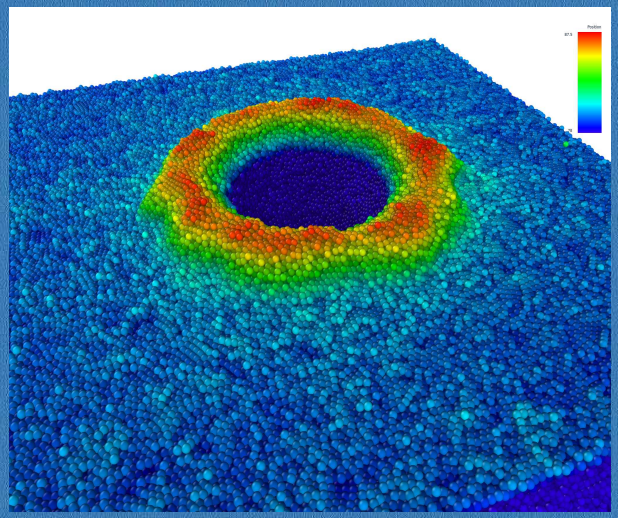
Computational and modeling challenges to simulate materials under extreme conditions



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Funding:

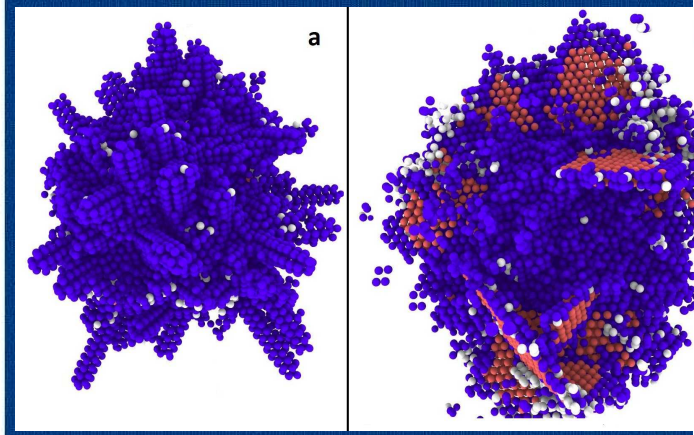
Agencia CyT, Argentina: PICT2008-1325

PICT2009-0092

SeCTyP, UN Cuyo

2015 LAMMPS Users' Workshop and Symposium

Albuquerque, USA
August 2015



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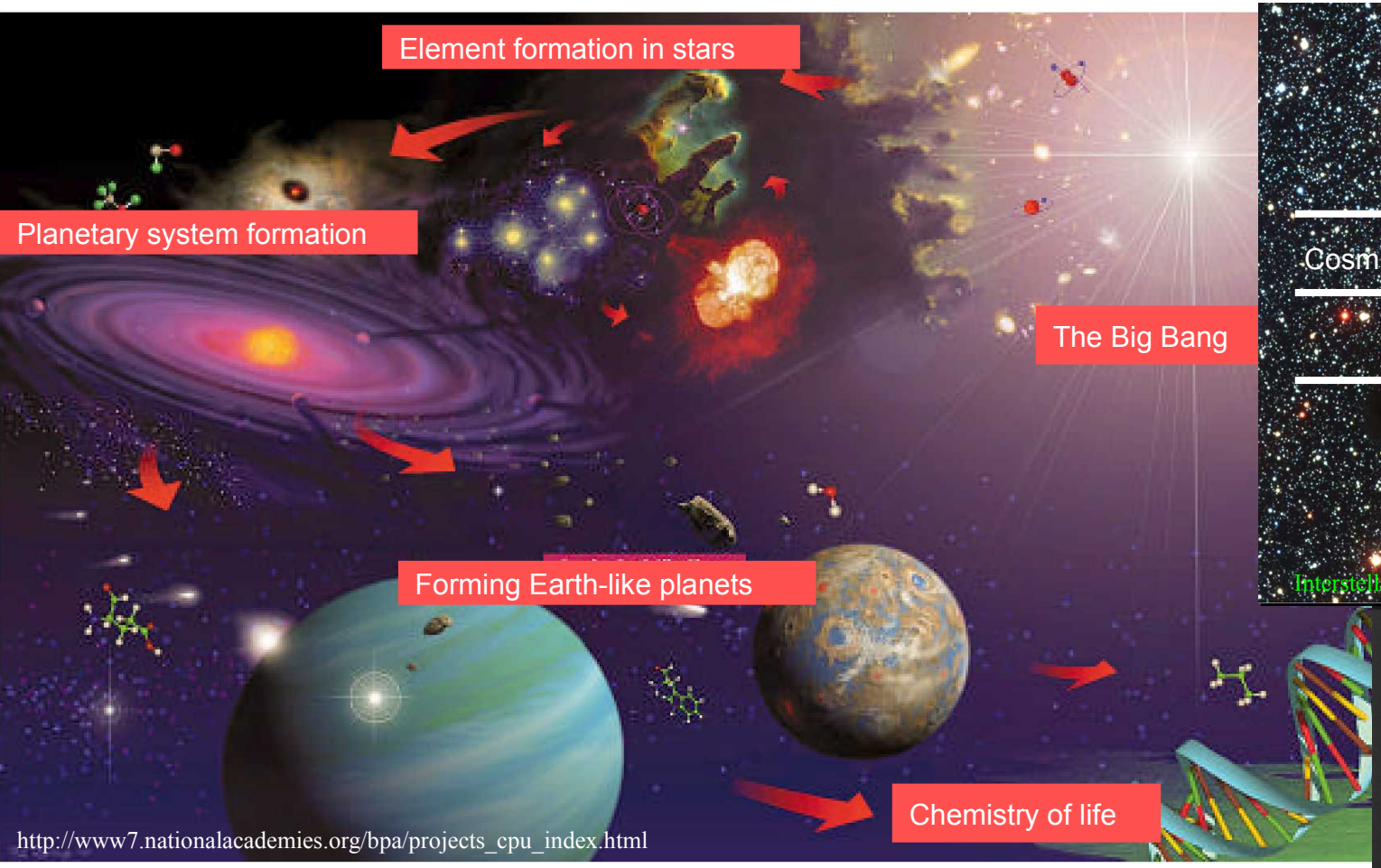
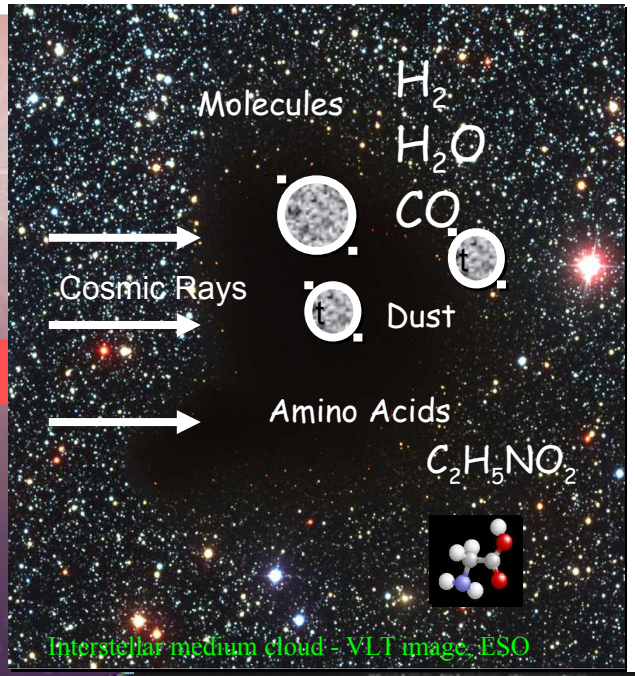
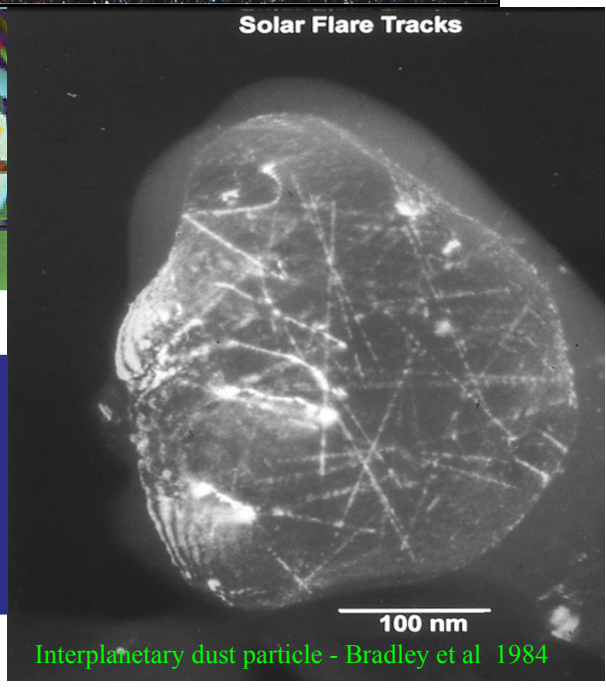
Our universe provides various regions of extreme conditions far from thermodynamic equilibrium

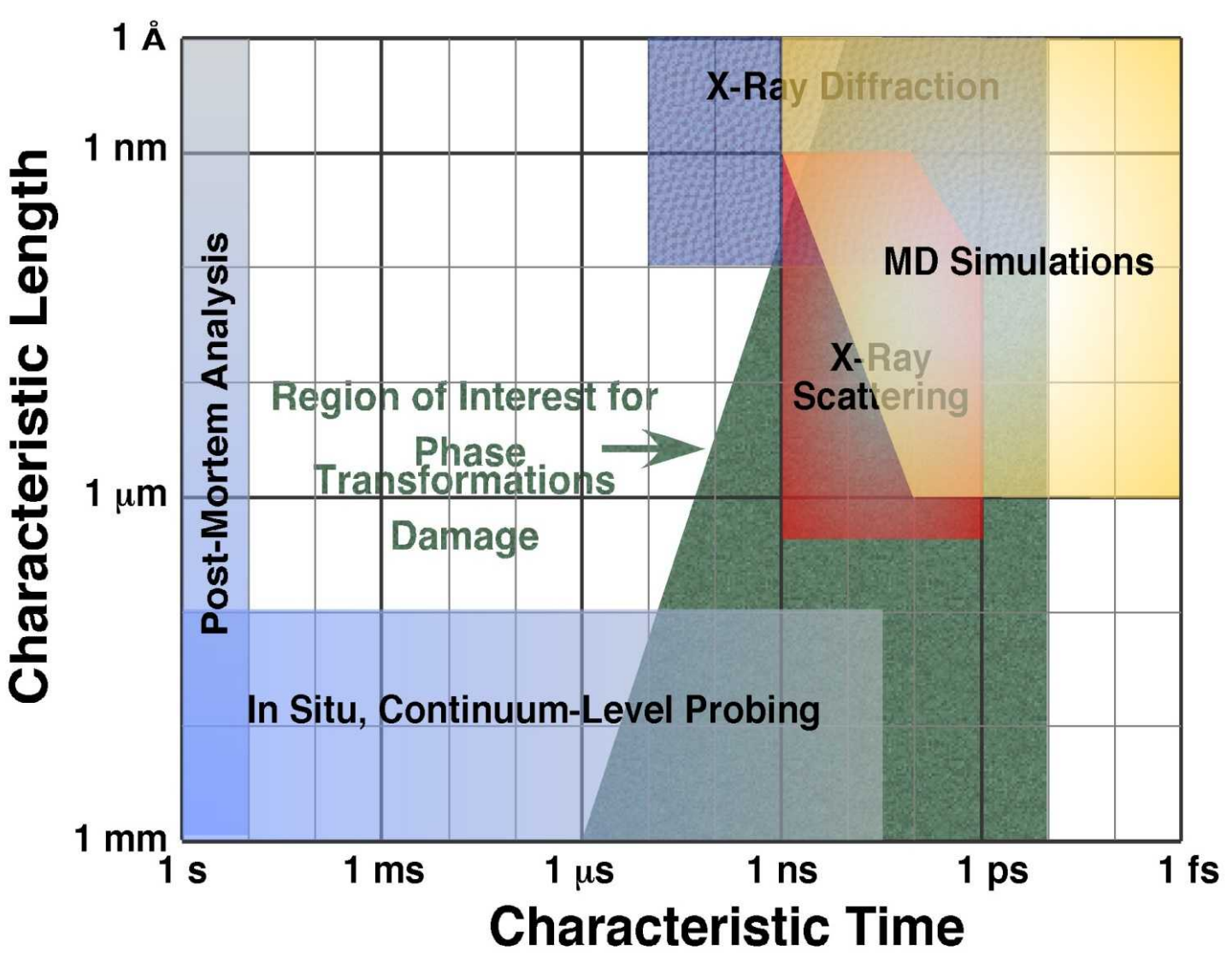






Nanoscale affects macroscale:
planet and star formation, dust clouds, astrobiology
Experiments too difficult/costly: need simulations

New experimental techniques are reaching time and length scales comparable to the ones in atomistic simulations



Process control under extreme conditions ➔
production of new materials y comprehension of astrophysical processes

MD limitations in materials sciences

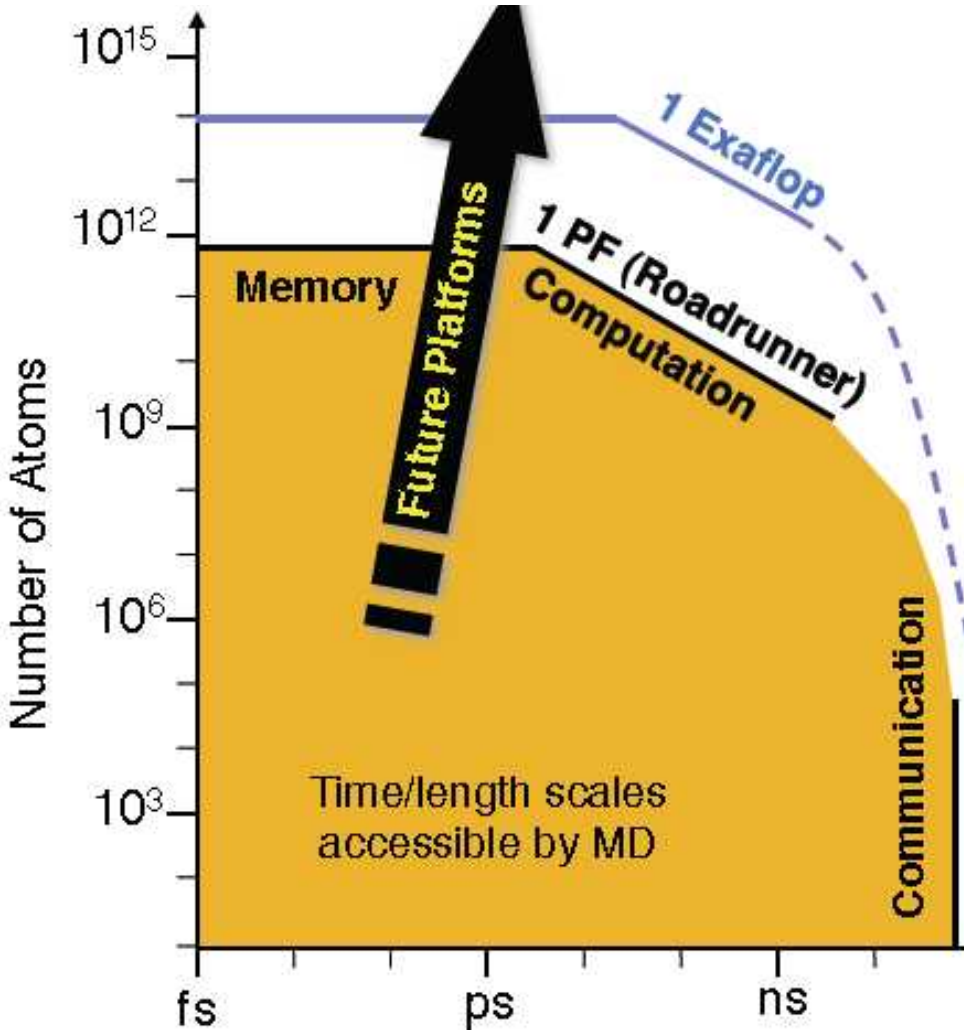


Figure by T. Germann for SPaSM (LANL)

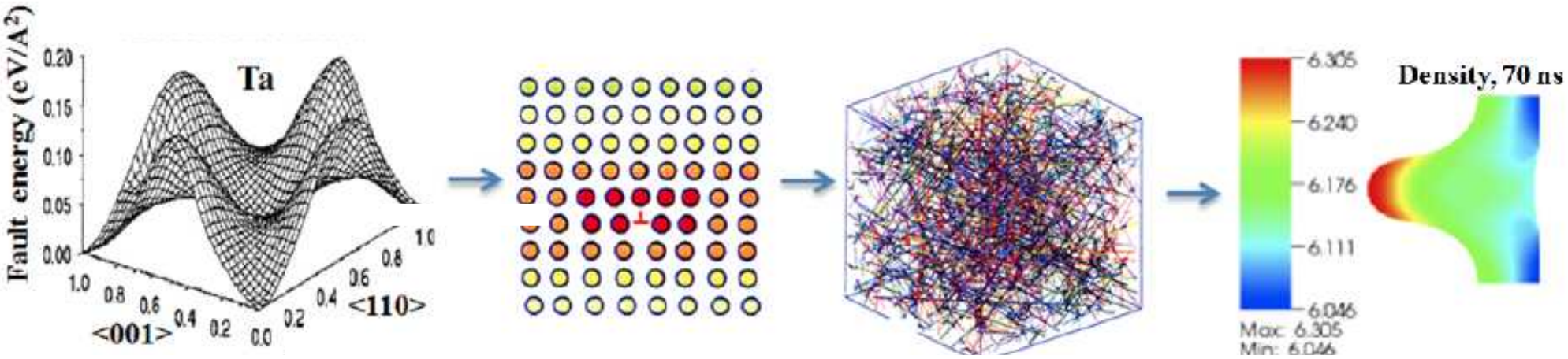
Main Challenges:
Memory limitations +
Communication limitations

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
Are we currently stagnating?

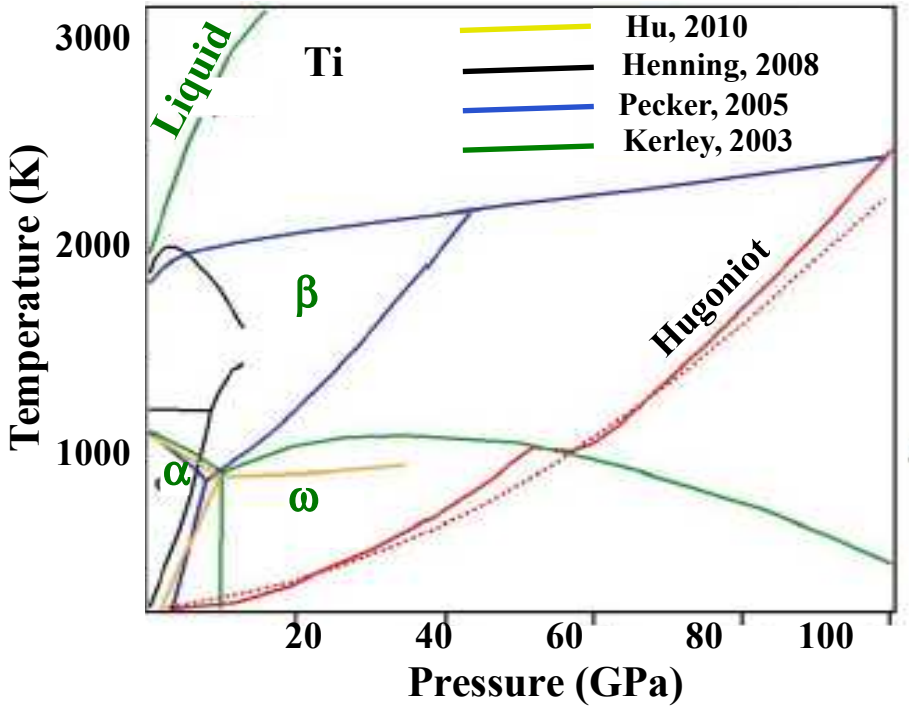
Example: Multi-scale models of plasticity and phase diagrams are needed to predict high pressure, high strain rate plastic flow in ductile metals (Remington *et al.*)

Electronic scale | Atomistic scale | Microscale | Macroscale continuum

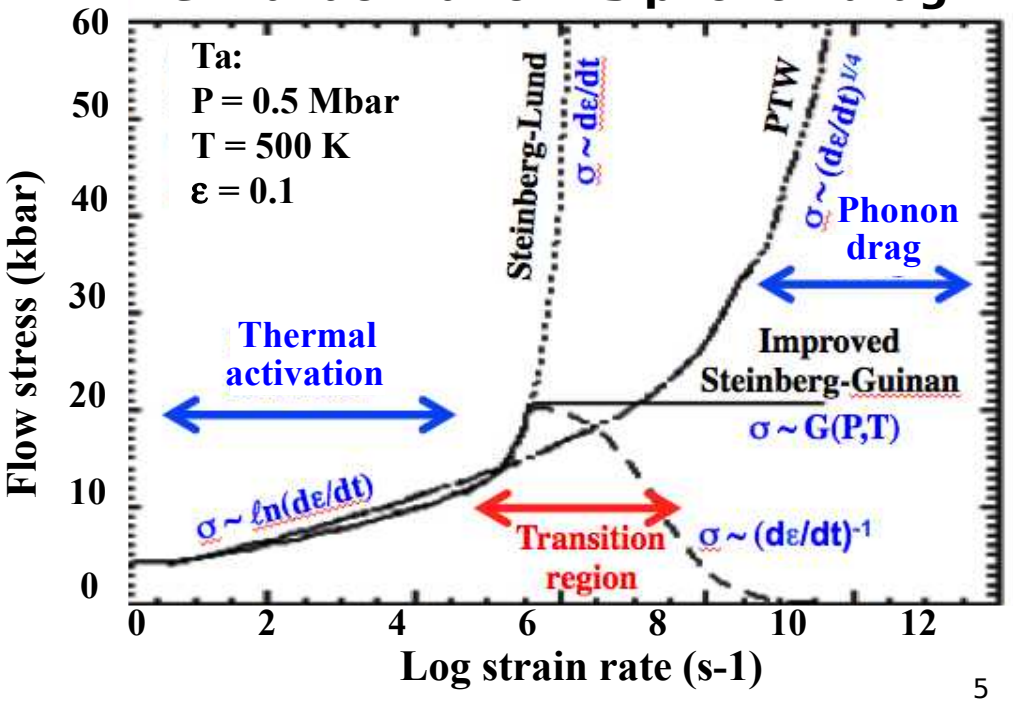


Rayleigh-Taylor exp.

Phase boundaries vs loading rates (kinetics)



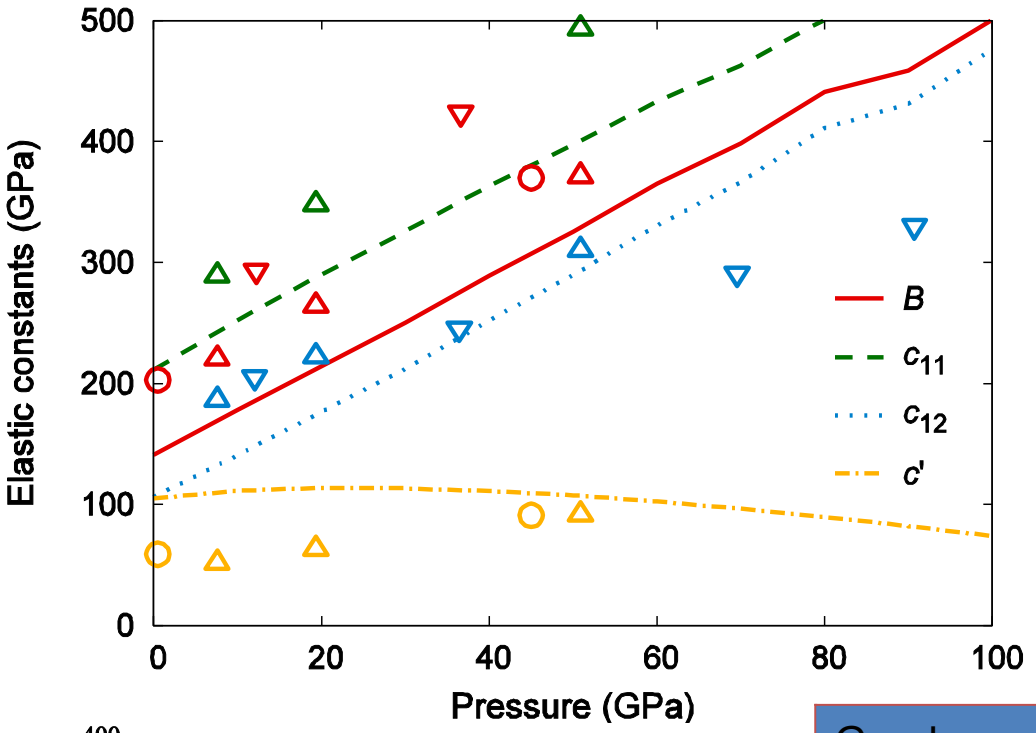
Thermal activation vs phonon drag

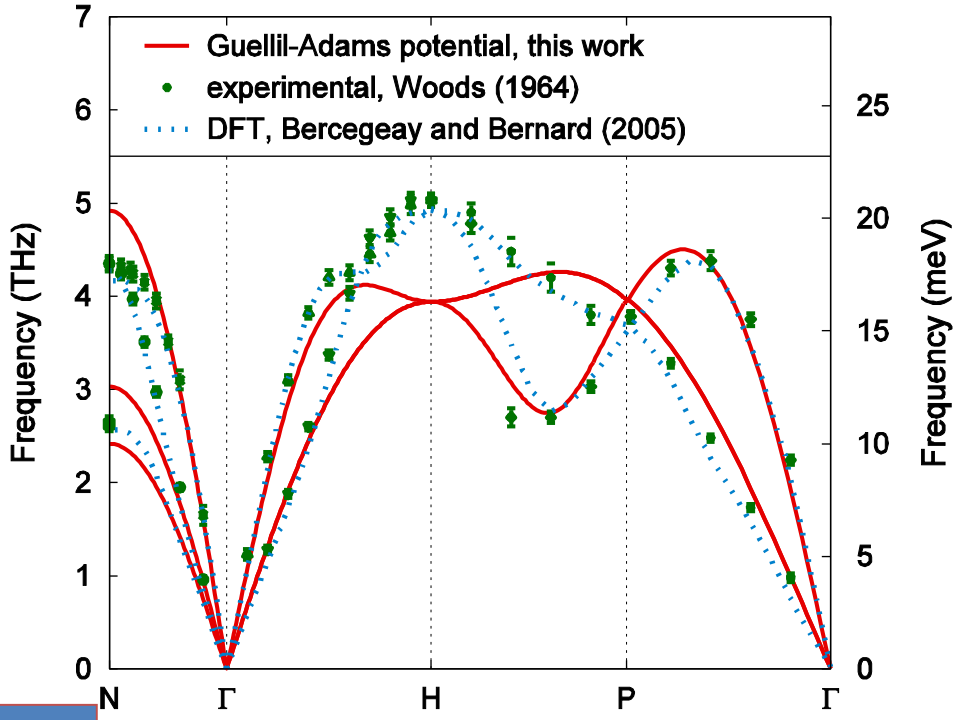


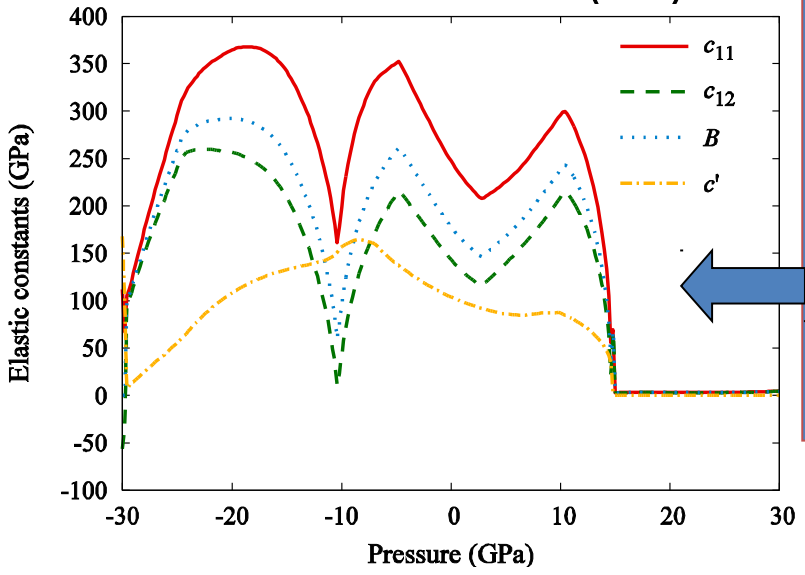
"Potential" problems: EAM potentials, phonons and elastic constants

or when, even if the PV EOS is OK, other things can go wrong

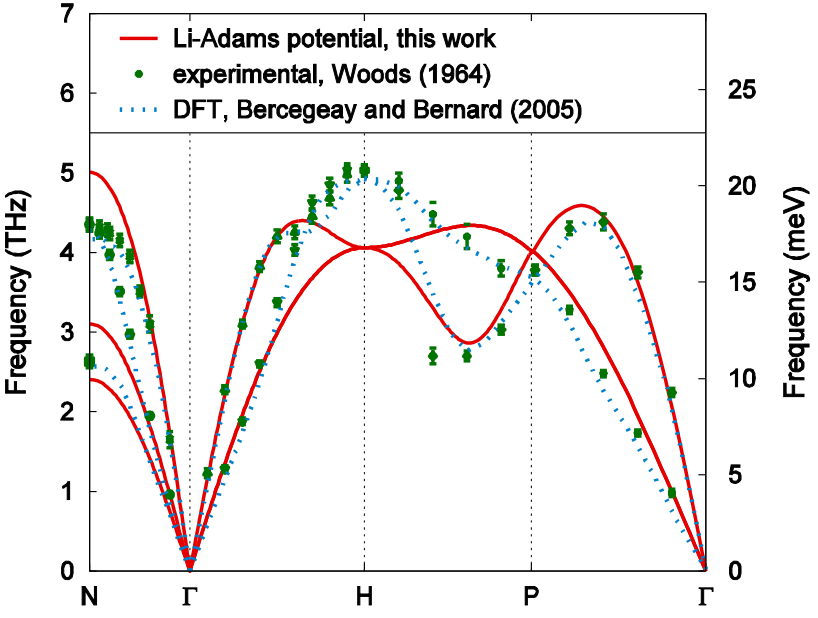
Ruestes *et al.*, Materials Science&Engineering A 613, 390 (2014)





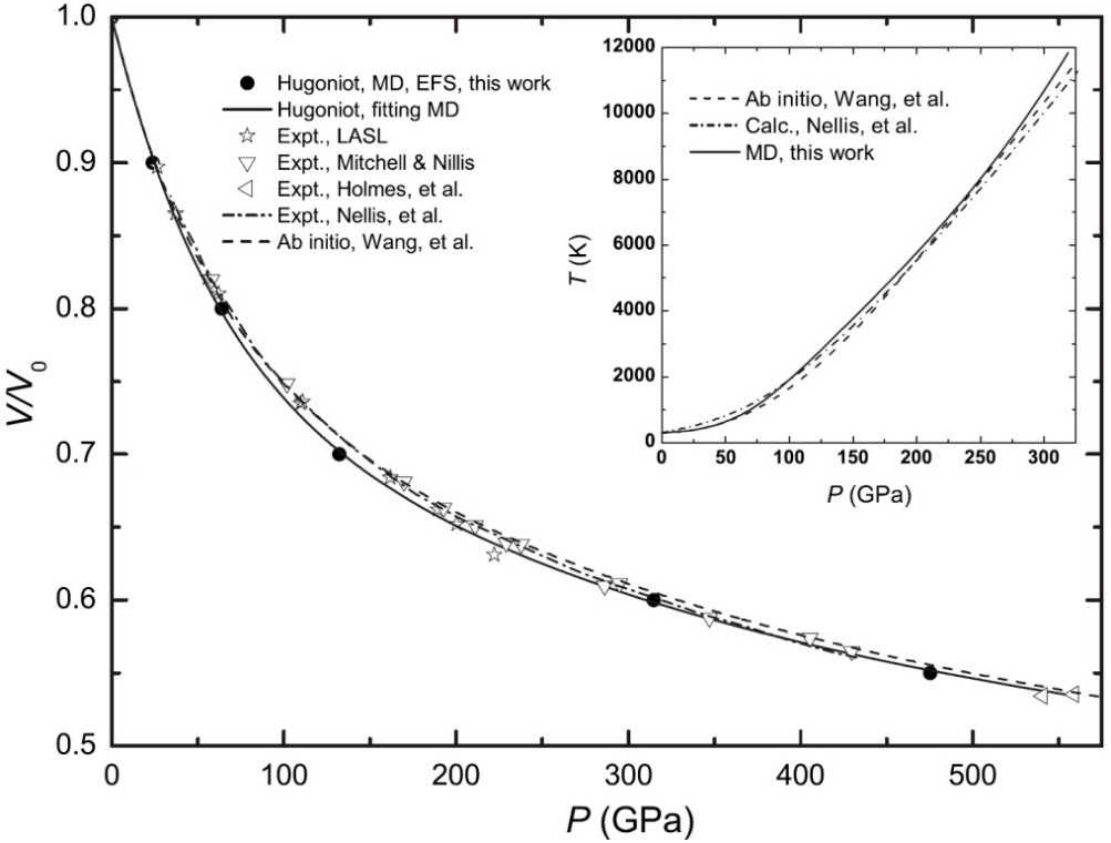


Good agreement with phonons at P=0 GPa, but discontinuities in elastic constants, due to splines in the potential, lead to multiple elastic fronts

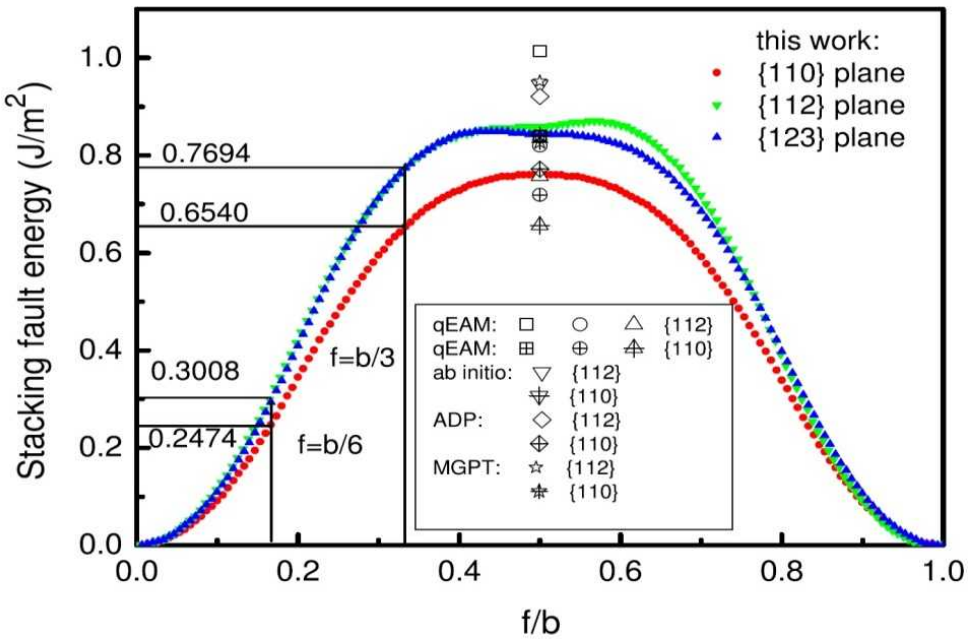


Another example: EFS Ta Potential

X.D. Dai, Y. Kong , J. Phys. Cond. Mat. **18** (2006) 4527



Z-L Liu, L-C Cai, Phys. Rev. B **77** (2008) 024103

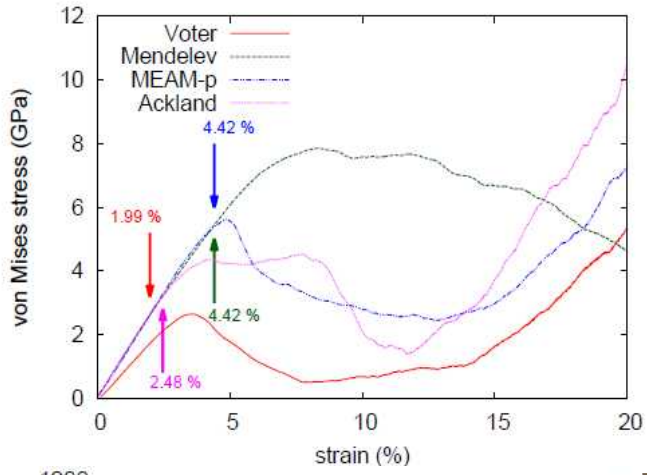


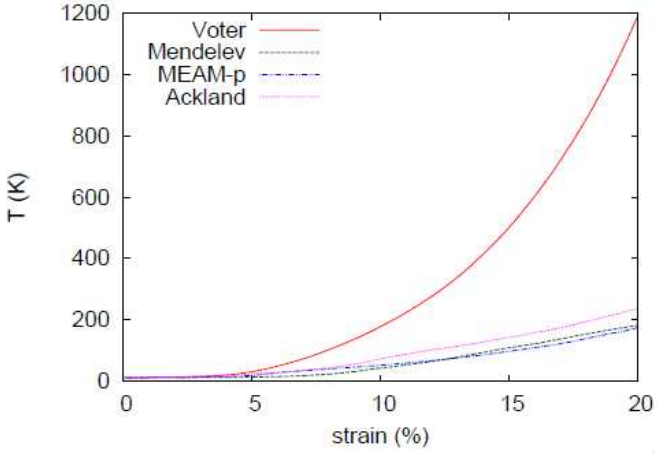
Tang, Bringa, Meyers, Acta Mat. **59** (2011) 1354

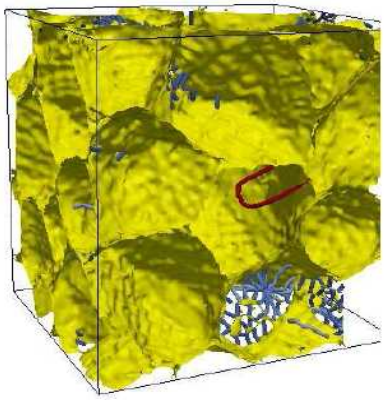
- Excellent agreement with PV, equilibrium Hugoniot, **melt line**, etc.
- Elastic constants OK up to ~1 Mbar.
- **BUT**… BCC→HCP at ~69 GPa (Ravelo *et al*., SCCM-2011).

Potential validity depends strongly on type of fit, which can emphasize a certain property, temperature & pressure range, structure, etc.
Potentials are often non-transferable ☹

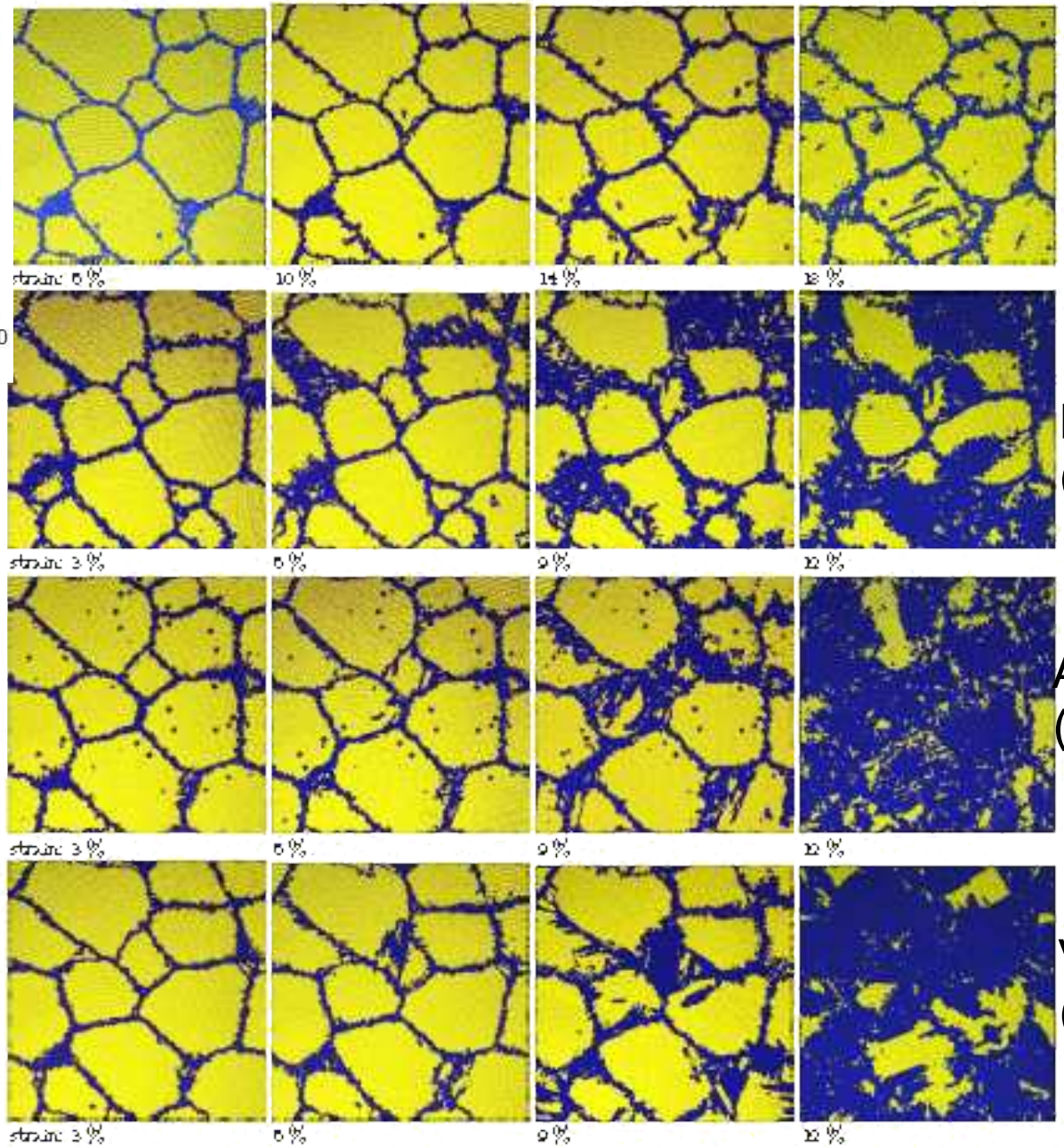
ncFe under pressure: plasticity + phase transition (bcc → hcp/fcc)







Potentials



Mendelev (~65 GPa)

MEAM-p (~13 GPa)

Ackland (~20 GPa)

Voter (~8 GPa)

Homogeneous compressive loading, *Gunkelmann et al.*, PRB **86** (2012) 144111

Simulation details need to include info on BC

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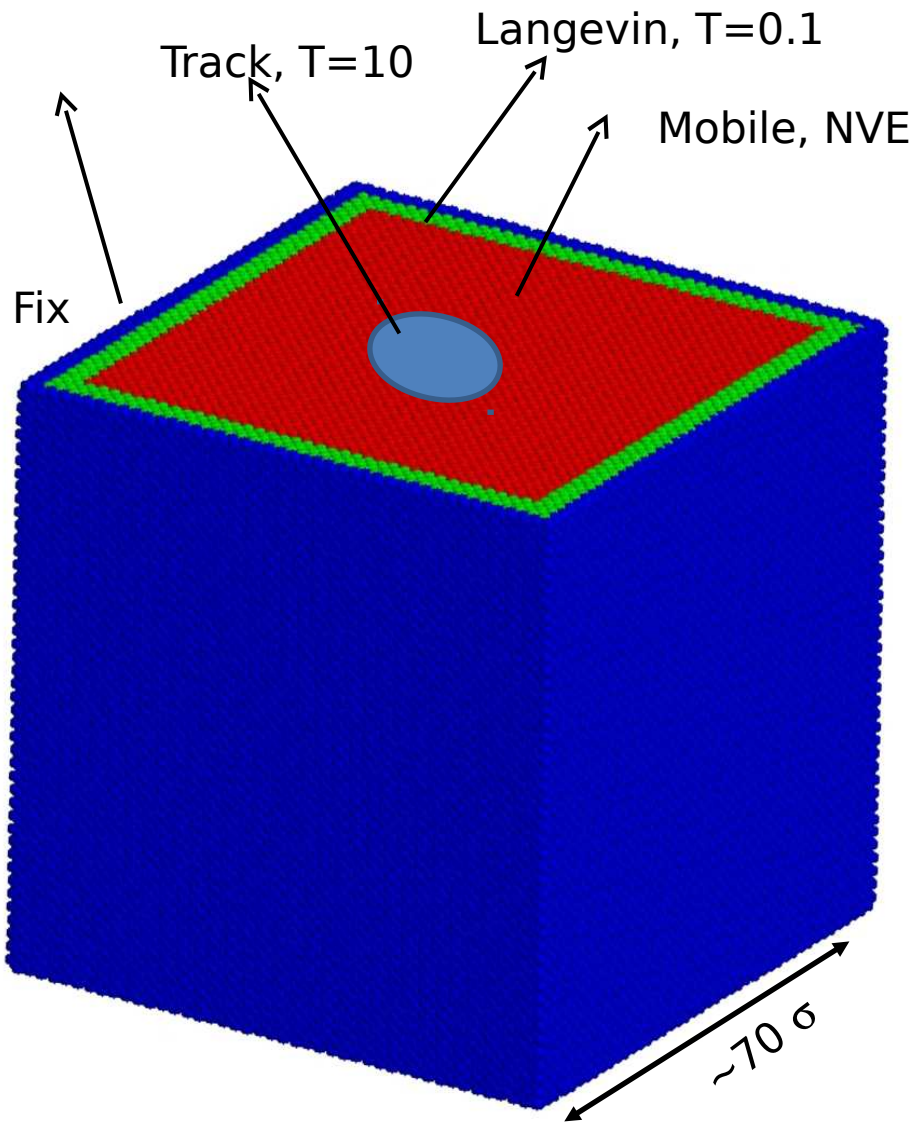
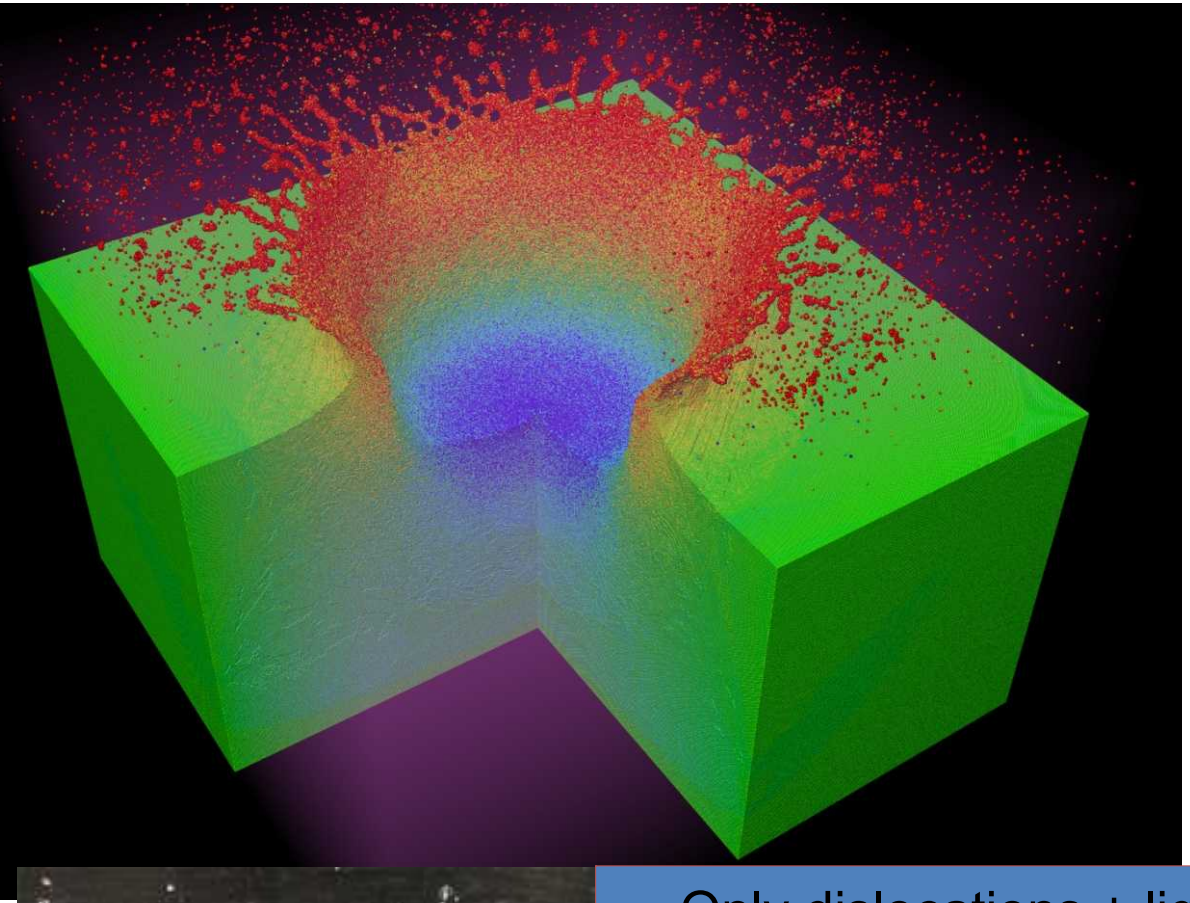
Coupling to continuum?

- PBC in (x,y), free BC with expansion (z). Langevin bath with critical damping at the sides.
- Need to re-calculate damping for each interatomic potential and bath condition.
- There are complex schemes to have impedance matching at boundaries, but none standard.
- Size has to be large enough to capture desired phenomena. Need to verify this by running simulations of different sizes: results should not change beyond certain size L, or they could be extrapolated versus 1/L.



Simulation of hot spot

Large-scale MD links nano and microscales in damage induced by nanoprojectiles [C. Anders *et al.*, PRL 108, 027601 (2012)]



Only dislocations + liquid atoms are shown

$R_{cluster}$=20 nm, 20 ps after impact, ~300 10^6 atoms, 15 hours using 3,840 CPU's in Thunder (LLNL)

Data analysis

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- On the fly and post-processing of data takes considerable time …
- Need to choose appropriate analysis tools to avoid artificial results.
- Whenever possible, carry out the analysis in parallel with domain decomposition and neighbor lists.
- Care must be taken with time averaging, thermodynamic variables.

Thermodynamics? Temperature in nano systems

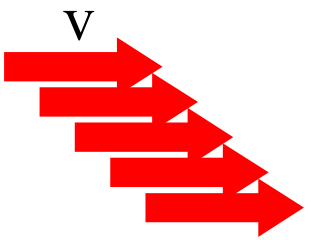
Usual: $(3/2)\, N\, k_B\, T = E_{kin}$

Nano Systems: $$T_\omega = \frac{1}{k}\left[\left(\frac{3N}{2} - 1\right)\left\langle E_{kin}^{-1}\right\rangle_\mu\right]^{-1}$$

Jellinek & Goldberg, Chem Phys. (2000)
Pearson et al, PRB (1985)

Correction due to non-zero flow velocity <v>:

$E_{kin} \rightarrow (m/2)\,(v - \langle v\rangle)^2$



$E_{kin} > 0$, but T=??

"Partial" T's: T_{rot}, T_{vib}, T_{ij}

Thermodynamics?

Can we define an atomic stress tensor? Only with caveats

Virial stress for atom I (lammps)

$$S_{ab} = -\left[mv_a v_b + \frac{1}{2}\sum_{n=1}^{N_p}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b}) + \frac{1}{2}\sum_{n=1}^{N_b}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b}) + \right.$$
$$\frac{1}{3}\sum_{n=1}^{N_a}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b} + r_{3_a}F_{3_b}) + \frac{1}{4}\sum_{n=1}^{N_d}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b} + r_{3_a}F_{3_b} + r_{4_a}F_{4_b}) +$$
$$\left. \frac{1}{4}\sum_{n=1}^{N_i}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b} + r_{3_a}F_{3_b} + r_{4_a}F_{4_b}) + \sum_{n=1}^{N_f} r_{i_a}F_{i_b} \right]$$

a, b= x,y,z . Includes thermal, pair, bond, angle, dihedral, improper, and “fix”

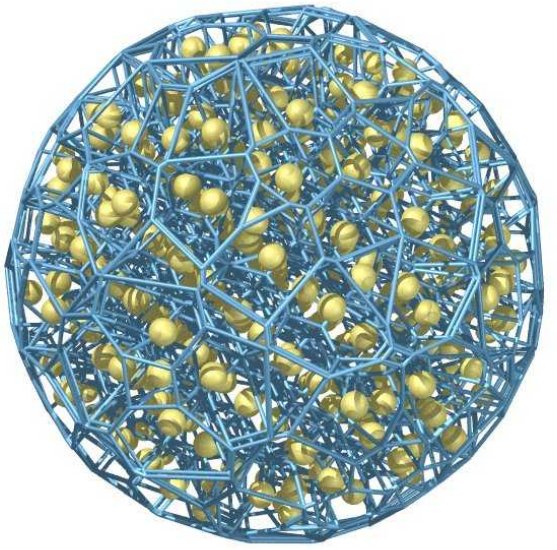
Be careful with Nk_BT term …it should discount flow velocity in calculation of T

S = σ V ➔ how do we define “atomic” volume to calculate momentum flux?

Possible solution: use Voronoi polyhedra

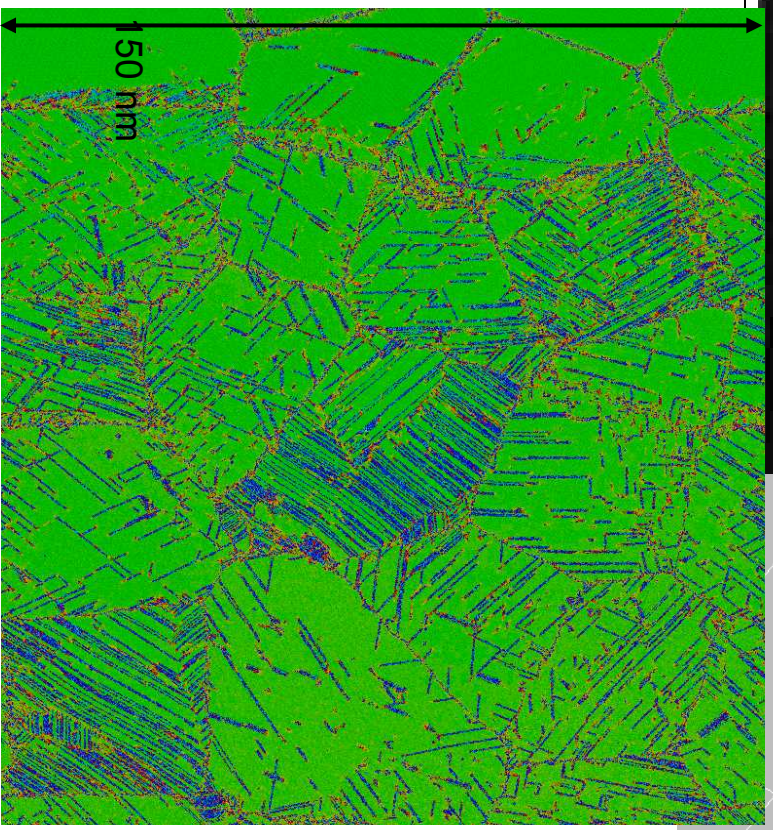
PdH nanoclusters. Using Voronoi or mean volume gives roughly the same results. Work with G. Bertolino, M. Ruda (Centro Atomico Bariloche), S. Ramos, E. Crespo (UN Comahue, Neuquen)

Int. J. Hydrogen Energy (2012)



Perfect crystals are the `spherical horse' of atomistic simulations (also for many model Hamiltonians)

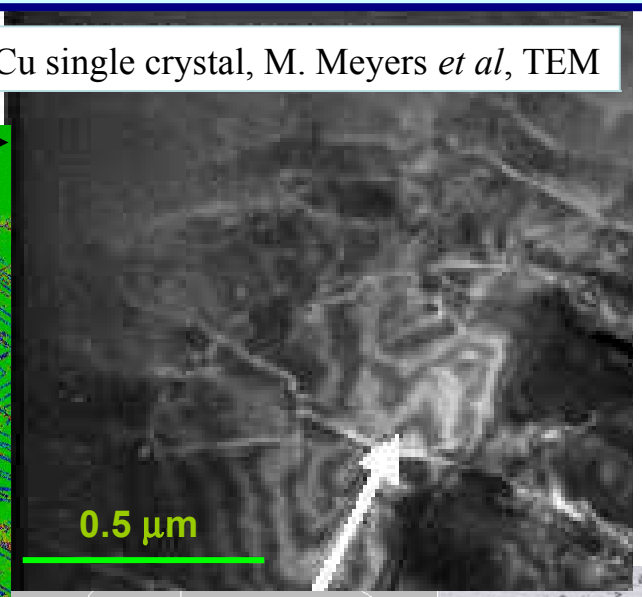
How to make more realistic simulations? Add defects:
vacancies → voids → bubbles, interstitials, dislocation loops/lines,
grain boundaries (bi-cristals → polycrystals), impurities, etc.

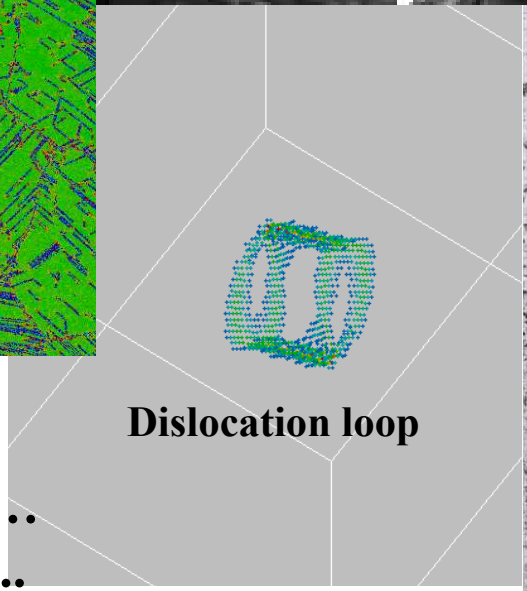


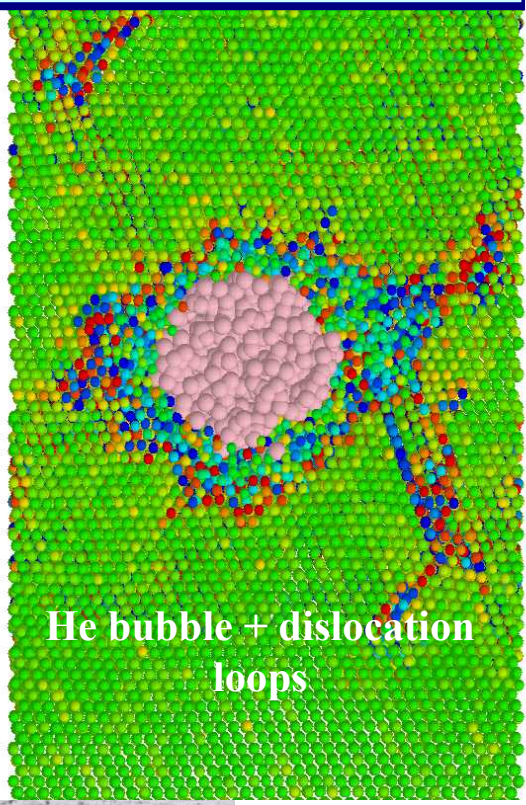
Polycrystal (50 nm grain size)
(400 million atoms)

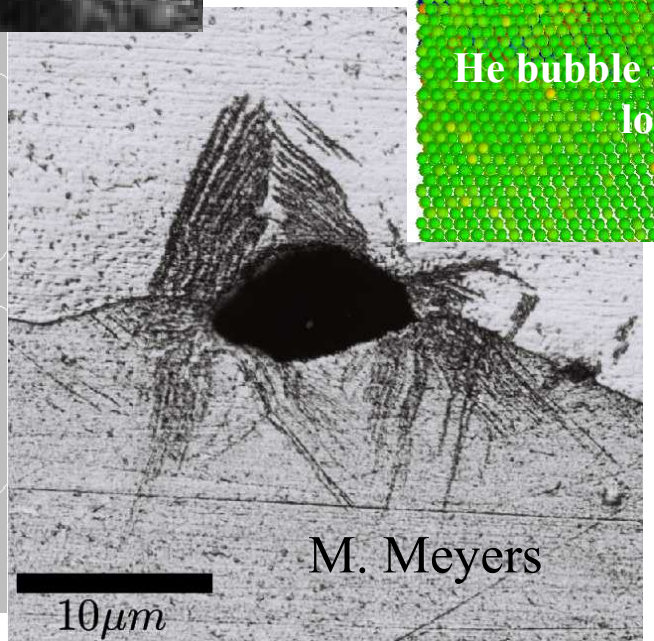
Few GB are Σ boundaries …

Not 1 dislocation but many ...









Common Neighbor Analysis

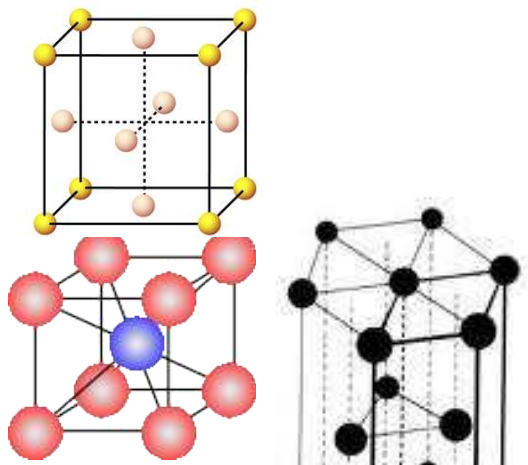
- **CNA***:* a parameter to measure the local disorder
- Sensitive to cutoff radius, **problems at large uniaxial strain**
- 12 nearest neighbor for perfect FCC and HCP crystals, 14 nearest neighbors for perfect BCC crystals

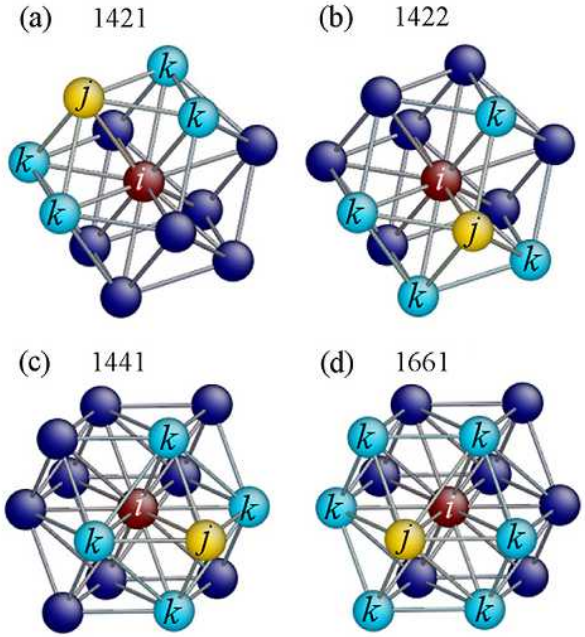
This is done for every atom in the sample ➔ high computational cost

$$r_c^{fcc} = \frac{1}{2}\left(\frac{\sqrt{2}}{2}+1\right)\mathrm{a} \simeq 0.8536\,\mathrm{a}$$

$$r_c^{bcc} = \frac{1}{2}(\sqrt{2}+1)\mathrm{a} \simeq 1.207\,\mathrm{a}$$

$$r_c^{hcp} = \frac{1}{2}\left(1+\sqrt{\frac{4+2x^2}{3}}\right)\mathrm{a}$$

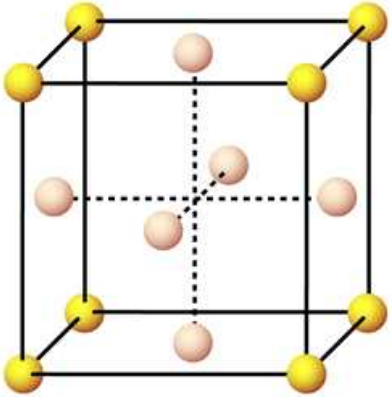




• Faken, Jonsson, Comput Mater Sci, 2, 279 (1994).
• Tsuzuki, Branicio, Rino, Comput Phys Comm, 177, 518 (2007).

Centro-Symmetry Parameter (centro)*

- **Centro-symmetry parameter** *(centro/CSP):* a parameter to measure the local disorder, particularly useful to study cubic structures. Problem at large temperatures.

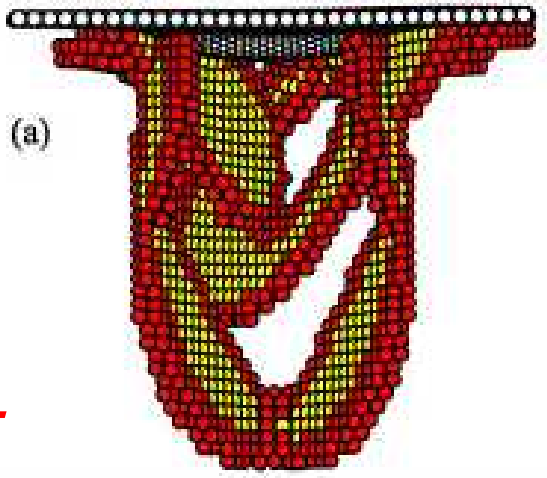


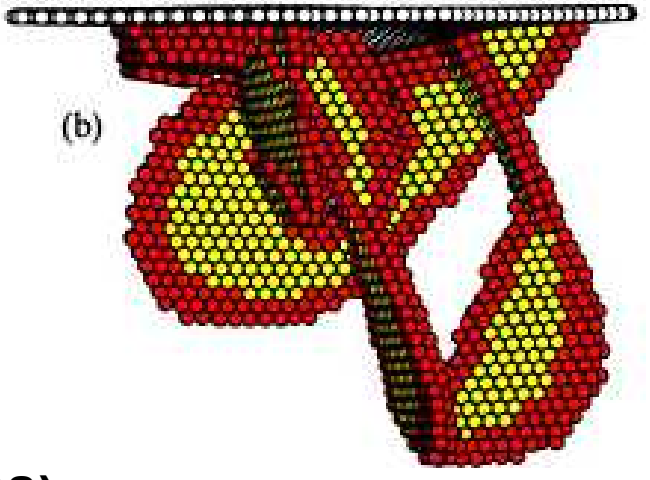
f.c.c structure

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

CSP expression for a f.c.c. unit cell

This is done for every atom in the sample ➔ high computational cost





Kelchner et al, FIG. 2, partial view. Defect structure at the first plastic yield point during indentation on Au (111), (a) view along [112], (b) rotated 45° about [111]. The colors indicate defect types as determined by the centrosymmetry parameter: partial dislocation (red), stacking fault (yellow), and surface atoms (white). Only atoms with P>0.5 are shown.

*** Kelchner, Plimpton, Hamilton, Phys Rev B, 58, 11085 (1998)**

DXA (Dislocation eXtraction Algorithm)

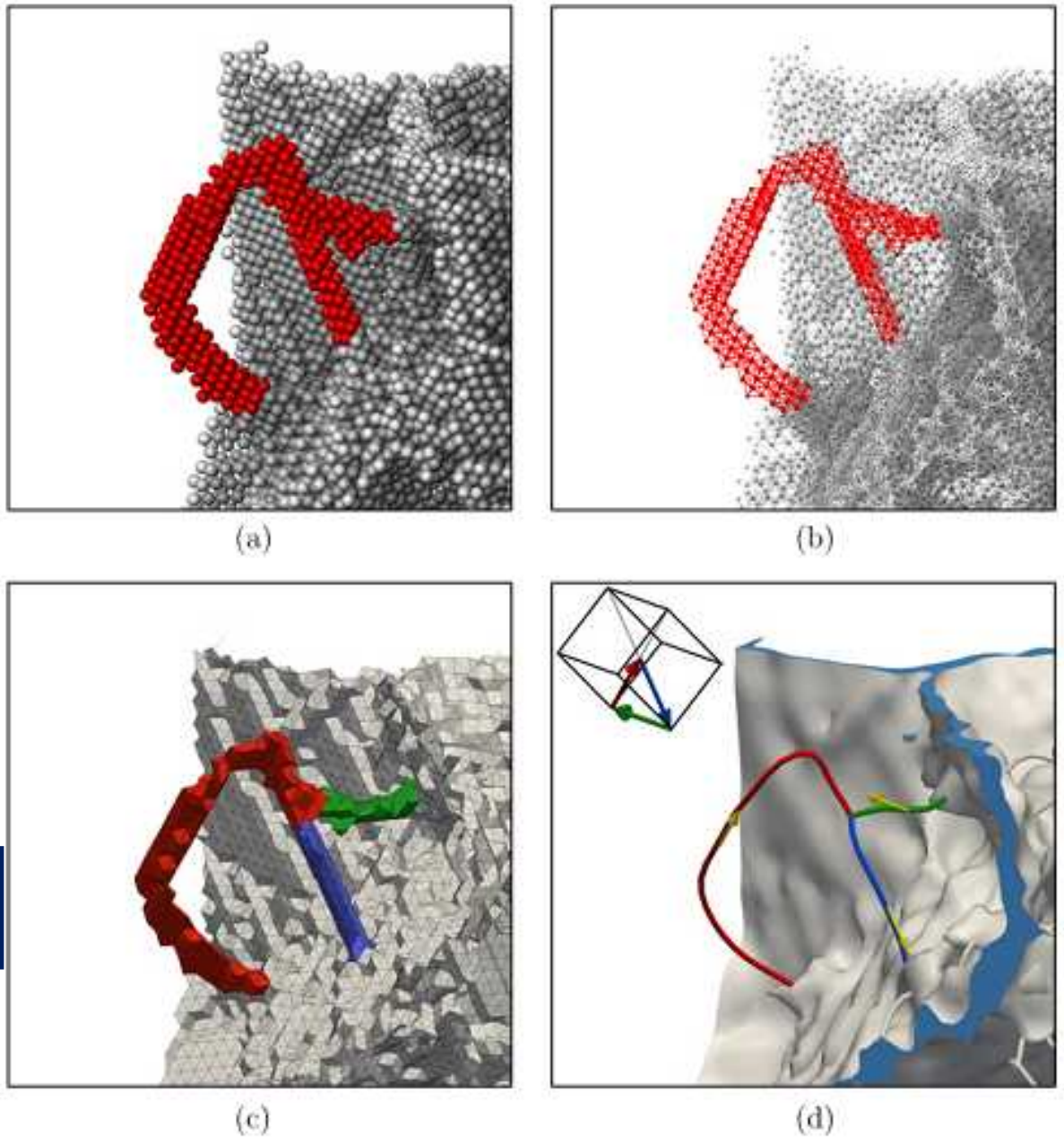
Stepwise conversion of atomistic dislocation cores into a geometric line representation.

(a) Atomistic input data.

(b) Bonds between disordered atoms.

(c) Interface mesh.

(d) Smoothed output.

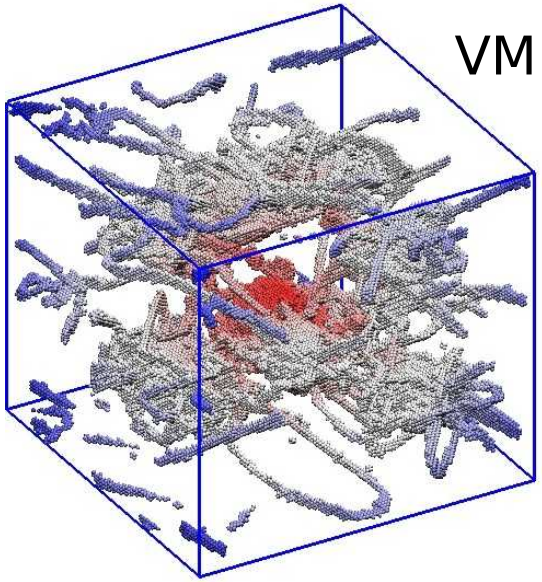


Changes in DXA parameters can have large effect on results

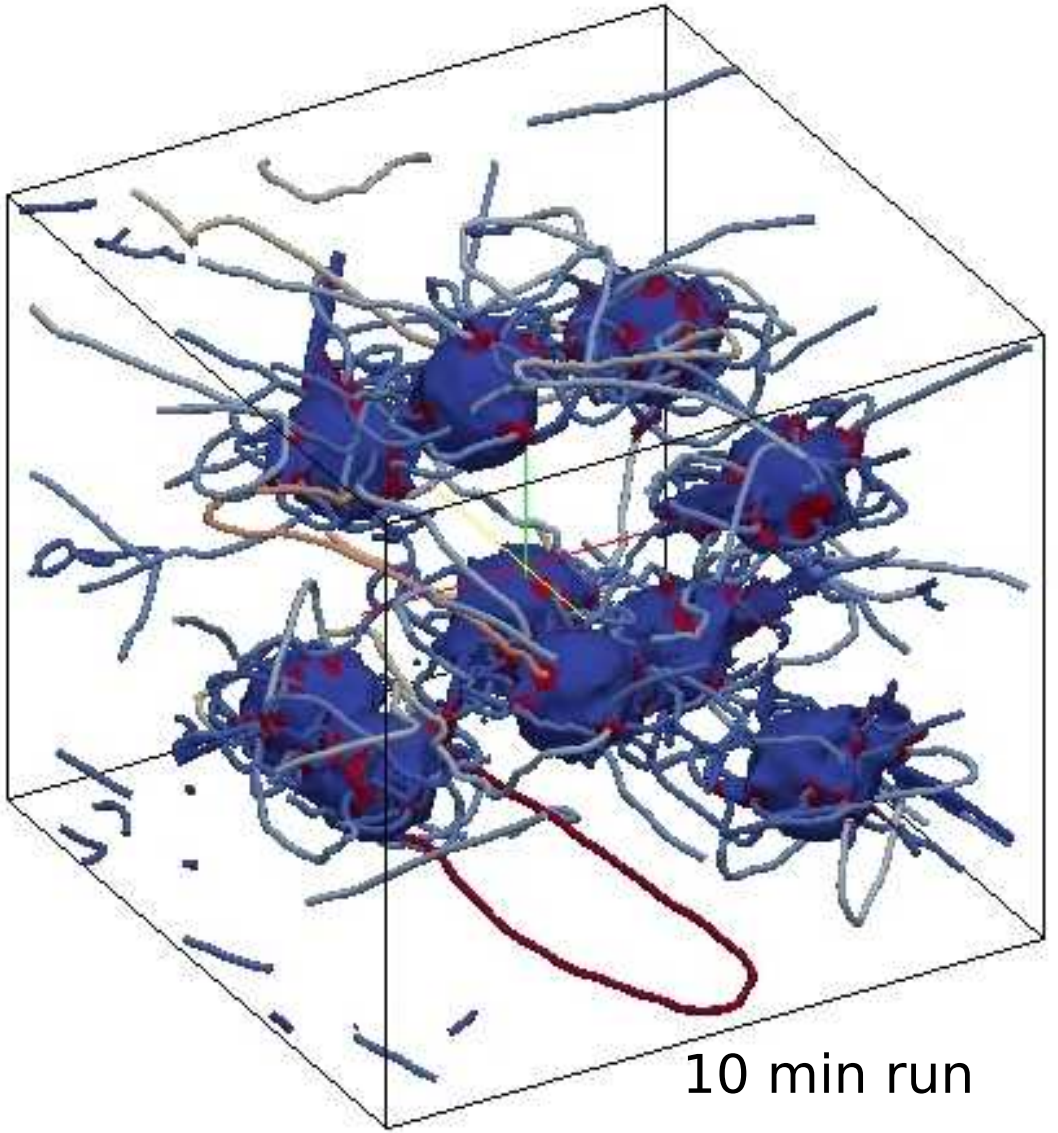
A. Stukowski and K. Albe, Modelling Simul. Mater. Sci. Eng. 18 (2010) 085001.

Modified DXA + ParaView

*Atomistic simulation of the mechanical properties of a nanoporous b.c.c. metal **



VMD



10 min run

DXA+ParaView

ParaView visualization of the results provided by DXA for a nanoporous Ta sample subjected to a 10^9/s uniaxial compressive strain rate at an 8% strain.
Preprocessed sample has 1.9 million atoms.
Run: 3 days in 32 cores
Analysis of each snapshot: 10 min run on AMD M520 + 4Gb RAM (dual core)

CNA analysis takes about 1/3 of the total analysis time

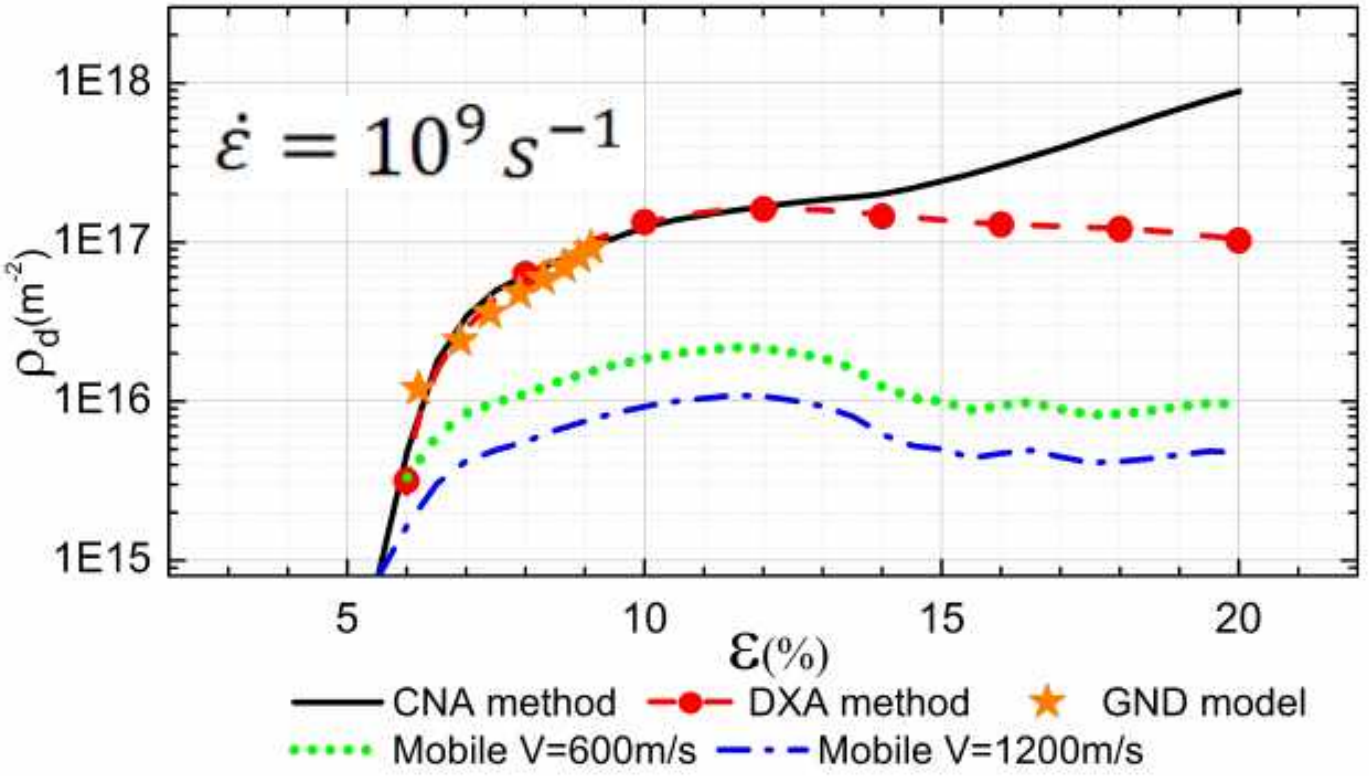
* Ruestes *et al.* , Scripta Materialia (2012)

Can we obtain dislocation densities?

•Rough estimate of total dislocation density calculated from the number of atoms with CNA not BCC, and dividing by n (2-10) to account for cross-section of dislocation cores.

• Mobile dislocation densities calculated from plastic heating* [A. Higginbotham *et al*., JAP (2011)].

$$dT = \beta \frac{V \sigma_{13}(t)\, \rho b v\, dt}{C}$$



Analytical GND model shows good agreement with MD

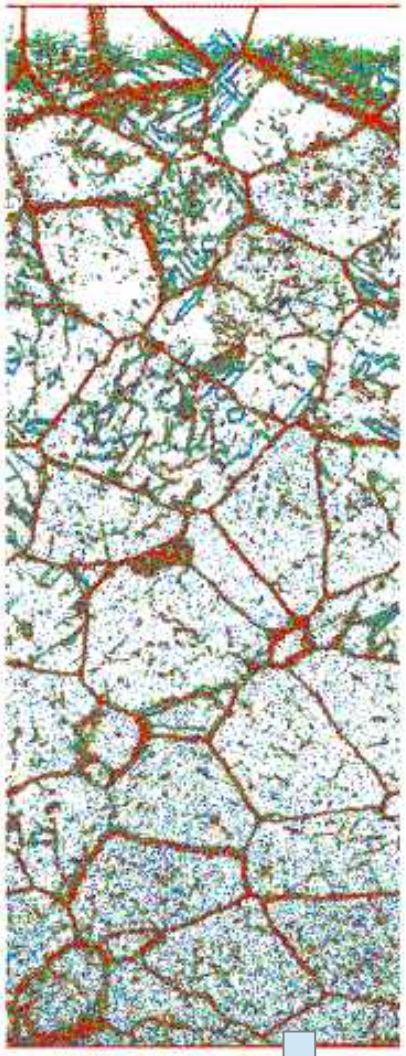
Ruestes *et al*., Mod. Sim. Mat. Sci. (2013)

Can we compare our results with experiments?

After relaxation to P=0. Possibly, because long-term recovery of the microstructure in bcc samples should have minor effects on total density. Note the absence of twins in the recovered sample, which can be checked with X-ray diffraction.

ncTa: twinning (CAT+OIM sim) and dislocations (DXA)

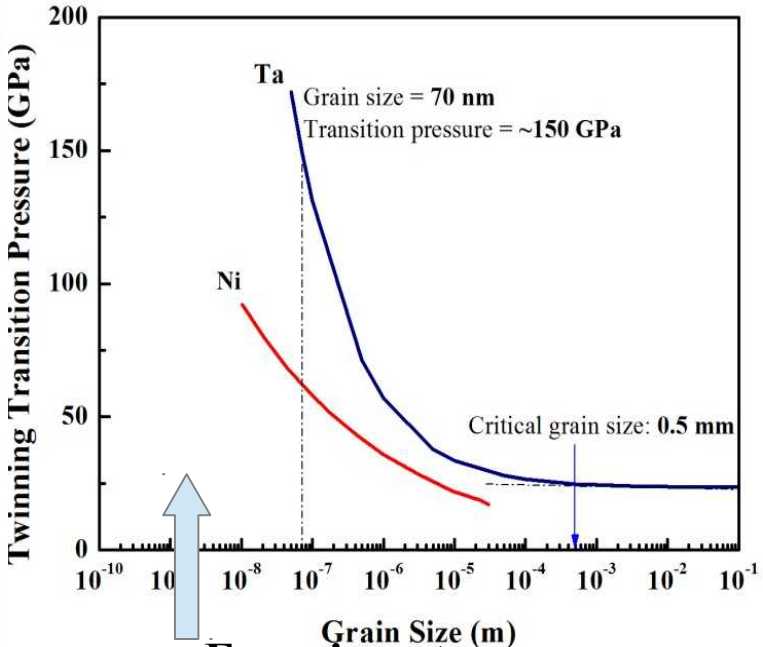
E. Hanhn (UCSD), D. Tramontina (U.N. Cuyo), T. Germann (LANL)



MD: d~5-30 nm

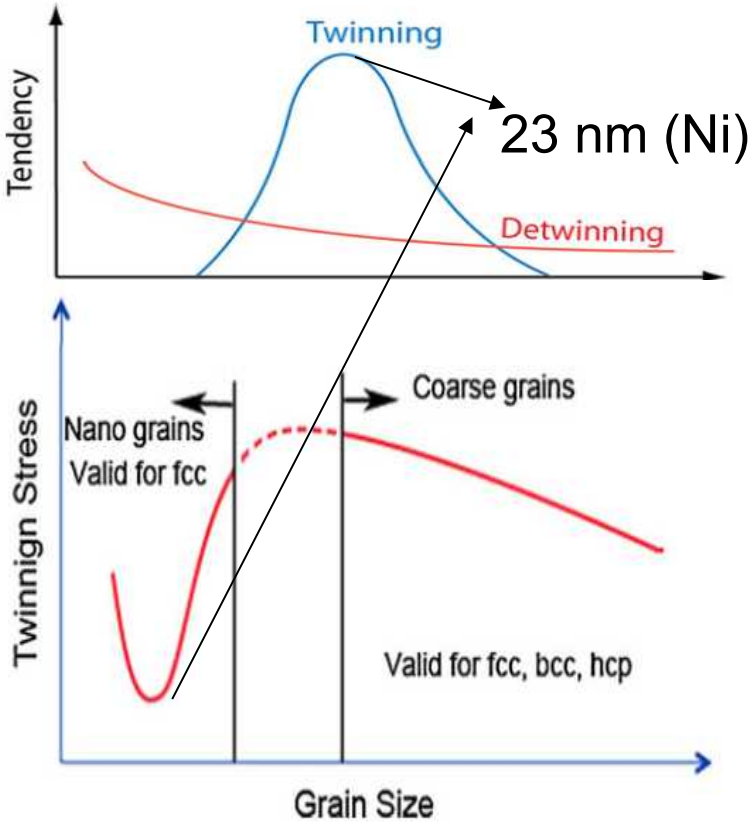
Inverse Hall-Petch for twinning

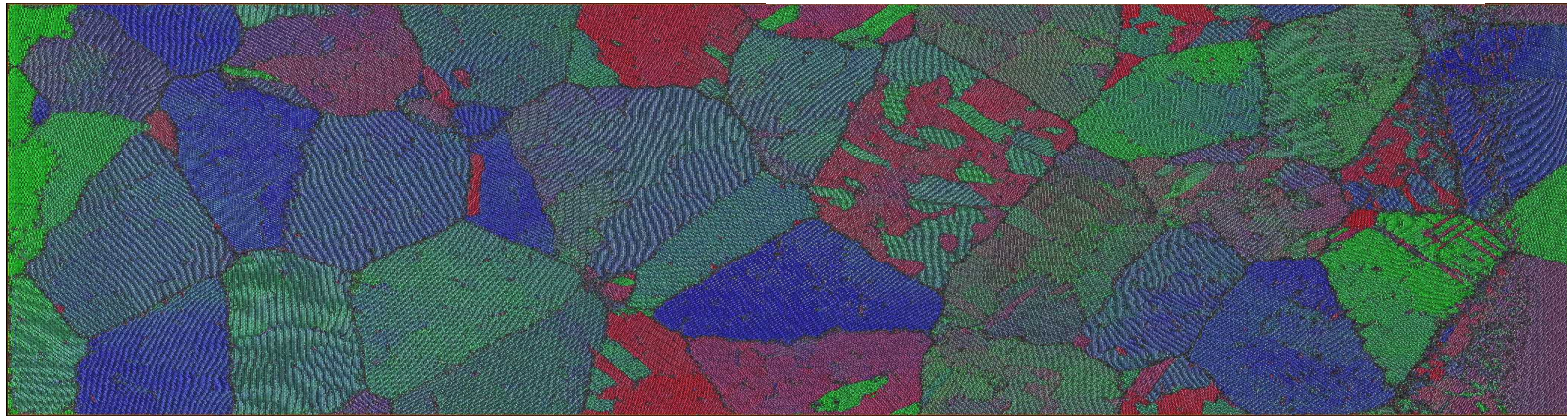
Hall-Petch for twinning



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

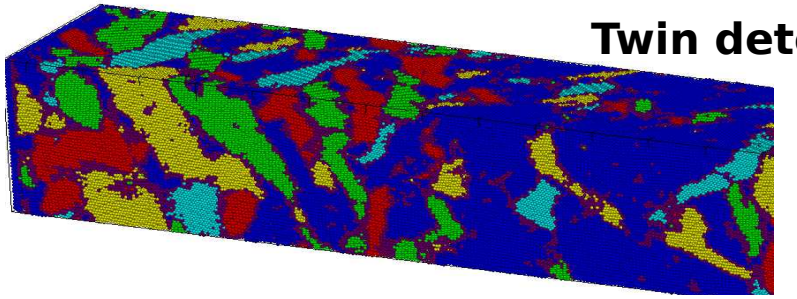
FCC: exp + model by Zhu *et al*.
J. Mater Sci (2013) 48, 4467





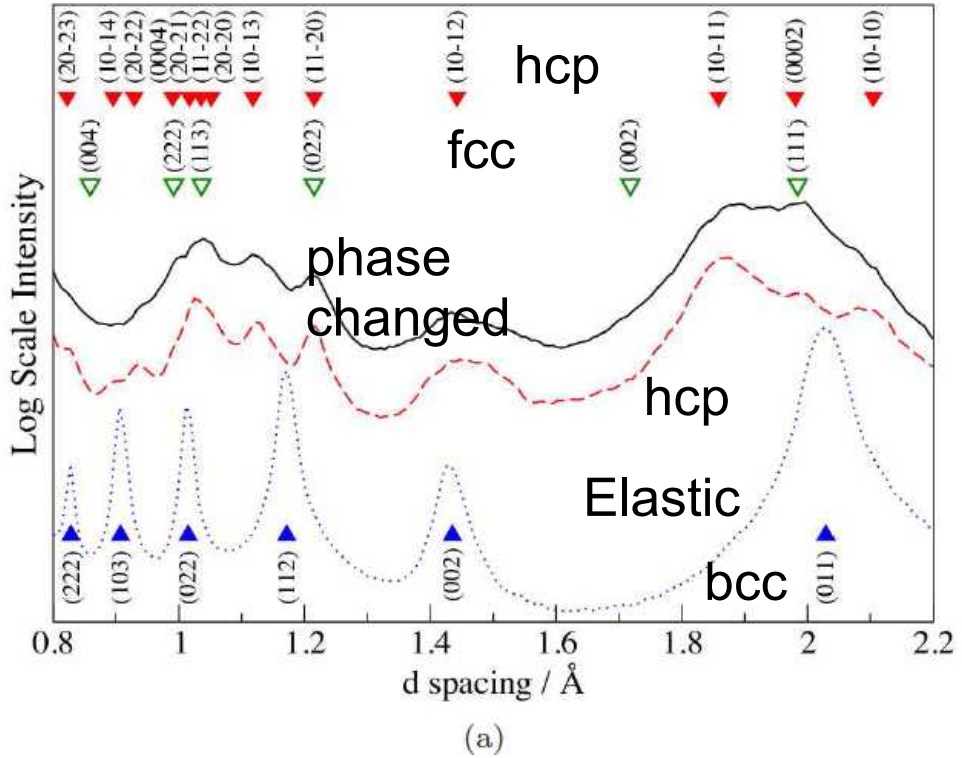
Simulated X-Ray diffraction (use cufftw)

A. Higginbotham, M. Suggit, J.S. Wark (U. Oxford).

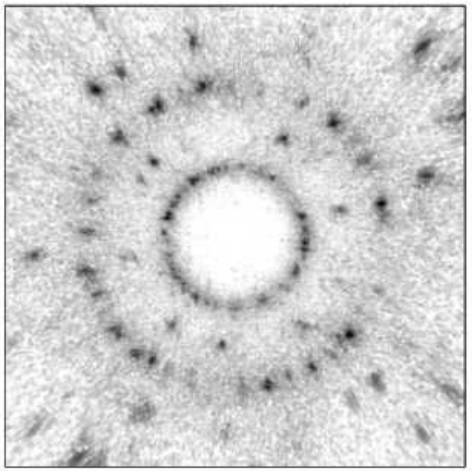


Twin detection in bcc metals: Suggit *et al*, Phys. Rev. B (2013)

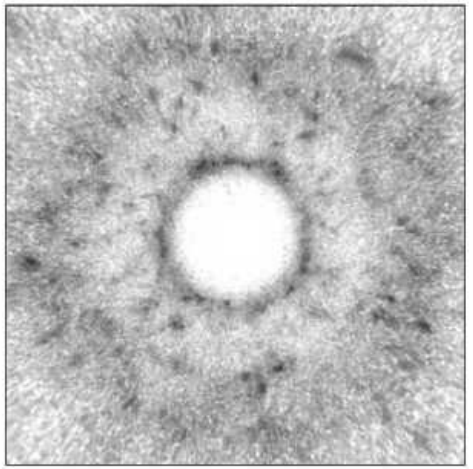
Fe phase change: Gunkelmann *et al*, Phys. Rev. B (2014)



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



unshocked

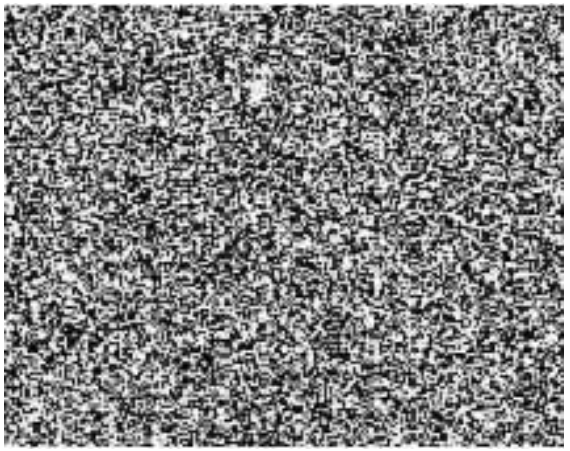


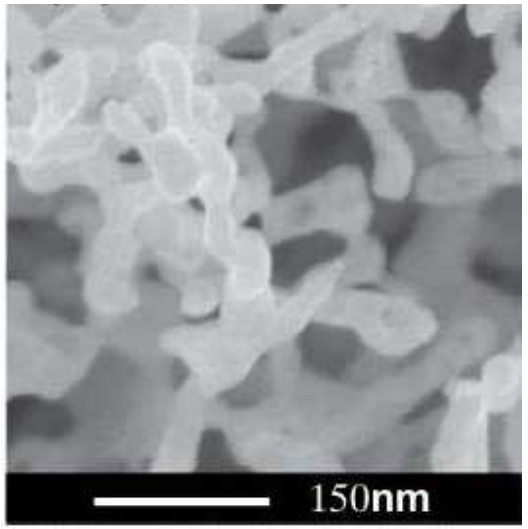
phase changed

“Reaction-diffusion equation” to obtain initial foam

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

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





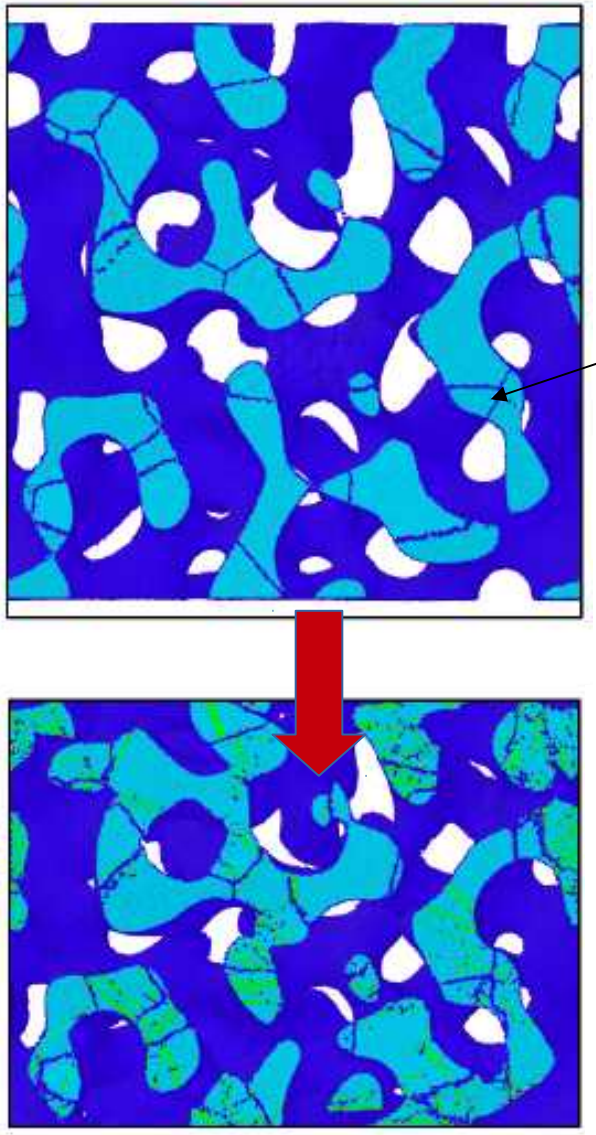
Plasma exposed W-C surface
Takamura et al., Plasma and Fusion Research 1, 51 (2006)

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

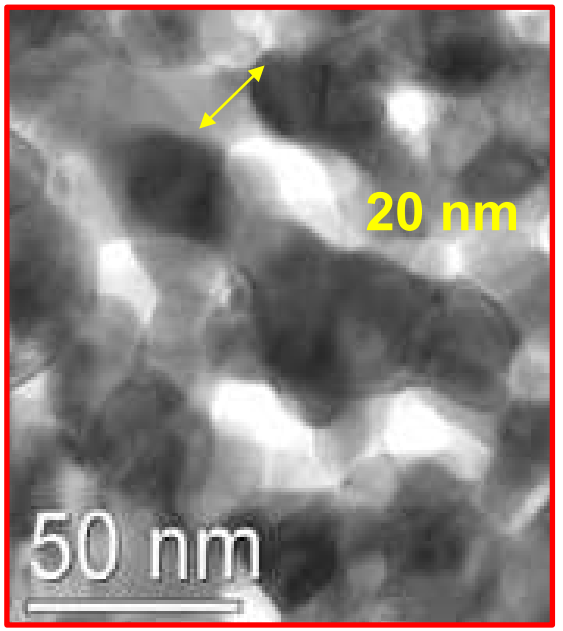
Bringa *et al*, NanoLetters (2012)

Loading of high porosity ncAu foams (2-15 nm filaments)

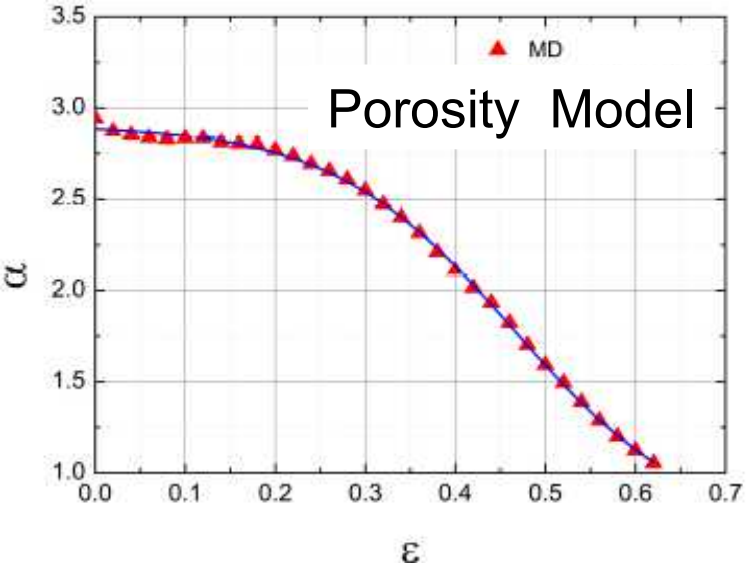
Carlos Ruestes, UNCuyo

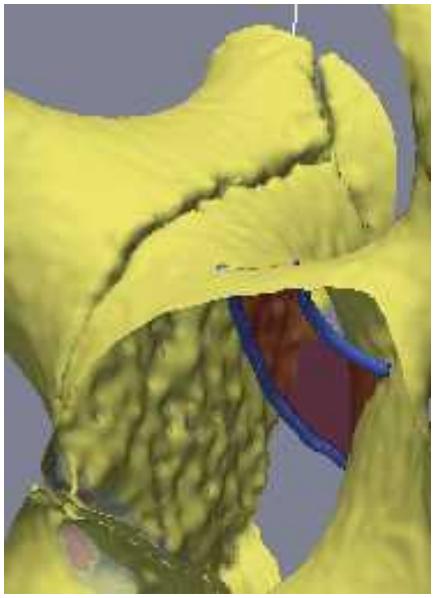


70% porosity foam
Elastic and plastic behavior



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

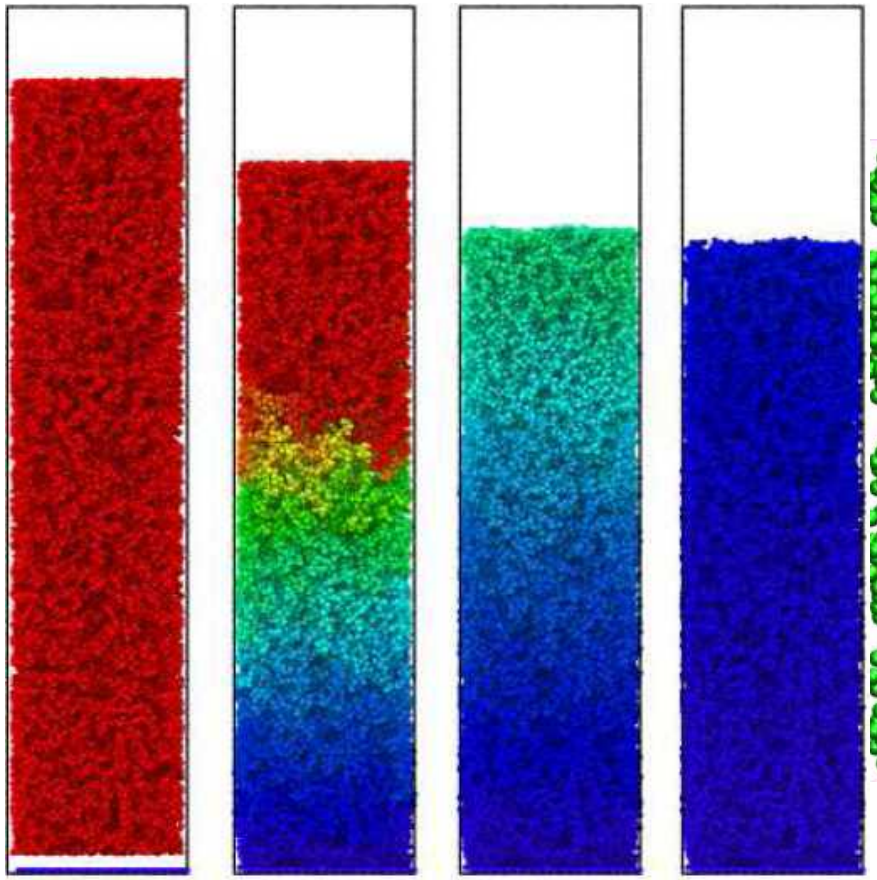




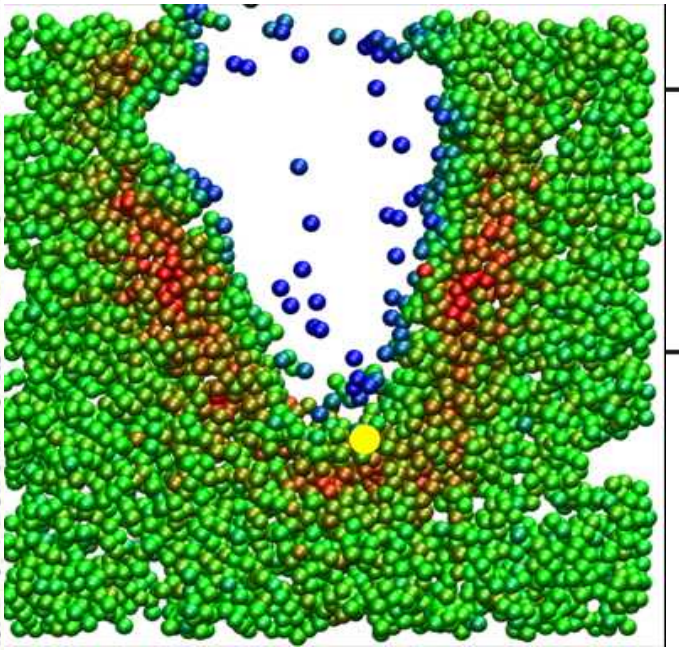
Loading: "realistic" foam includes full dislocations in addition to SFs and twins. New porosity evolution model.

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

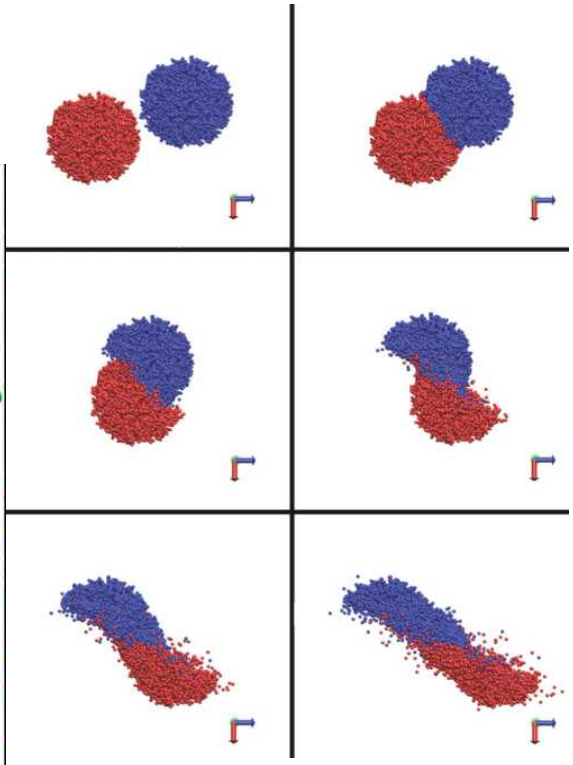
Porous samples simulated by granular mechanics



Compaction wave for impact against hard wall
Ringl *et al.*,
PRE **91**, 042205 (2015)



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

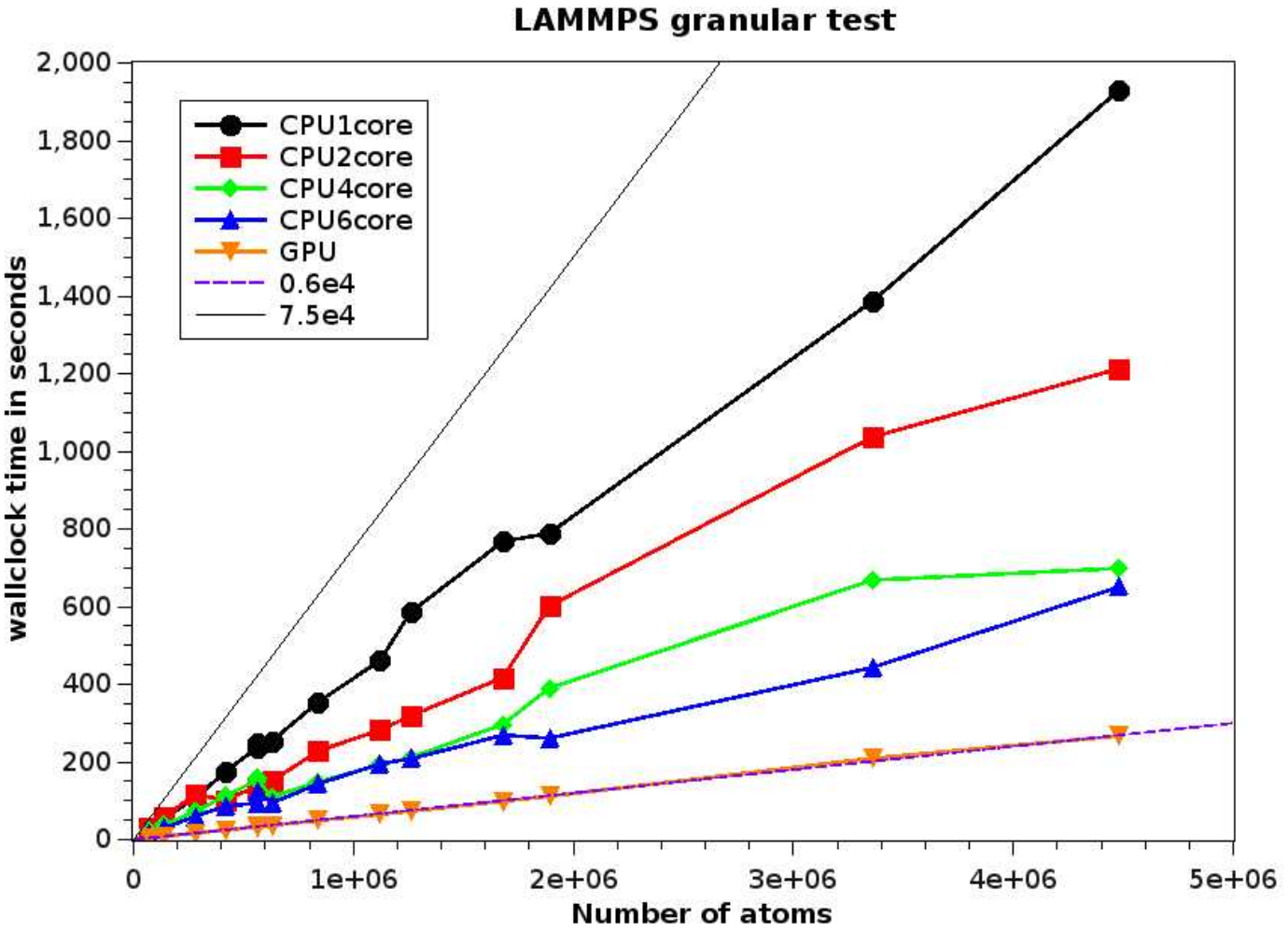
GRANULAR simulations Benchmarks in GPU (extension of USER-CUDA)

GPU version by E.N. Millán
CPU version by C. Ringl and H. Urbassek, Comp. Phys. **183**, 986 (2012)
Code submitted to LAMMPS repository

The 7.5e4 curve represents the results obtained in C. Ringl (2012).

CPU: AMD Phenom x6 1055t 2.8GHz
GPU: NVIDIA Tesla c2050

AVG speedup
GPU vs **1** CPU core = 7x
GPU vs **6** CPU core = 2.95x



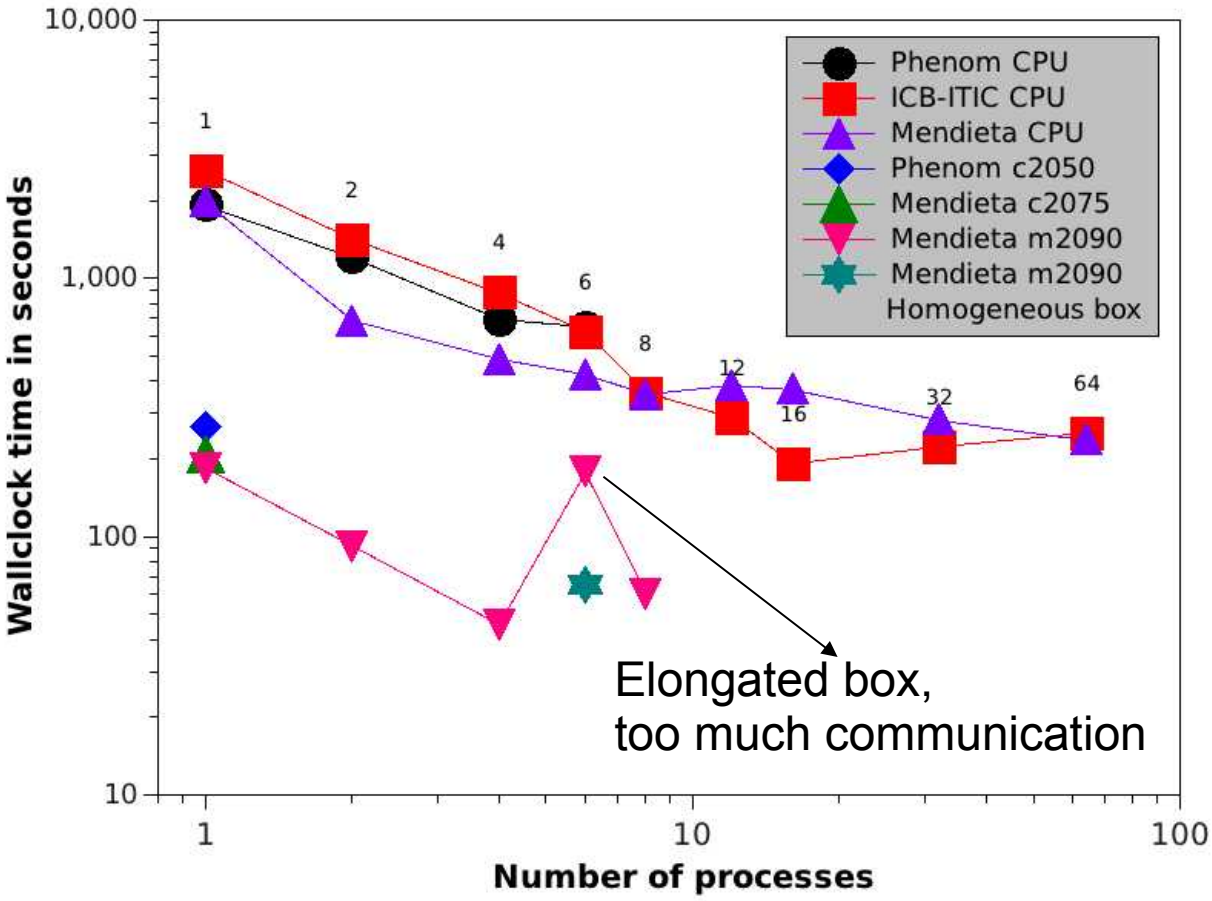
Millan et al. A GPU implementation for improved granular simulations with LAMMPS. HPCLatAm 2013, pp. 89-100 (full paper). Session: GPU Architecture and Applications. C. Garcia Garino and M. Printista (Eds.) Mendoza, Argentina, July 29-30, 2013. http://hpc2013.hpclatam.org/papers/HPCLatAm2013-paper-10.pdf

Granular benchmarks in small clusters

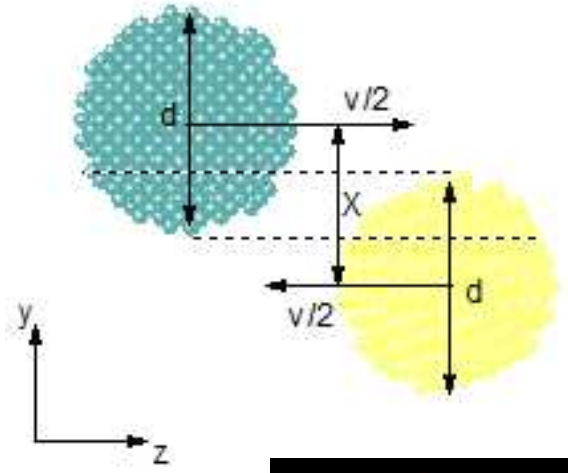
Granular simulation with the GranularEasy pair style, with **4.48e6 grains** and 1000 steps, for 1-64 processes, in Mendieta and ICB-ITIC clusters.
Various NVIDIA GPUs are tested: C2050, C2075 and M2090.

Tesla c2050 GPU ~
16 CPU cores ICB-ITIC cluster.

Mendieta Tesla M2090
GPUs best performance using 4 GPUs in two cluster nodes.
speedup of ~4.2 x against the best CPU result (ICB-ITIC cluster with 16 CPU cores).

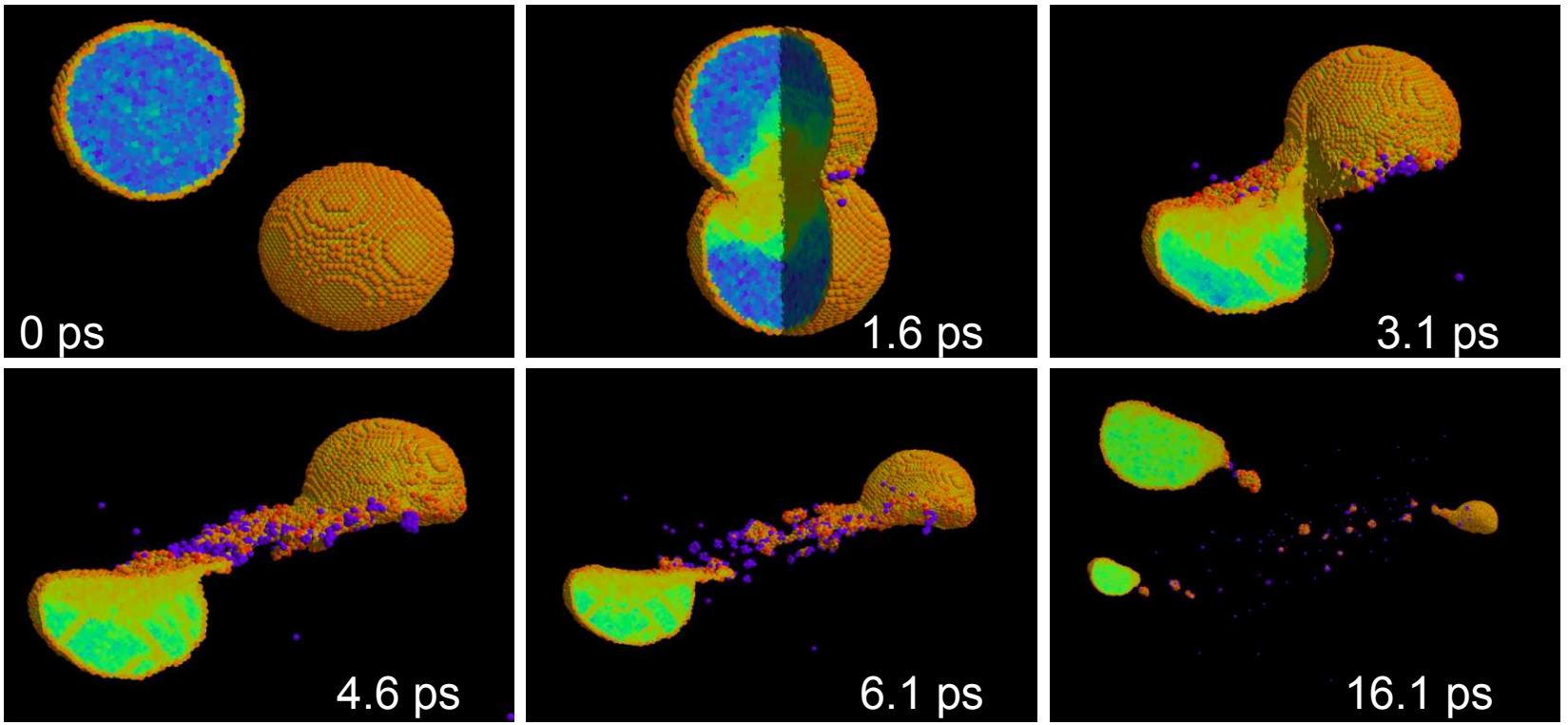


COMPLEXITY in cluster collisions



Parameters:

- ✓ **Velocity (v)**
- ✓ **Impact parameter (x)**
- ✓ **Radius (d/2)**
- ✓ **Structure**
- ✓ **Orientation of the lattice**



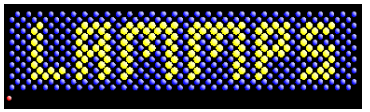
N. Ohnishi, et al. “Numerical analysis of nanograin collision by classical molecular dynamics,” J. Phys. Conf. Series **112** (2008) 042017. Run in 256 cores (LLNL)

“Numerical” experiments using LAMMPS: parameter sweep for cluster collisions

Need to sweep over relative orientation, velocity, R, etc. (1e6 sims)

Goal: reduce the total wall-clock time of multiples jobs executing parallel processes both in the CPU and GPU.

Ad-hoc strategy: split jobs bewteen CPU&GPU. Could be improved further with other job scheduling tools.

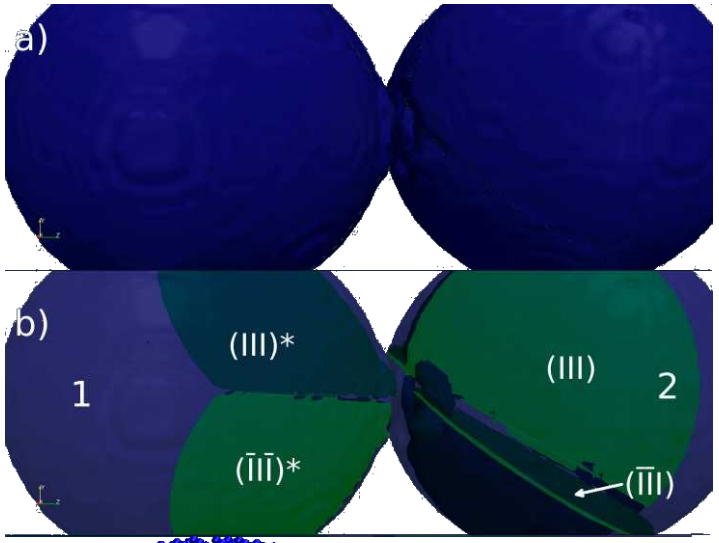


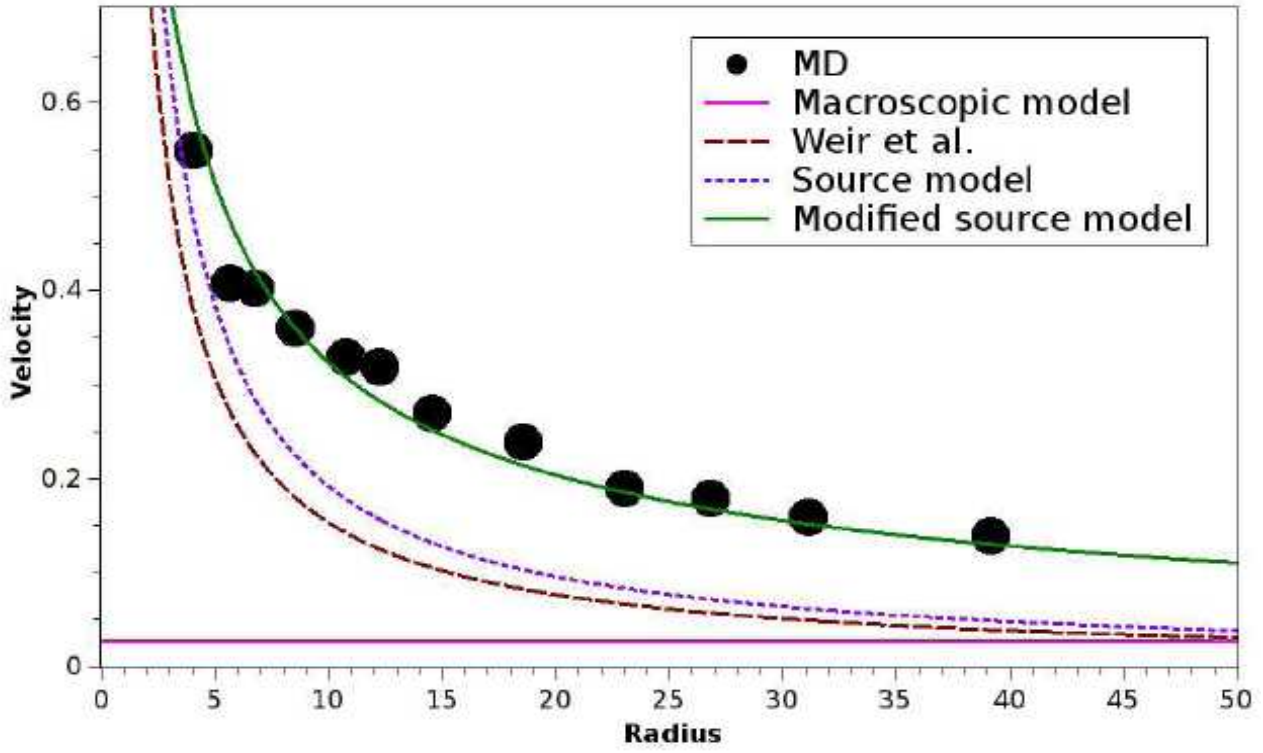
Different parallel modes considered:

- Process parametric study on multicore CPU workstation using OpenMPI.
- Process parametric study on the GPU.
- Hybrid studies: RUBY script to assign workload both to CPU and GPU according to predefined strategy. MPI plus Dynamic or Static load balancing.
- Only up to 10 simultaneous jobs in single GPU, due to memory limitations.

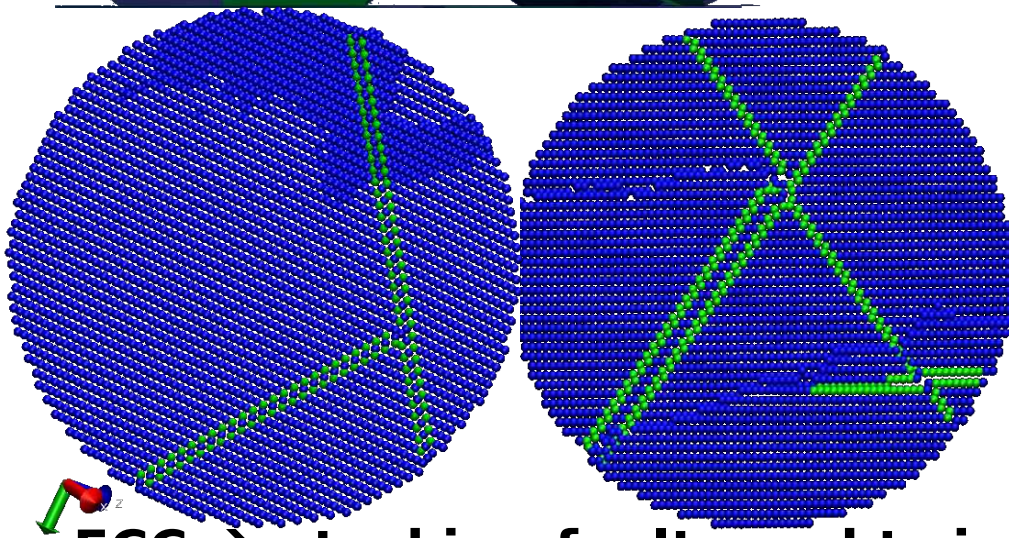
Plasticity threshold in grain-grain impacts

Granular models typically assume lack of plasticity





Dislocation-based model by Lubarda *et al*. agrees with MD. Millan, Tramontina, *et al*., submitted (2015)



FCC → stacking faults and twins

GPUs + CPUs to run ~1,000,000 independent MD simulations

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

Future (?) of MD

- **Sample size:** in 10 years, ~tens of μm, but most simulations still sub-μm.
- More/better **hybrid codes** to extend time and length scales: MD+MC, MD+kMC, MD+DD, MD+continuum, MD+BCA, MD+TB, MD+CPMD, MD+QMMM. Examples in LAMMPS ...
- **Time scale problem**: new algorithms to extend time scale and simulate thermal evolution.
- Better description of **electronic effects** by:

  I) Physics + Chemistry + Biology ➔ "reactive" potentials that are accurate and efficient for full periodic table. Need reactive potentials which work for radiation (ZBL) and high P.

  II) coupling to CPMD, tight-binding, etc. (TDDFT?)

  III) TTM, Ehrenfest dynamics, inclusion of magnetic effects, etc.

<u>Major roadblocks (need brave volunteers!)</u>

- Computers are becoming faster and larger, but algorithms for **long range potentials** (biology & oxides), ab-initio and continuum simulations typically do not scale well beyond couple thousand CPUs ➔ expect better results within the next 10 years.
- No set recipes to build **better potentials**, specially if chemistry (reactive potentials) or electronic effects (charge transfer, potentials for excited states, etc.) are involved.
- Nobody knows yet what to do to efficiently solve the time scale problem beyond some relatively simple model problems.
- **Data mining and viz** for TBs datasets? Open source simulated X-ray and TEM imaging (talk)

Summary: there are many opportunities for MD

- **Petascale➔Exascale! (USA & EU initiatives).** Science **335**, 394 (2012).
- **New software: novel algorithms and preferably open source** (Nature 482, 485 (2012)**]. Still need significant advances in visualization (**Visual Strategies: A Practical Guide to Graphics for Scientists and Engineers, F. Frankel & A. Depace, Yale University Press, 2012**), TB dataset analysis [**Science **334**, 1518 (2011)**], self-recovery & fault tolerance, etc.**
- **New hardware :** better (faster/greener/cheaper) processors, connectivity, memory and disk access; MD-tailored machines (MD-GRAPE-4, Anton, etc.); GPUs, Phi, MICs, hybrid architectures (GPU/CPU); cloud computing, etc.
- **Experiments going micro-nano/ns-ps ➔ same as MD**
- **Can go micron-size, but still have to connect to mm-m scale ➔** novel approaches needed, including smart sampling, concurrent coupling, dynamic/ adaptive **load balancing/refining** for heterogeneous systems, asynchronous simulations, etc.
- Need **better and cheaper reactive potentials** to handle non-equilibrium scenarios
- **Need human resources with mix of hardware, software & science expertise.**

That's all folks!!

SiMAF: Simulations in Materials Science, Astrophysics, and Physics

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

Web master: M.J. Erquiaga; design: E. Rim.

Funding: Agencia CyT, Argentina, PICT2008-1325 & PICT2009-0092

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