated, the properties of nanocrystals can be controlled to increase their strength.**



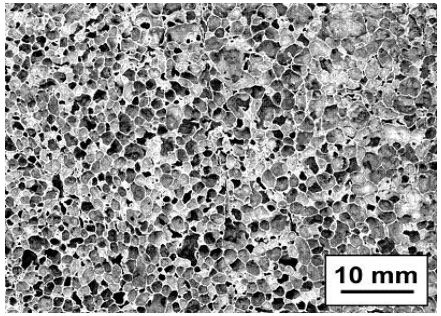
MODELING & UNDERSTANDING METALLIC FOAMS:

* Metal foams are very challenging materials as their manufacture involves the simultaneous occurrence of solid, liquid and gaseous phases at varying temperatures and the morphology of the solidified foam is quite complex.

* As new advanced porous materials offer a lot of possibilities:

- High specific surface area (”surface density”).
- Resistance to harsh environments (high temperature & humidity).
- Thermal, electrical & other properties related to the base metal.
- High strength-to-weight ratio.
- Lightness (material is composed of 70% to 95% air).
- Good impact energy absorption.
- Great noise attenuation.

* Are metal foams good candidates for inertial fusion targets?:



Our metal foam *size dilemma*:

- Current manufactured minimum porous size > 0.5 μm. Pore morphology still not fully controlled. i.e. METAFOAM pore size min. 100 μm. Sizes up to now bigger than 100 nm pore size.

  NO experimental data available for LOWER pore sizes !!!

- Unfortunately we work **in MD** design in a lower scale**. At maximum 400 fcc** → aprox. 150nm. Using the top world five supercomputers.

- May the "nano" porous scale be able to bring benefits to the mechanic properties of these new materials?

- One possible approach: ***"De novo"* Molecular design**. Using MD techniques study the molecular properties (atomic scale) of new compounds.

New non-tested materials *"in silico"* !!!

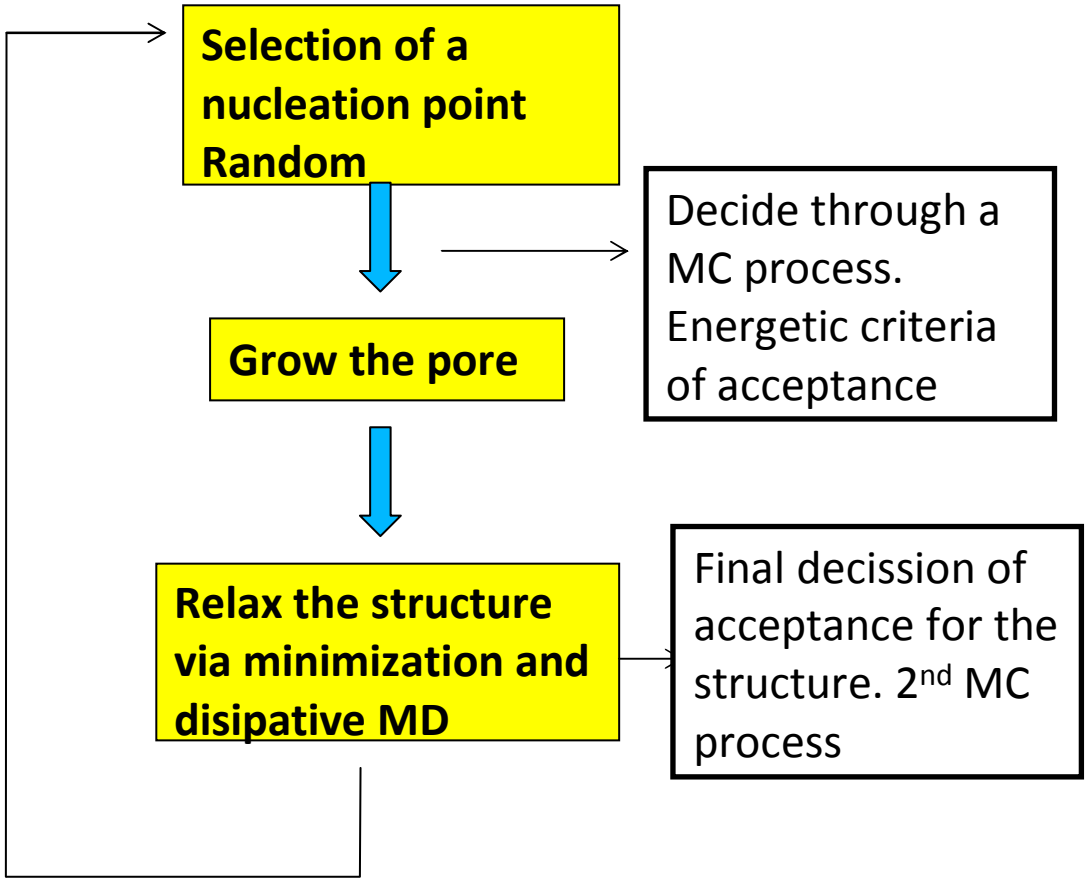
- Study the mechanical properties of porous molecular materials of porous size < 50nm. Response versus T,P, non-linear P, shear, tension ...

Pore sizes < 2-35/50 nm almost straightforward

Pore sizes up to 50nm we need an strategy !!

"In silico" design of a nano pore material. (atomistic simulation):

Pore sizes between 5-35nm. Pores are constructed through a double MC process.

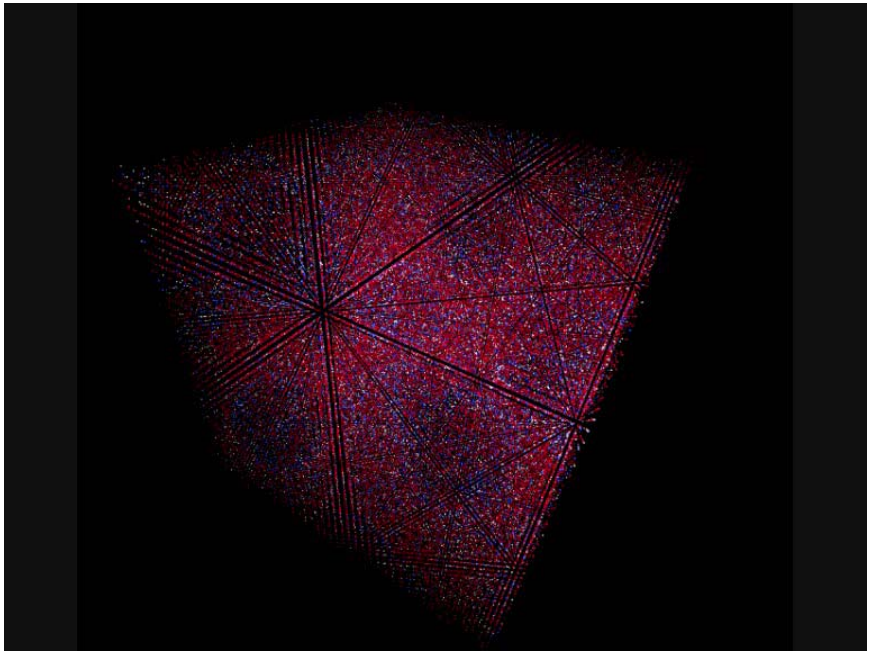


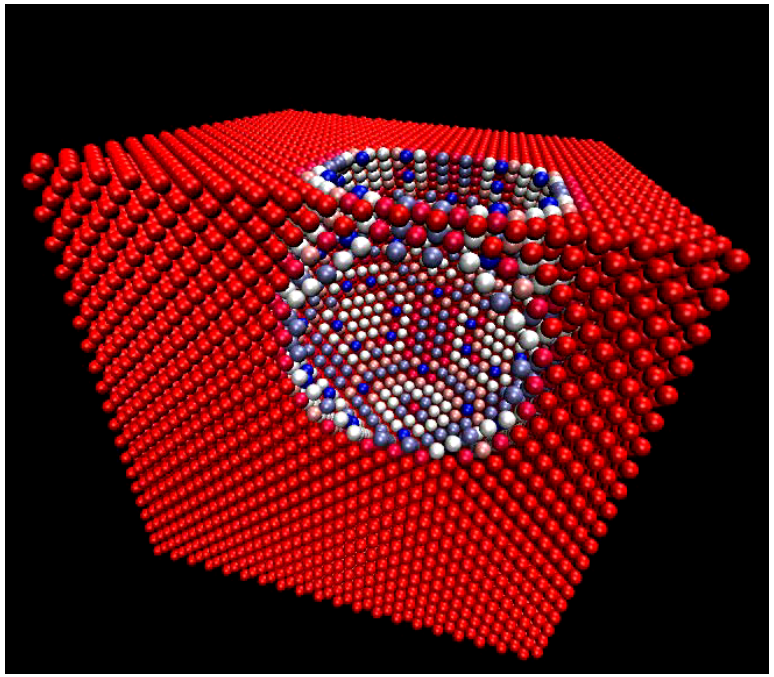
* Final Fe porous structure with pores of 10nm.

After 1000 MC movements. 10 pore relaxation using MD, QMD and dissipative Brownian MD.

Final structure has finally been accommodated to work conditions (room and high T (800K)).

Total supercomputer time 400.000 hrs/cpu !!!





movie

2nd Proposal:
"Meso-scale" model of nano-porous materials:

- We have developed a project to build up a ***"meso-scale"* model** (*coarse grained approach*) for metal foams. However the model is susceptible to be applied to any porous material whatever the grain/pore size (from nm to μm).

- We are working now in the integration of this model as part of a multi parallel MD code embedded in LAMMPS package.

- Still the model needs for parameters. A parametric study is under development.

- We plan to start a close collaboration at UPM to extract experimental data from SiC-Based porous ceramics via naturally derived scaffolds. Experimental studies in commercial metallic foams may also be possible.

And in addition:

Possible structure determination experimental techniques to complement *"in silico"* analysis:

- **Conventional:**

Powder diffraction. Precession electron diffraction. (Nanocrystals).
TEM (HRTEM).
SEM
STM
AFM
High resolution X-ray tomography. ESRF facility (Grenoble).

- **Advanced:**

Small angle atom neutron scattering (SANS). Mean grain radius. Grain boundary thickness. Ideal for nanocrystals !!. Collaboration with ILL (Grenoble)

Coherent X-ray diffraction Imaging. XFELs new sources. Ideal for mesoscale systems: nano-scale condensed matter.

THANKS !!!