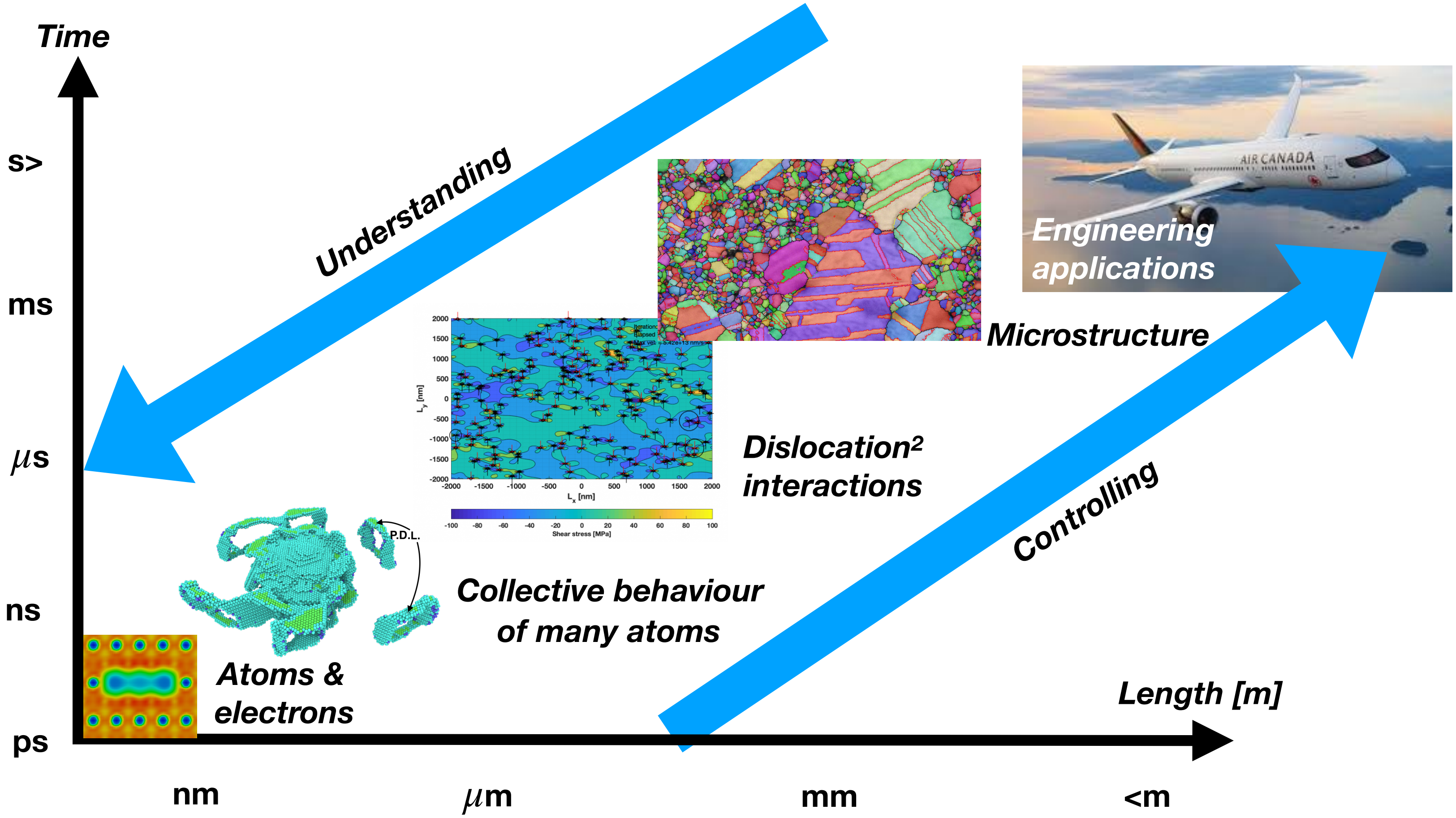
Developing ultra-strong and ultra-tough metallic materials with gradient nano-grained structures

Radiate - TRIUMF - Vancouver

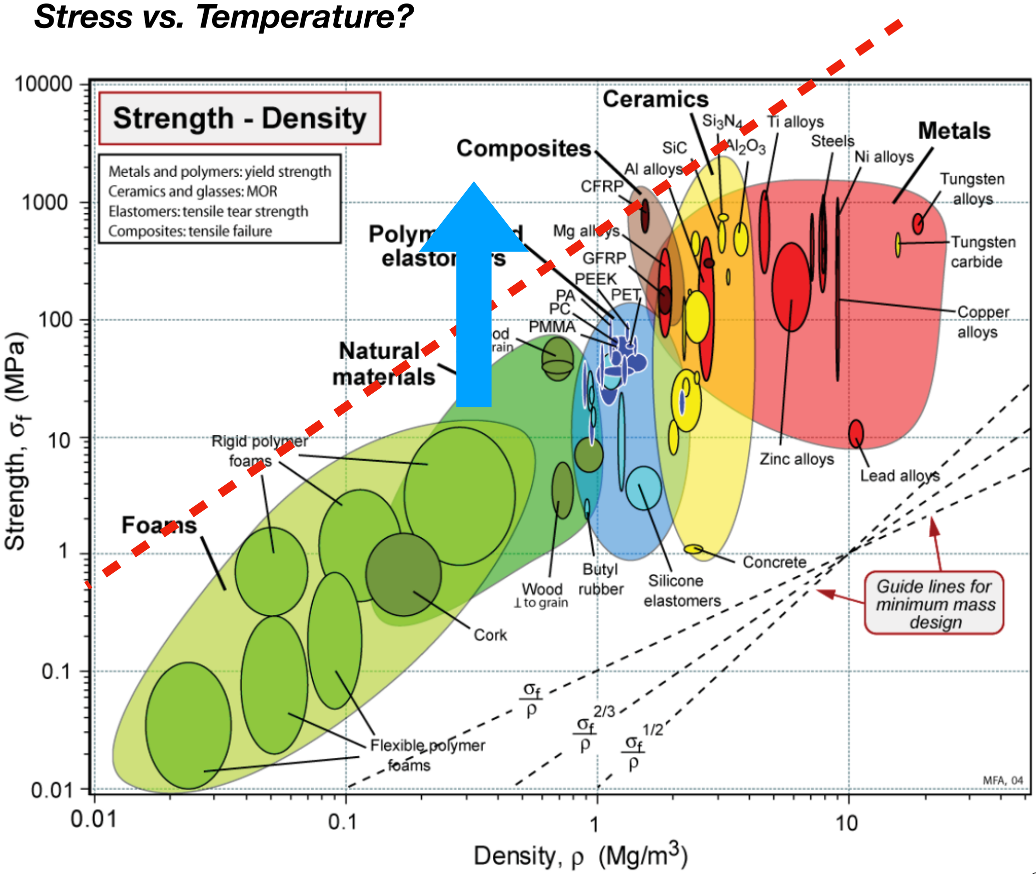
Assistant Prof. Mauricio Ponga
Department of Mechanical Engineering, UBC
December 11, 2019

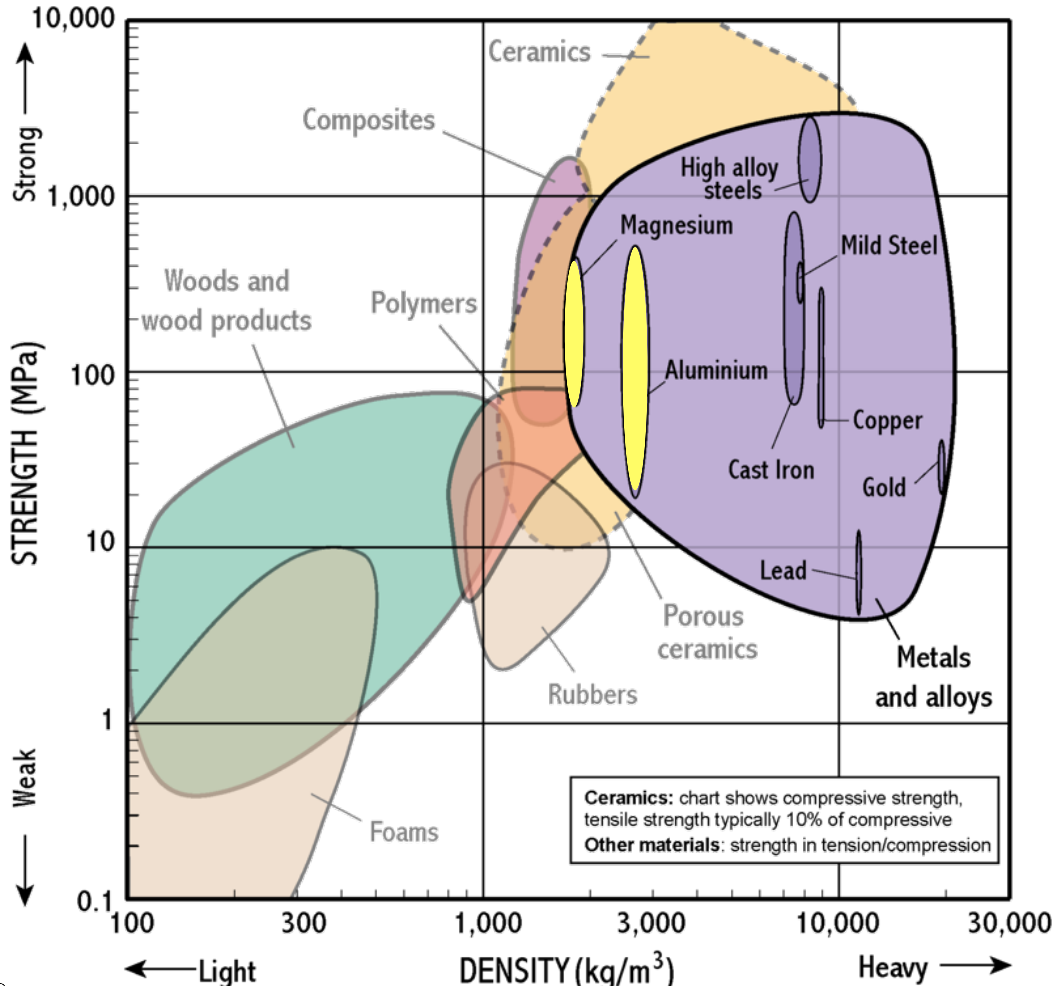
Multiscale modelling of materials
Investigating the scales



Materials selection and properties

What is the figure of merit for targets?
Temperature vs. Time?
Stress vs. Temperature?



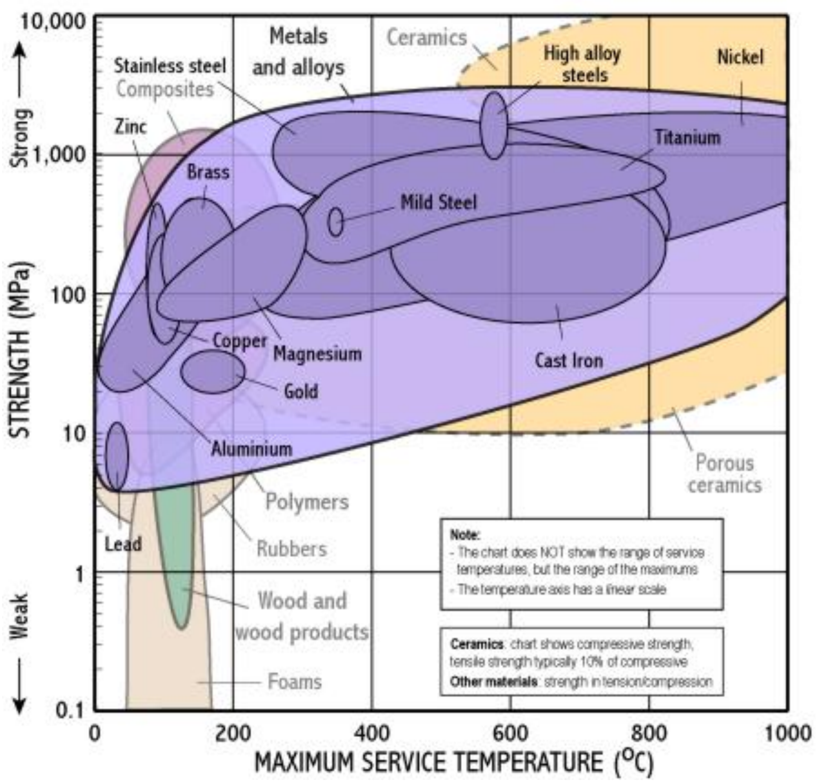


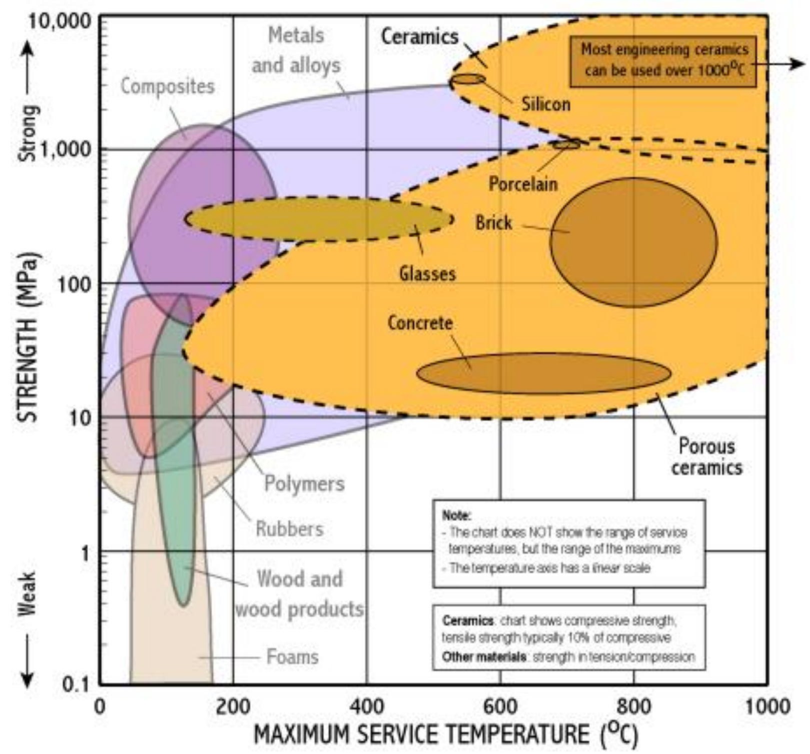
Materials selection and properties

What is the figure of merit for targets?

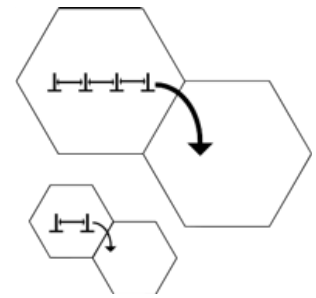
Temperature vs. Time?

Stress vs. Temperature?

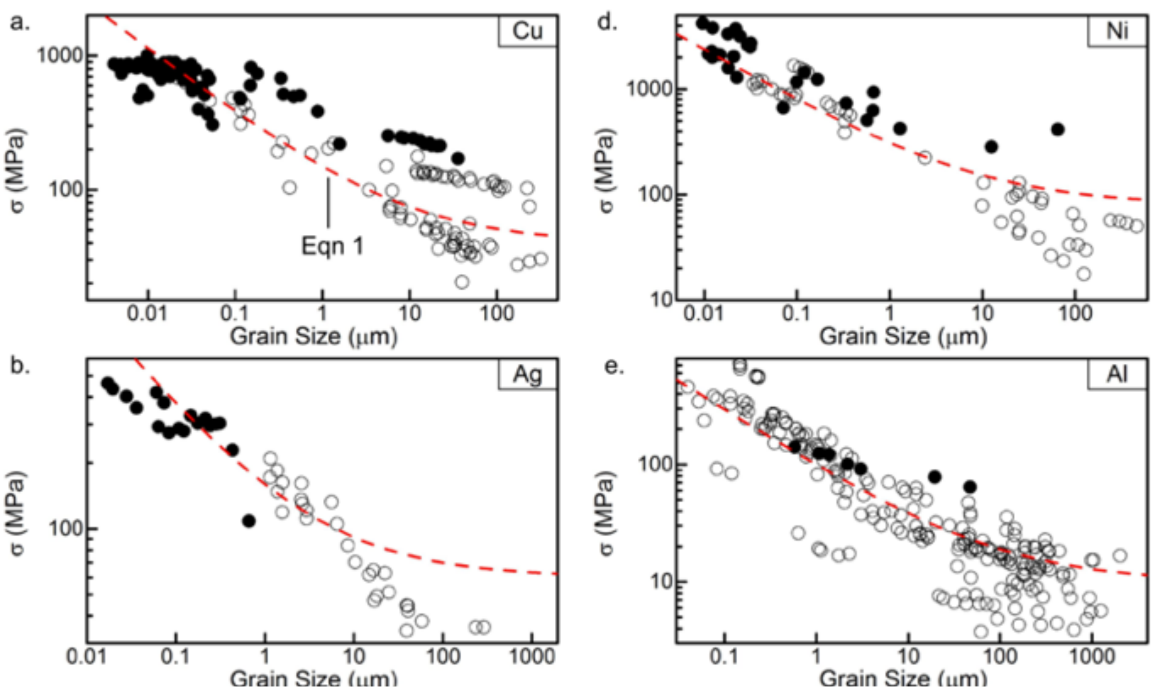


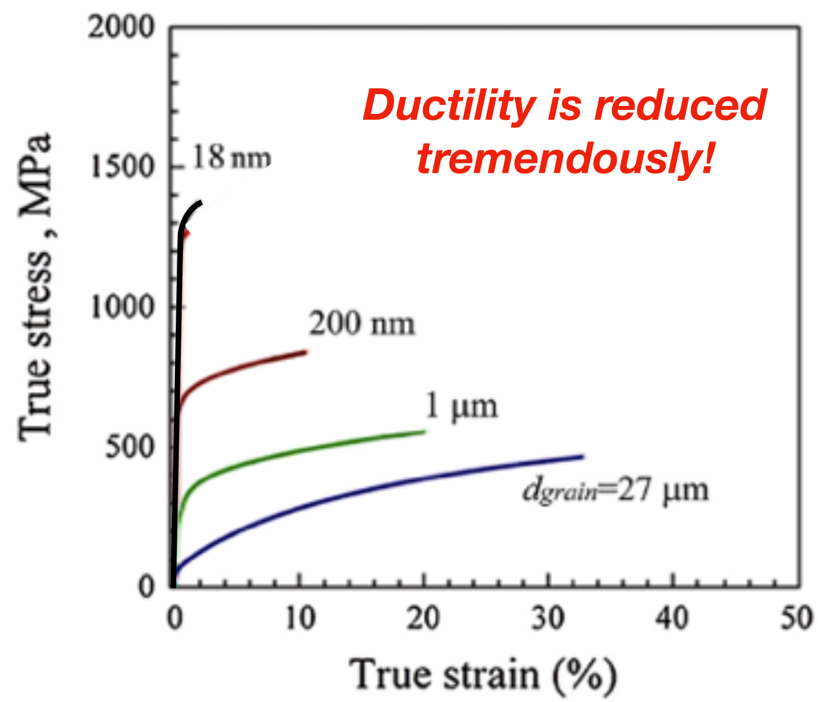


Nano-grained materials are very strong!



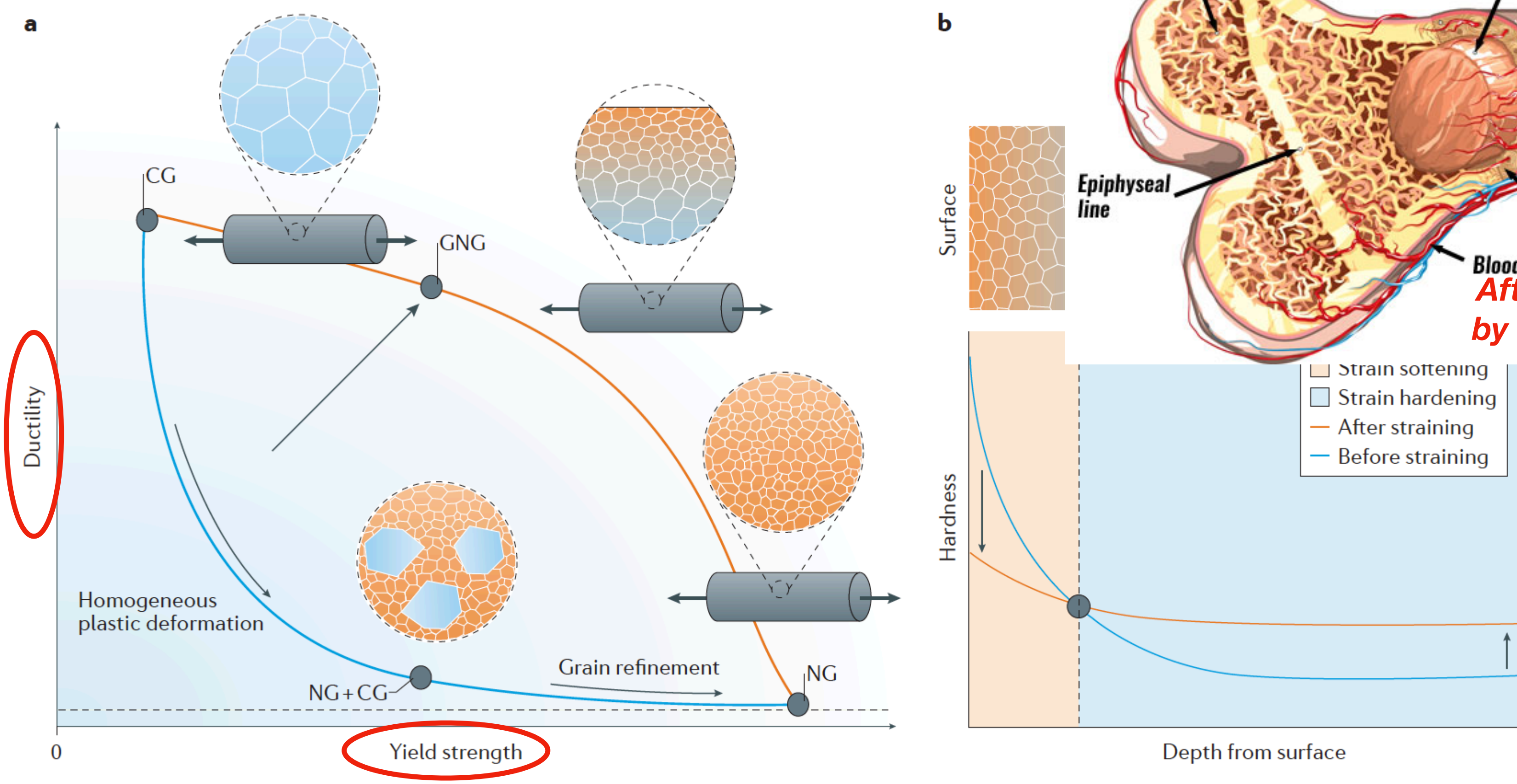
Dislocation provide extra hardening, at the expense of toughness

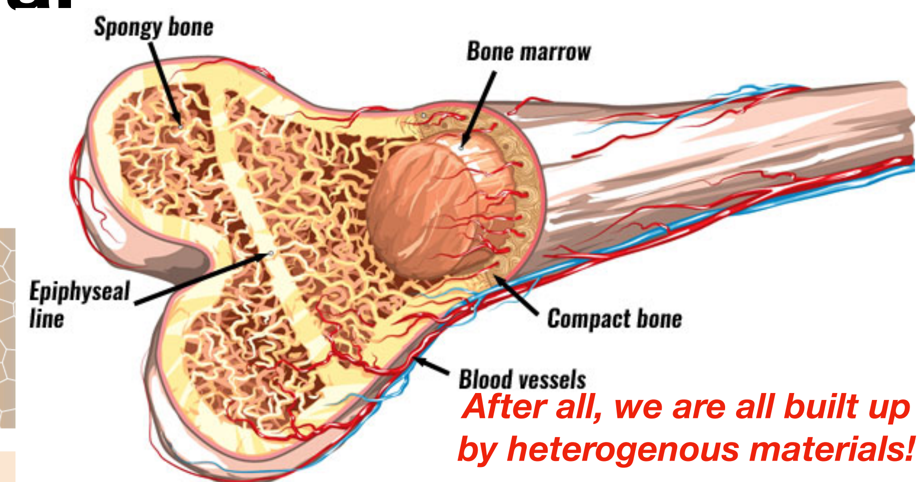




Towards strength–ductility synergy through the design of heterogeneous nanostructures in metals, Evan Ma and Ting Zhub

Heterogenous MS have shown to have good potential

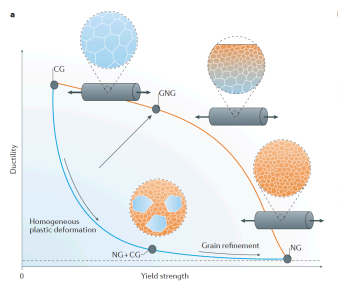


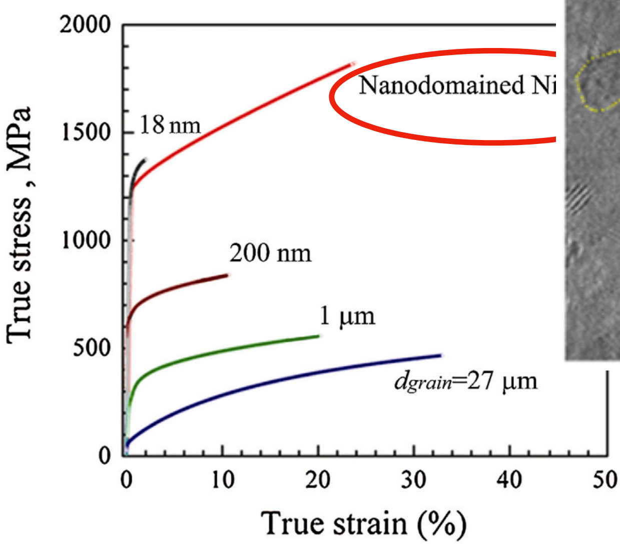


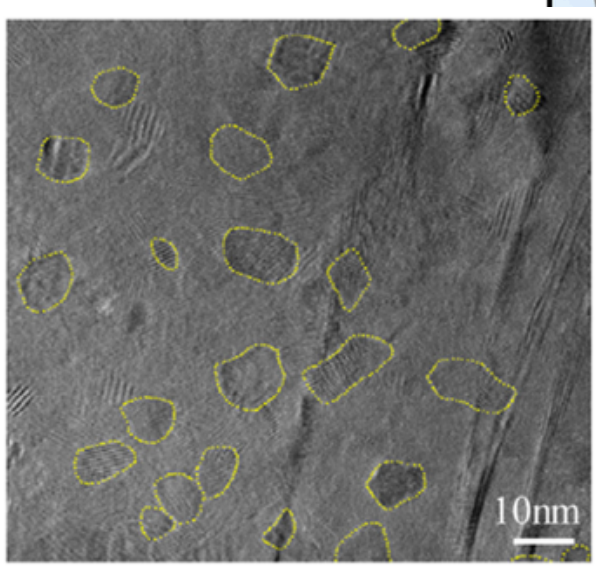
After all, we are all built up by heterogenous materials!

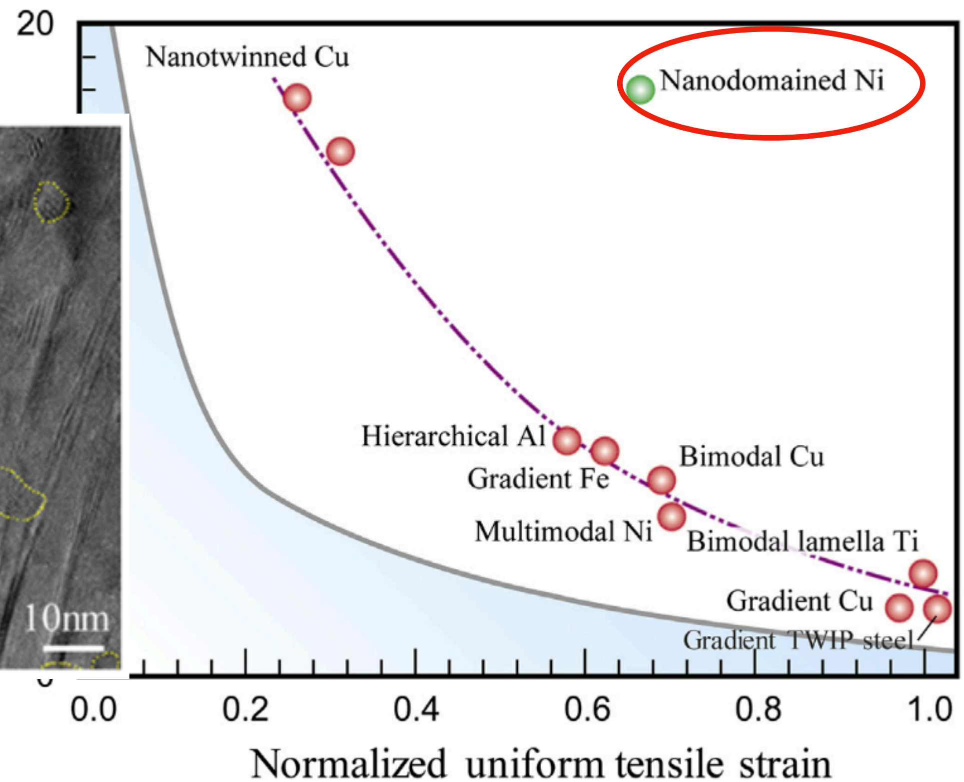
Stabilizing nanostructures in metals, K. Lu Nature Reviews Materials ***volume 1****, 16019 (2016)*

Heterogenous MS have shown to have good potential



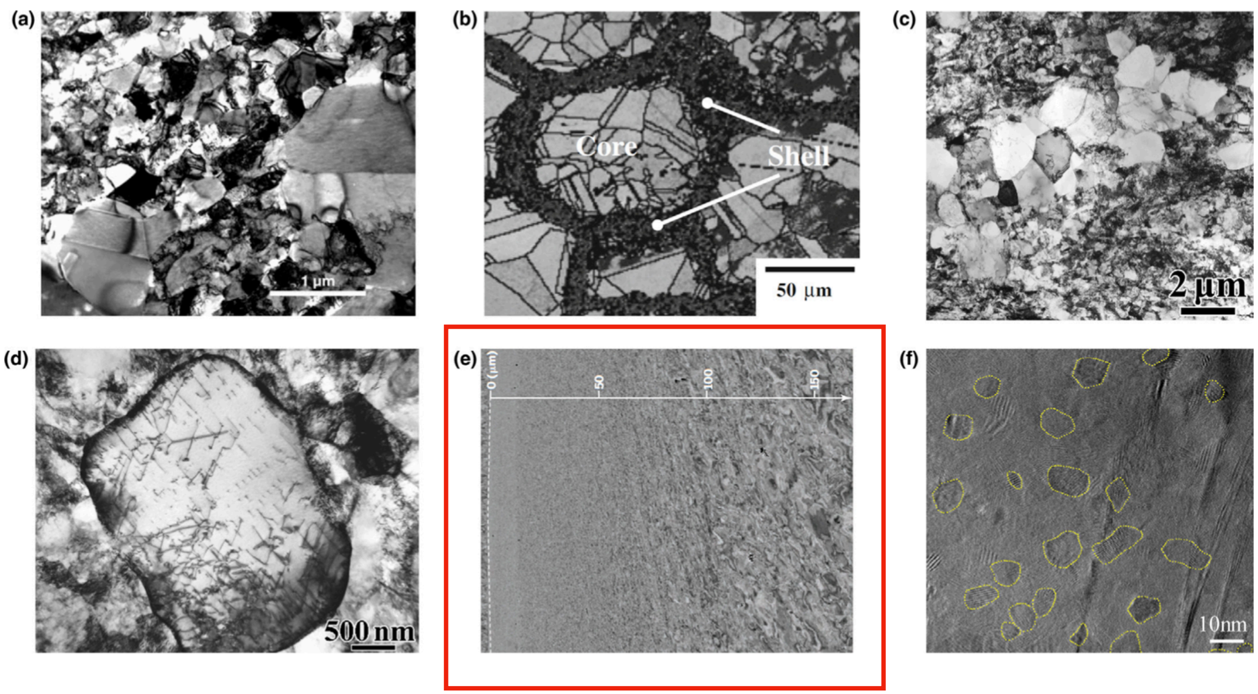


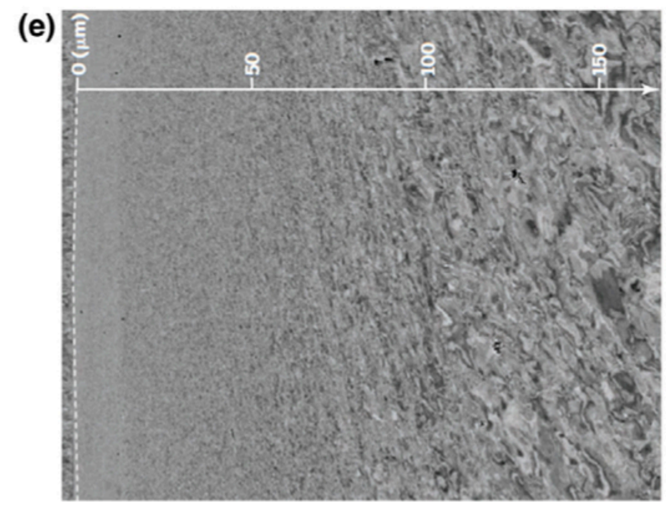




Towards strength–ductility synergy through the design of heterogeneous nanostructures in metals, Evan Ma and Ting Zhub

Examples of Heterogenous MS



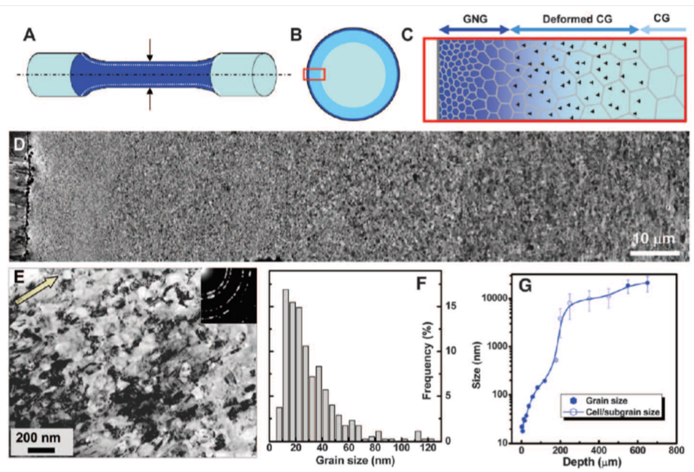


Gradient nano-grained (GNG) materials

Towards strength–ductility synergy through the design of heterogeneous nanostructures in metals, Evan Ma and Ting Zhub

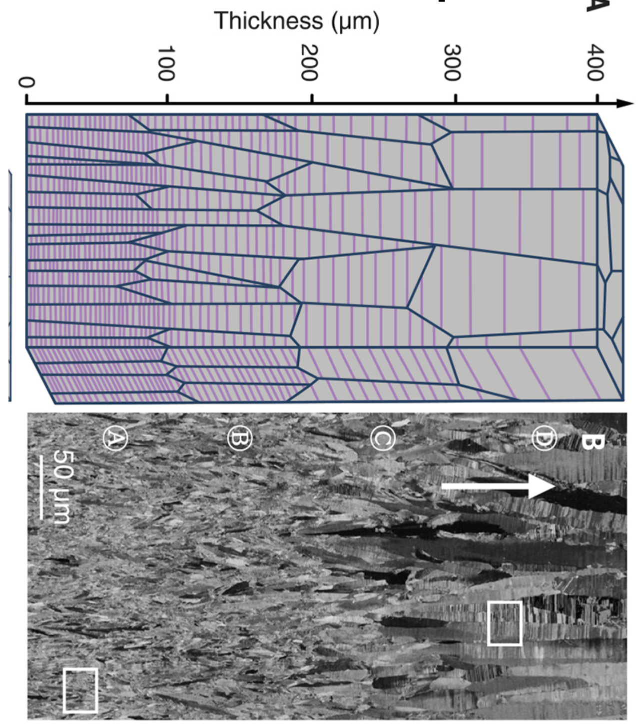
How can we obtain heterogenous MS?

Surface mechanical grinding

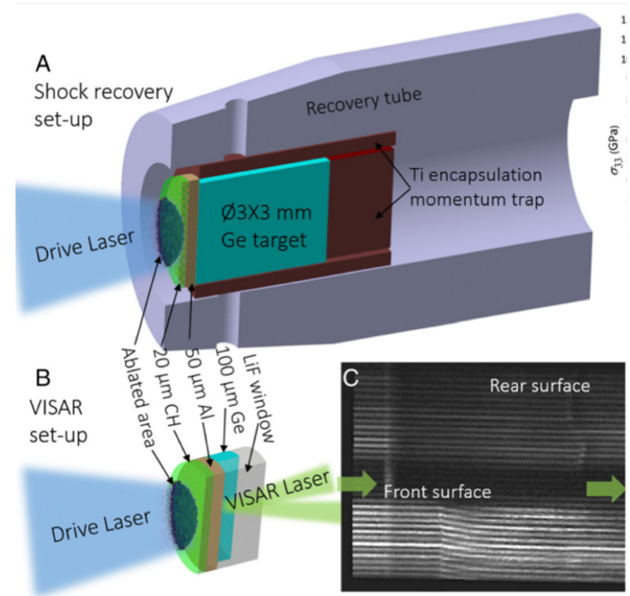


☑ **Today's presentation**

Electro-chemical deposition



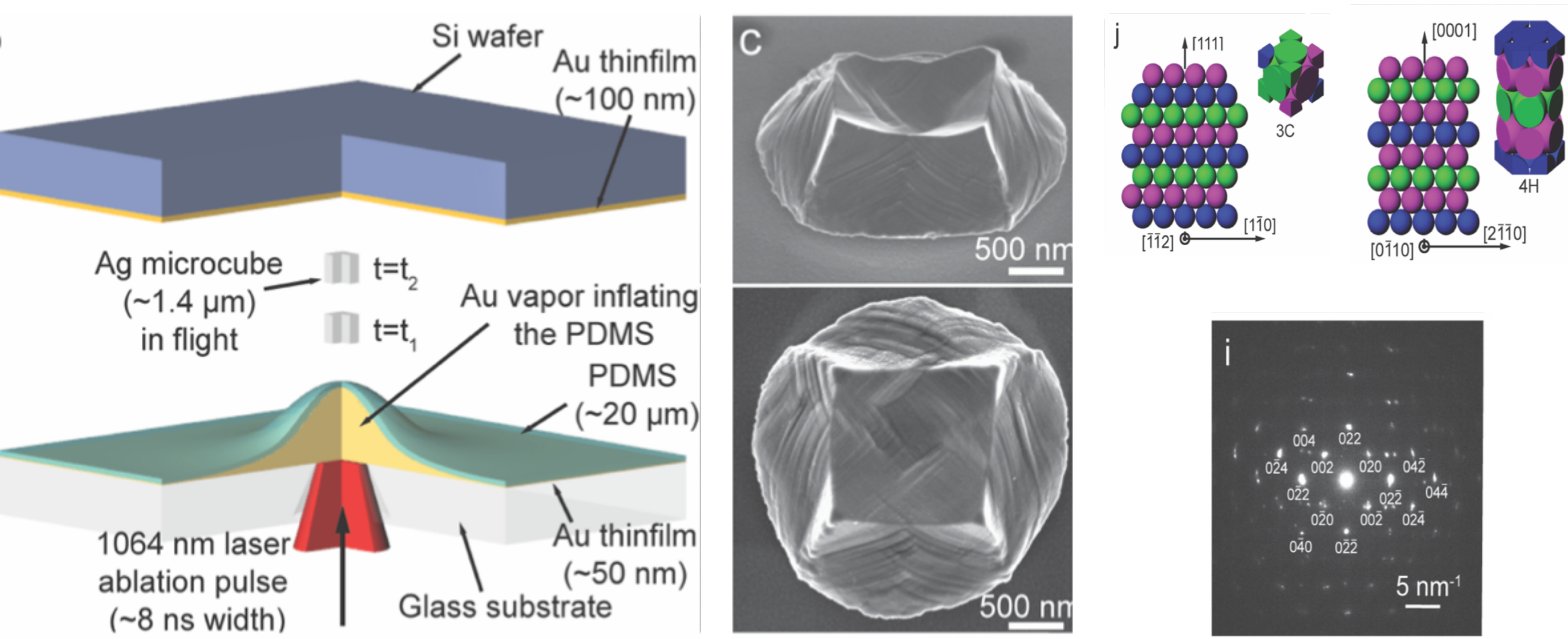
Severe plastic deformation through shock waves



☑ **Today's presentation**

Revealing Extraordinary Intrinsic Tensile Plasticity in Gradient Nano-Grained Copper, T. H. Fang, W. L. Li, N. R. Tao, K. Lu, Science, 2011.
Extra strengthening and work hardening in gradient nanotwinned metals, Z, Cheng et al. Science, 2018.
Generating gradient germanium nanostructures by shock-induced amorphization and crystallization, Shiteng Zhao, Bimal Kad, Christopher E. Wehrenberg, Bruce A. Remington, Eric N. Hahn, Karren L. More, and Marc A. Meyers, PNAS, 2017.

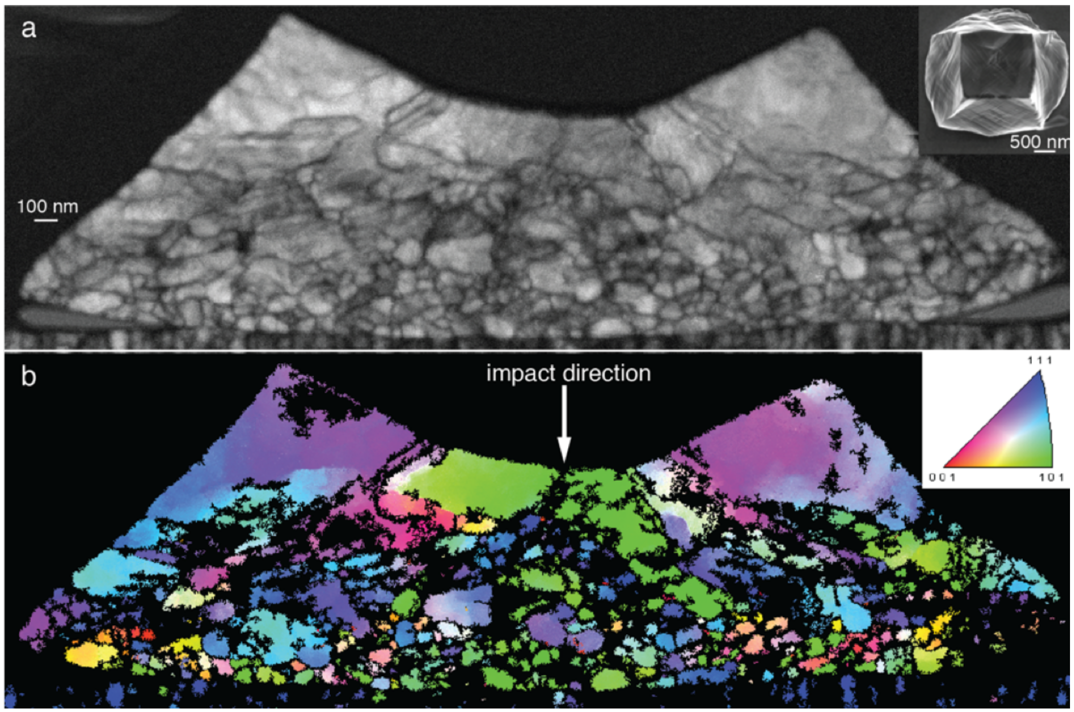
High-Velocity impact of Ag particles



Ramathasan Thevamaran, Sadegh Yazdi, Mauricio Ponga, Hossein Alimadadi, Olawale Lawal, Claire Griesbach, Seog-Jin Jeon, Edwin L. Thomas, Dynamic Martensitic Phase Transformation in Single-crystal Silver Microcubes, ActaMat, 2019.

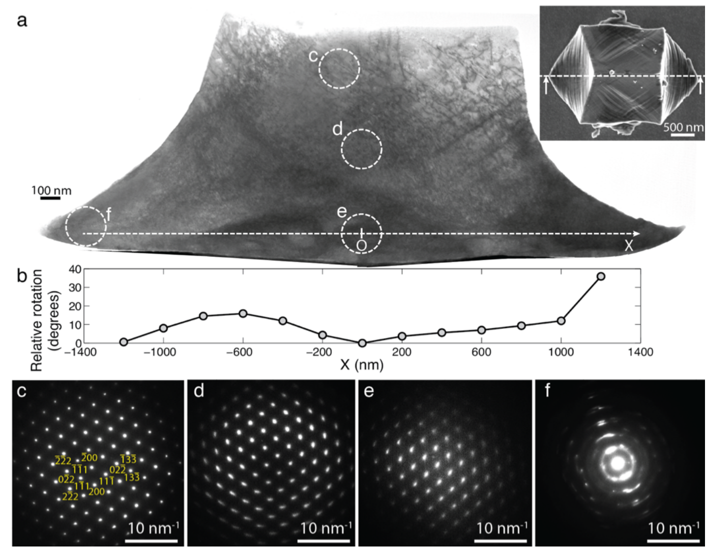
High-Velocity impact of Ag particles

Grain recrystallize,
and their size changes with distance



What dominates this transformation remains unclear!

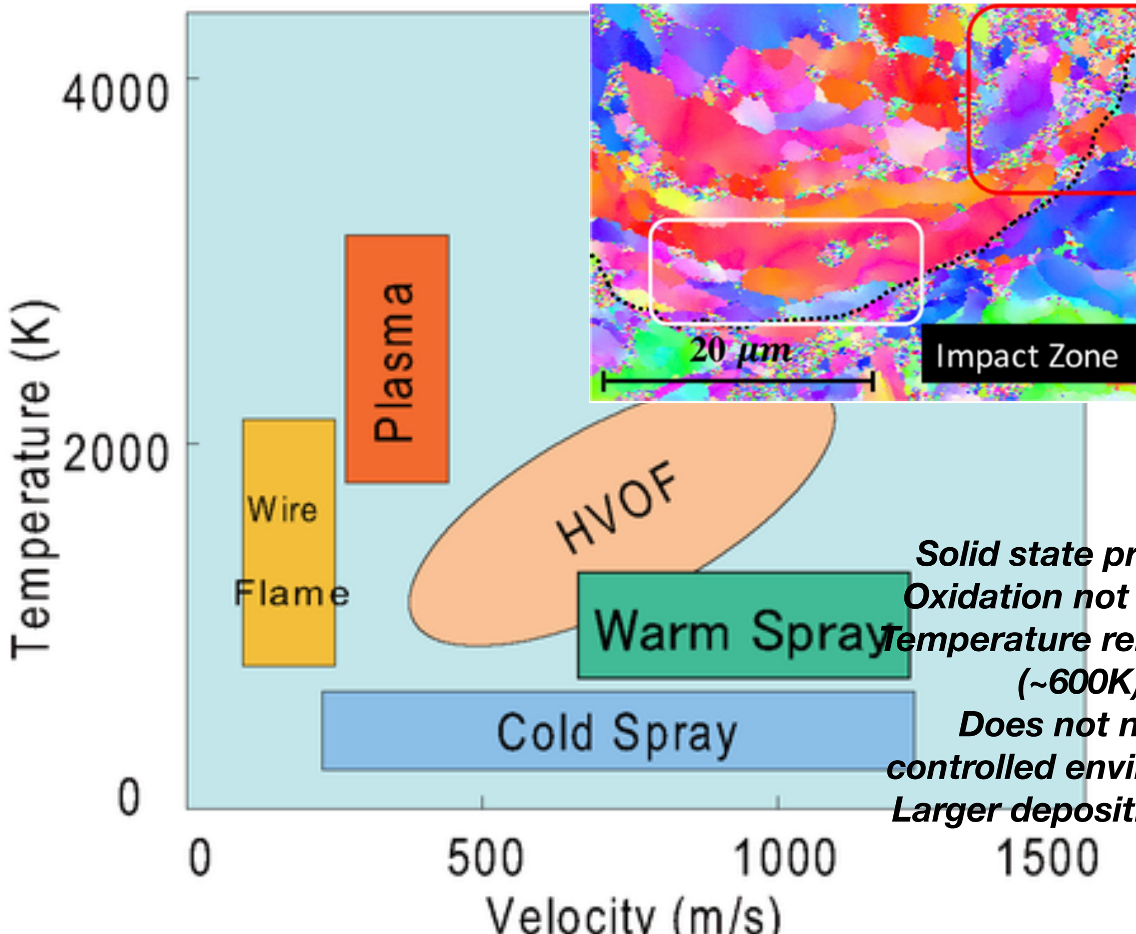
Several questions need to be answered:
1- Is a critical velocity for obtaining recrystallization?
2- Does the shape matters?
3- Does the orientation matters?
Intrinsic vs. Extrinsic effects!

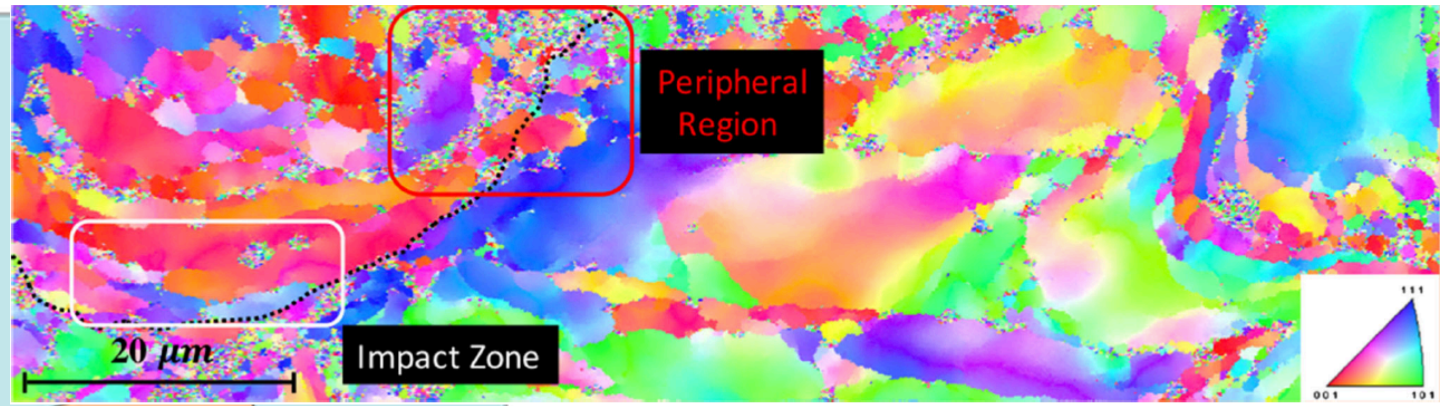


Ramathasan Thevamaran, Sadegh Yazdi, Mauricio Ponga, Hossein Alimadadi, Olawale Lawal, Claire Griesbach, Seog-Jin Jeon, Edwin L. Thomas, Dynamic Martensitic Phase Transformation in Single-crystal Silver Microcubes, Acta Materialia, 2019.

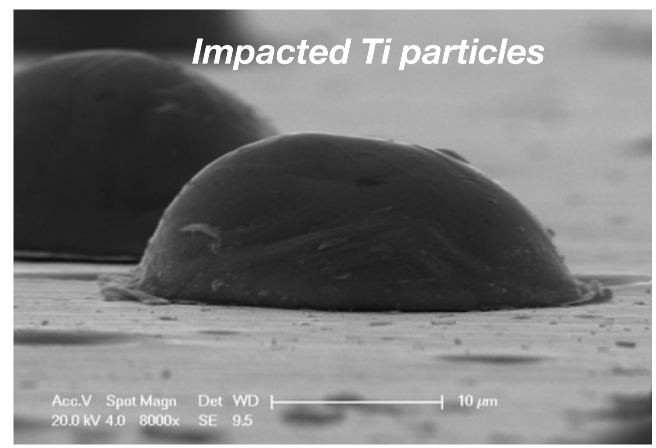
Cold spray can be used as 3D printing technique

What dominates this transformation remains unclear!





Solid state process.
Oxidation not critical.
Temperature remain low (~600K)
Does not need controlled environment
Larger deposition rate.



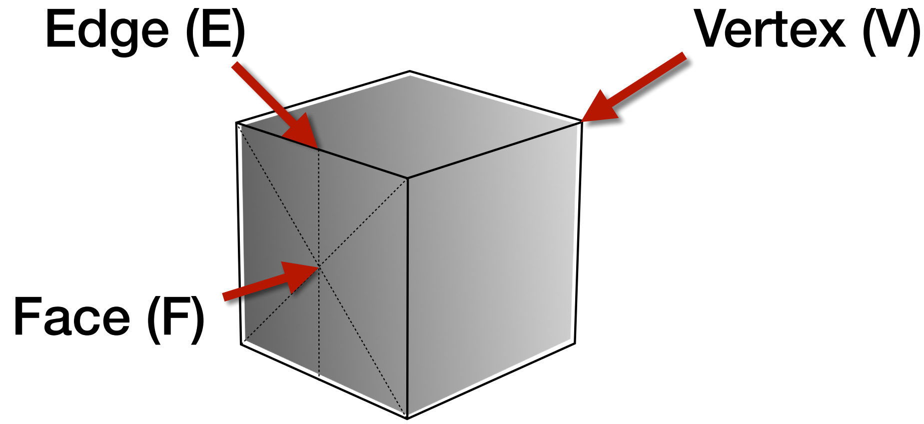
Effects of Preprocessing on Multi-Direction Properties of Aluminum Alloy Cold-Spray Deposits, Rokni et al. JTST, 2018.
Cold spray - Wikipedia.

Methodology

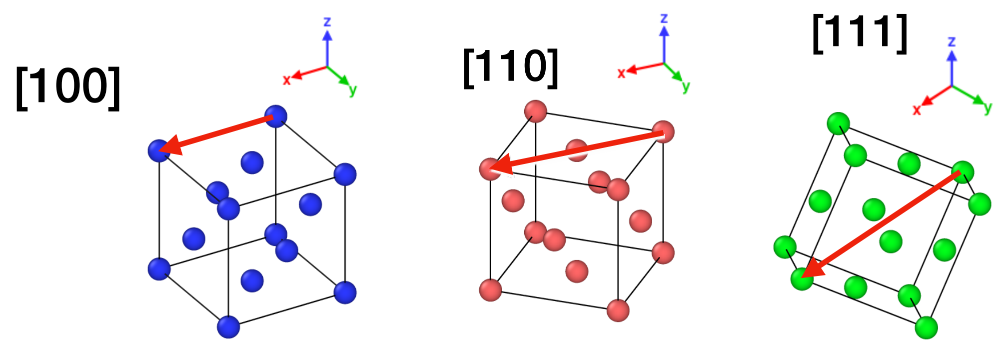
- Impacting the cube on face, edge and vertex
- Changing lattice orientation.

Orienting [100] [110] [111] with *x*-axis

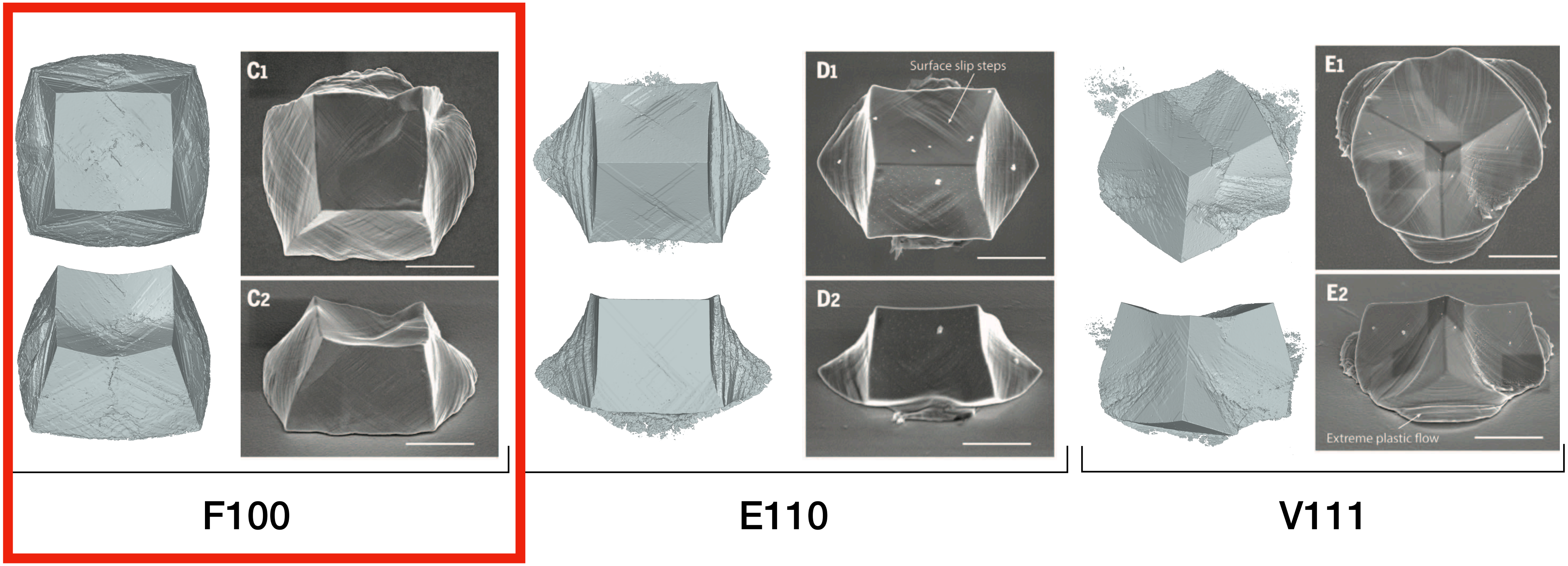
→ 9 cases



- Molecular dynamic simulations - LAMMPS
- Impact velocity **400 m·s**$^{-1}$
- About ~**16 millions** of atoms
- Single crystal
- Dimensions: **L = 65 nm**
- **Potential EAM - Sheng et al. 2011**

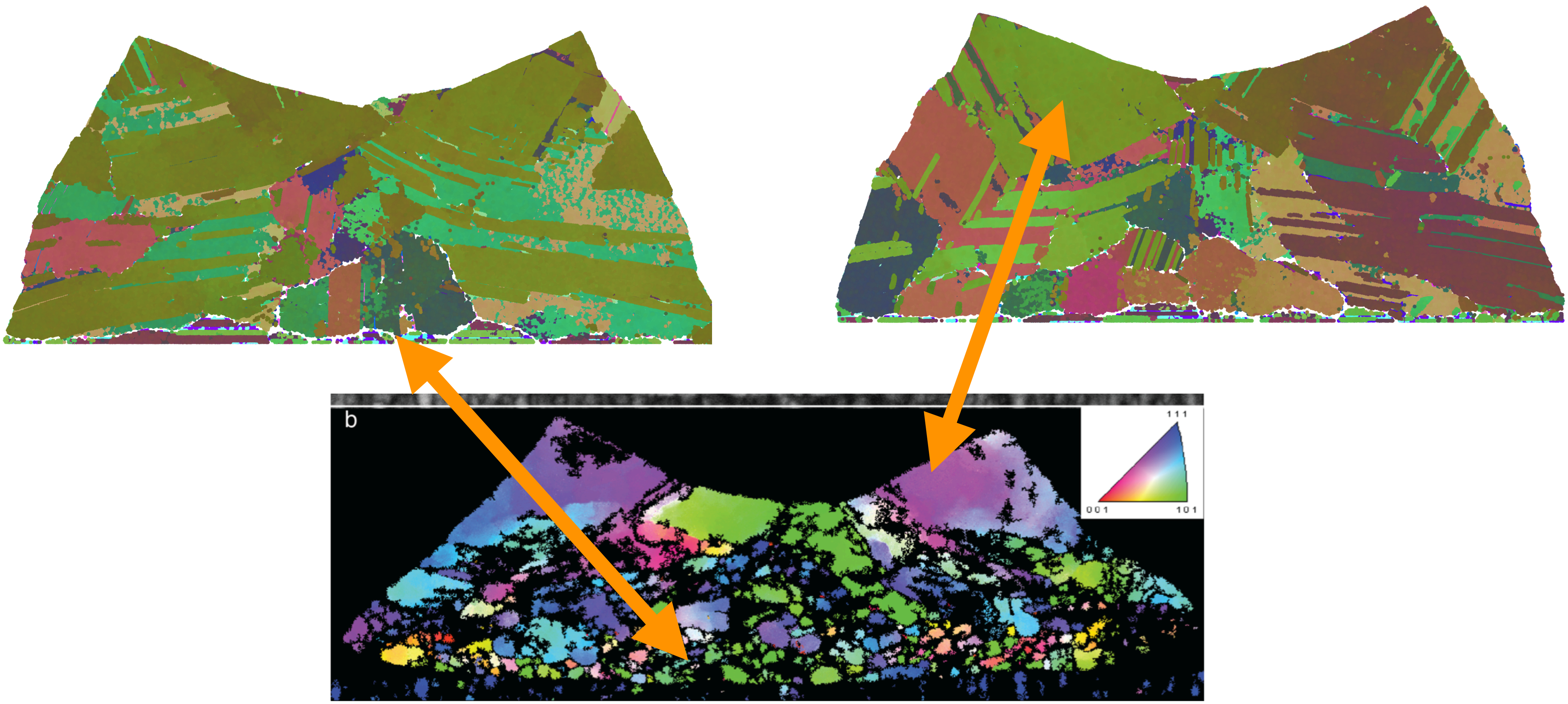


Comparison with experiments



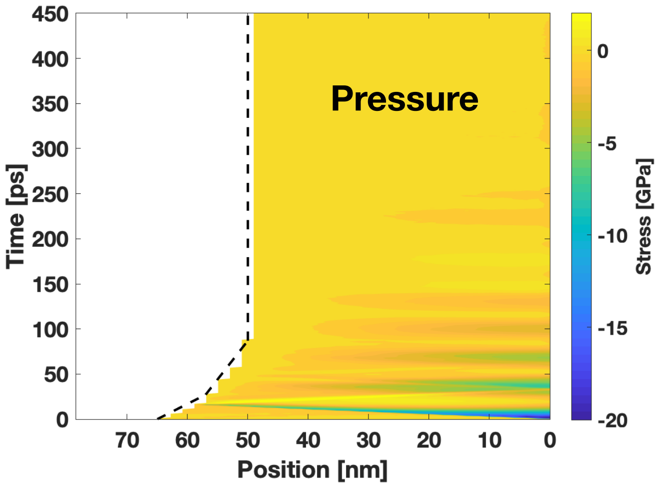
Cubes after the impacts. Simulation results compared with experiments, Thevamaran el al. 2016
The impacts shown are along [100], [110] and [111] directions, targeting the face, edge and vertex of the cube respectively

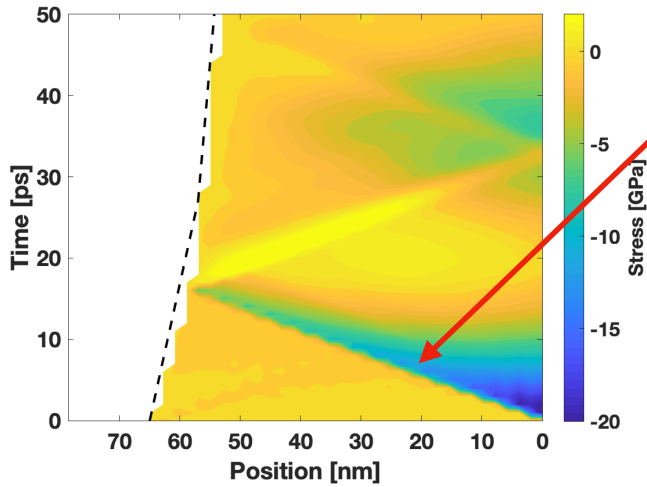
Comparison with experiments



What is really happening

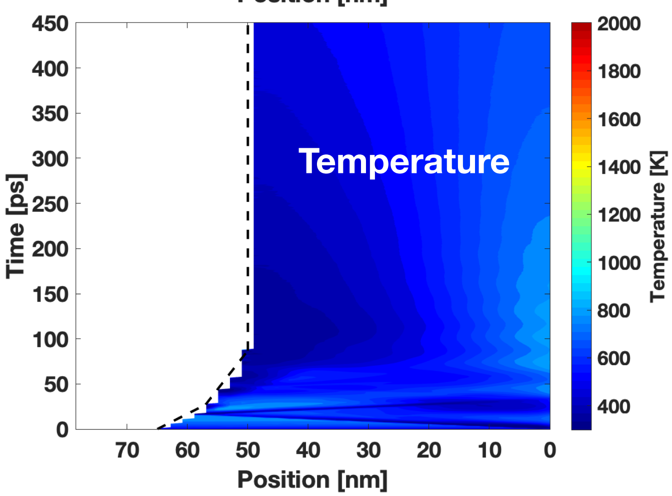
F100

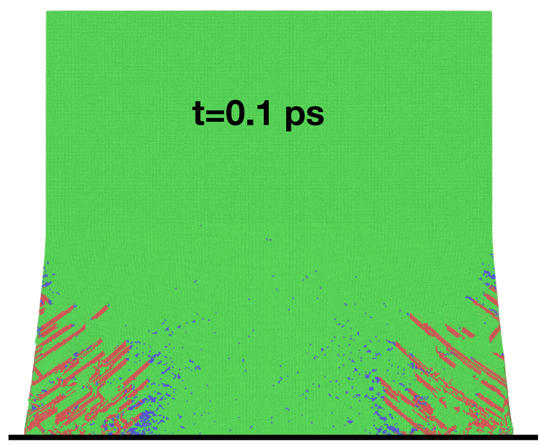




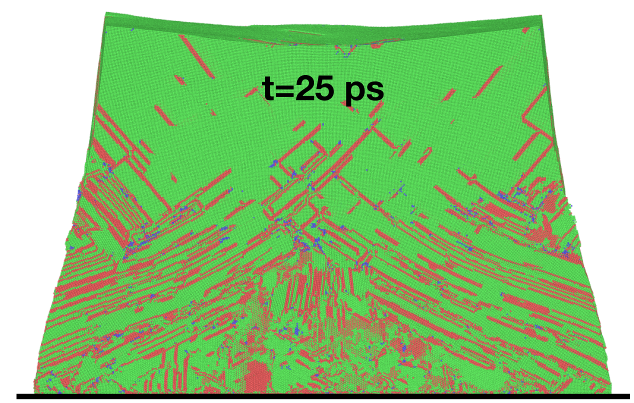
Shock wave propagating in the material

Avalanche of dislocations!





Microstructural changes happen in a sub nanosecond scale! Temperature way below melting point.

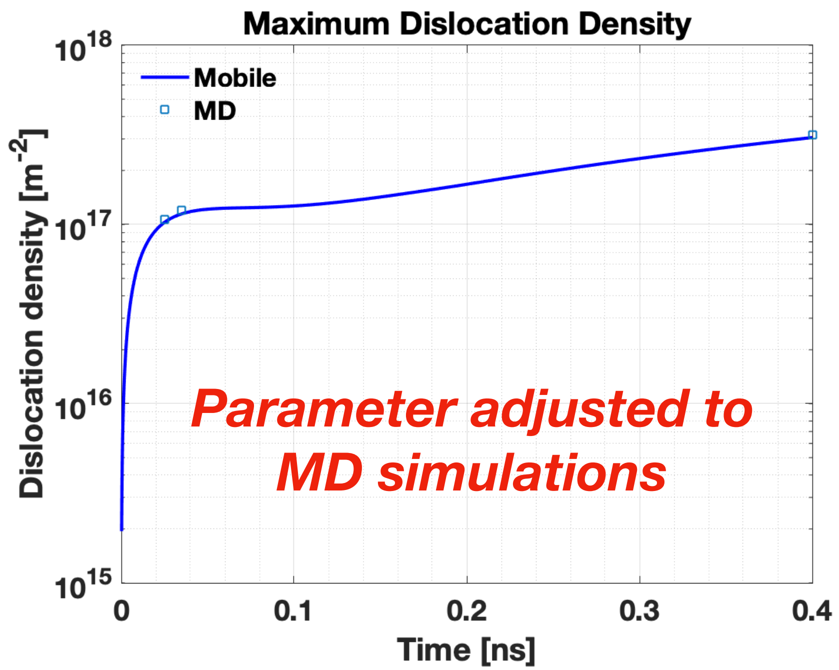


Dynamic recrystalization model based on dislocation density

$$\frac{\partial \rho_m}{\partial t} + \nabla \mathbf{j}_m = \left[p_m(\rho_m, \rho_i) + q_m(\rho_m, \rho_i, \dot{\epsilon}_p, \tau) \right] \dot{\epsilon}_p$$

Interaction terms *Flux terms*

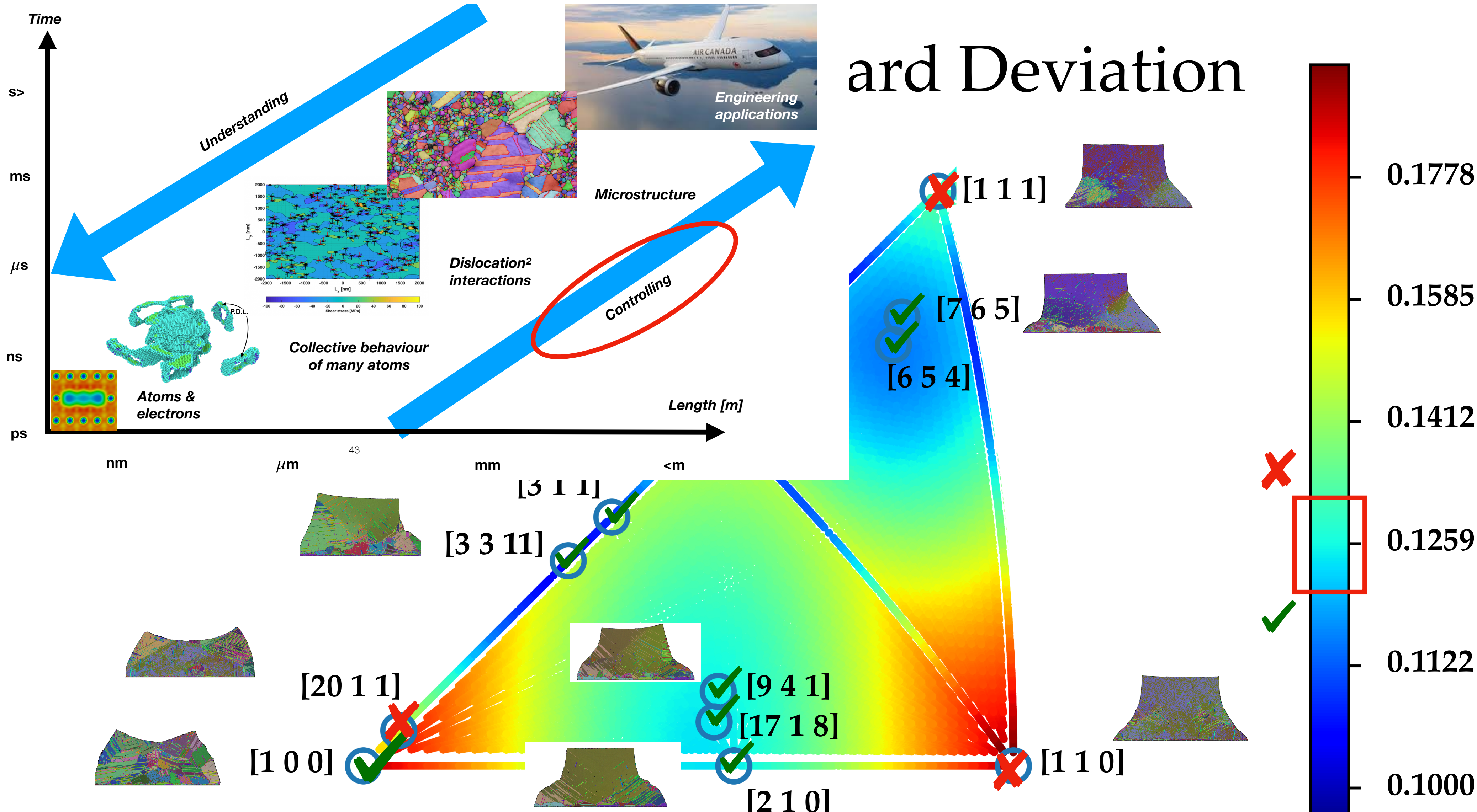
$$\frac{\partial \rho_i}{\partial t} + \nabla \mathbf{j}_i = \left[p_i(\rho_m, \rho_i) + q_i(\rho_m, \rho_i) \right] \dot{\epsilon}_p$$



Flux terms for mobile dislocation has to be modified due to large shock wave!

$$\tau = \frac{l_0}{c_L}$$

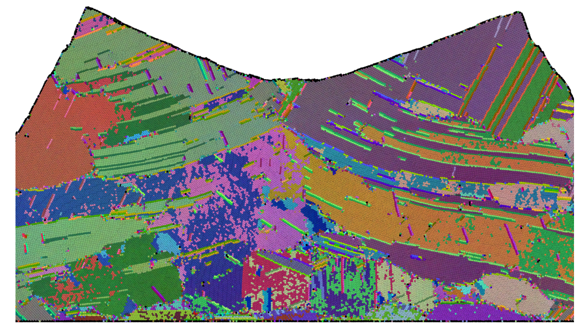
Characteristic time that depends on wave speed



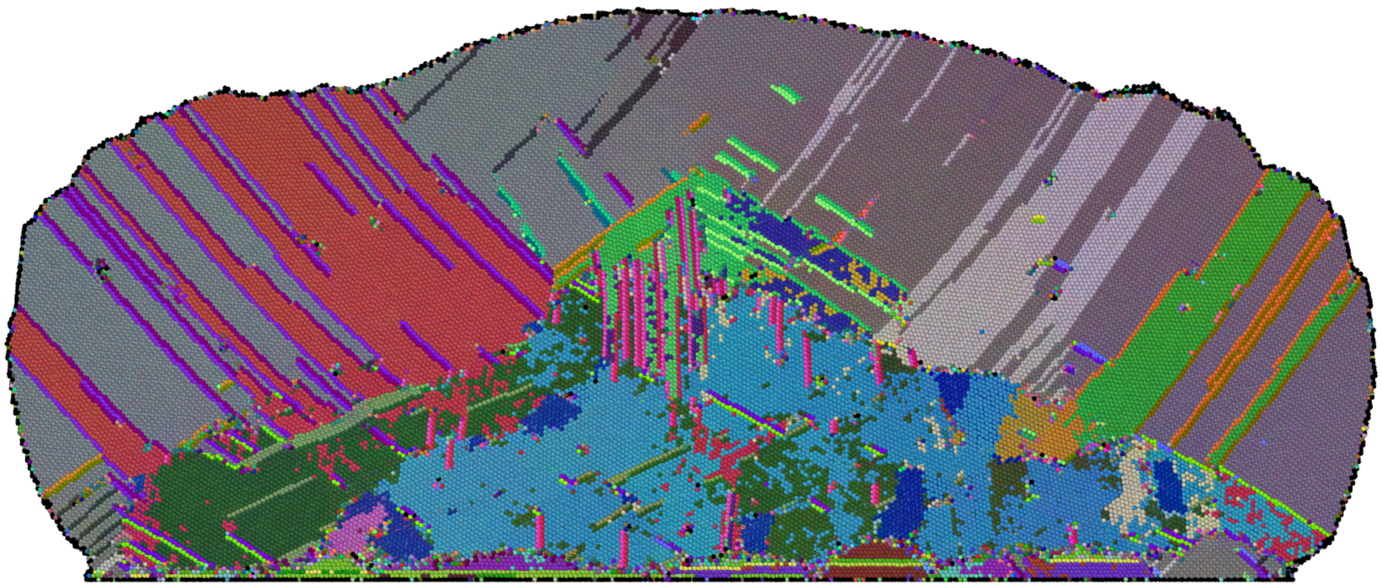
ard Deviation
Time
s>
ms
μs
ns
ps
nm
μm
mm
<m
43
Length [m]
Understanding
Controlling
Engineering applications
Microstructure
Dislocation² interactions
Collective behaviour of many atoms
Atoms & electrons
[1 1 1]
[7 6 5]
[6 5 4]
[3 1 1]
[3 3 11]
[20 1 1]
[1 0 0]
[9 4 1]
[17 1 8]
[2 1 0]
[1 1 0]
0.1778
0.1585
0.1412
0.1259
0.1122
0.1000

Shape of the particle and material

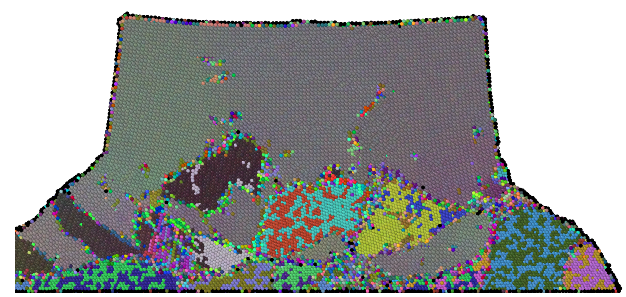
Copper FCC



Sphere [100]

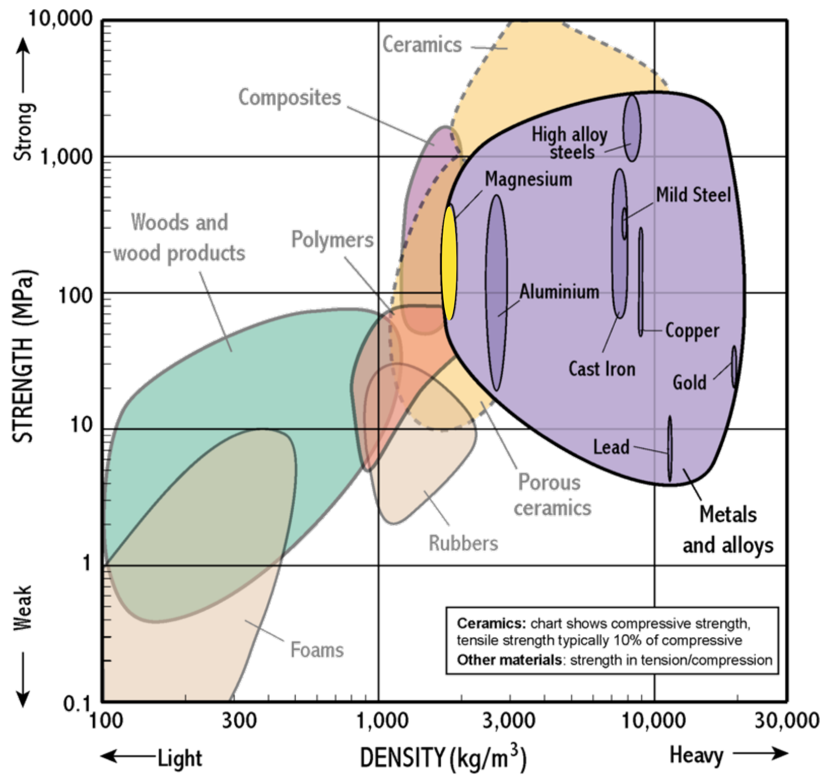


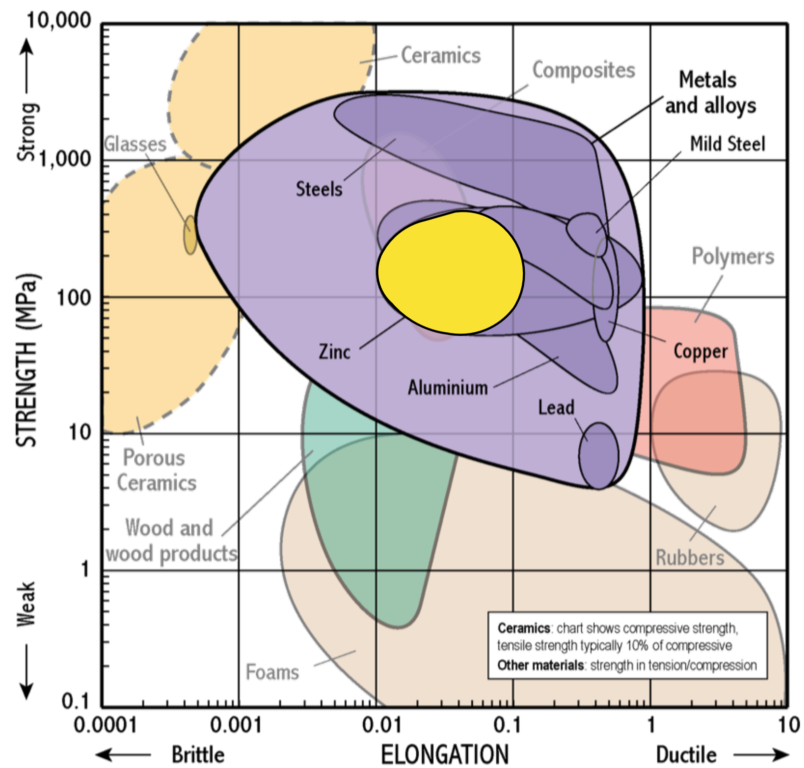
Iron BCC



Lightweight structural materials with GNG structure

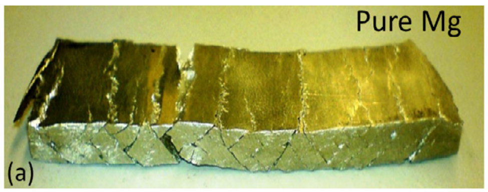
Metals dominate this sector.
Good strength, good ductility, good fracture toughness.
Heavy and exhausted - Same alloys used since the last two decades!
Innovation: Introduce more exotic materials (e.g., Mg).

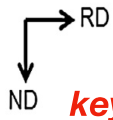




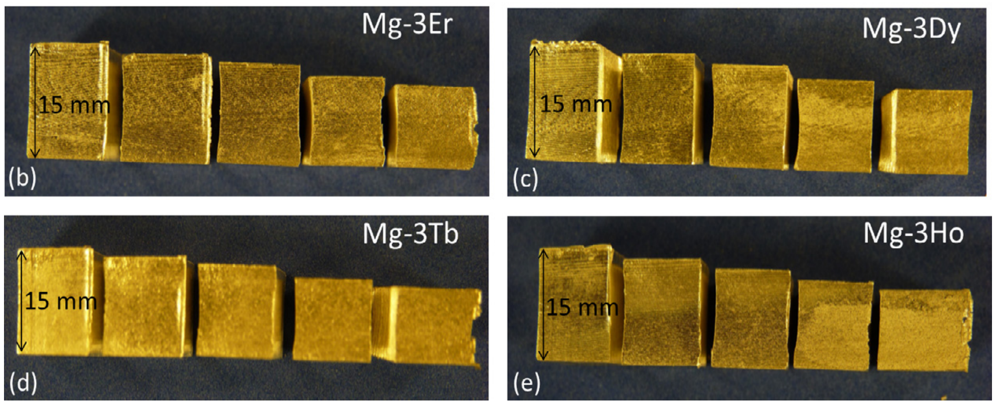
Alloying and microstructure

Controlling microstructure is one key to achieve better properties!





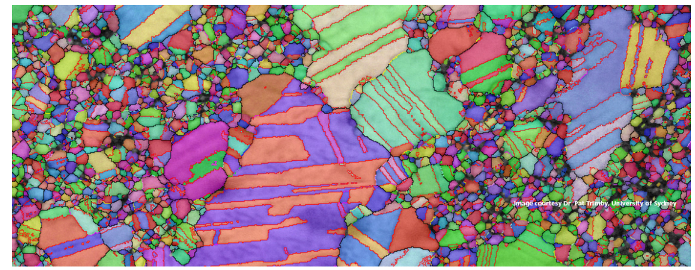
Alloying materials is one key to achieve better properties!

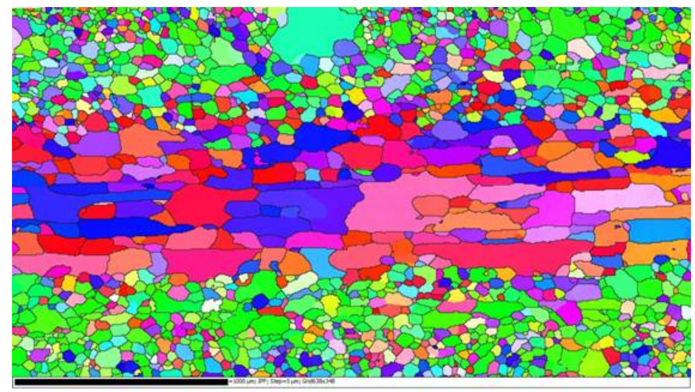


1 RE-atom per 1000 atoms - Alloying plays a critical role in materials properties

But the questions is:
What is the optimal microstructure?
Can I control the microstructure?
What are the key factors involved in generation of MS?

S. Sandlöbes, Z. Pei, M. Friak, L.-F. Zhu, F. Wang, S. Zaefferer, D. Raabe, J. Neugebauer, Acta Materialia 70 (2014) 92–104
Oxford instruments - EBSD maps of different materials
Towards strength–ductility synergy through the design of heterogeneous nanostructures in metals, Evan Ma and Ting Zhub

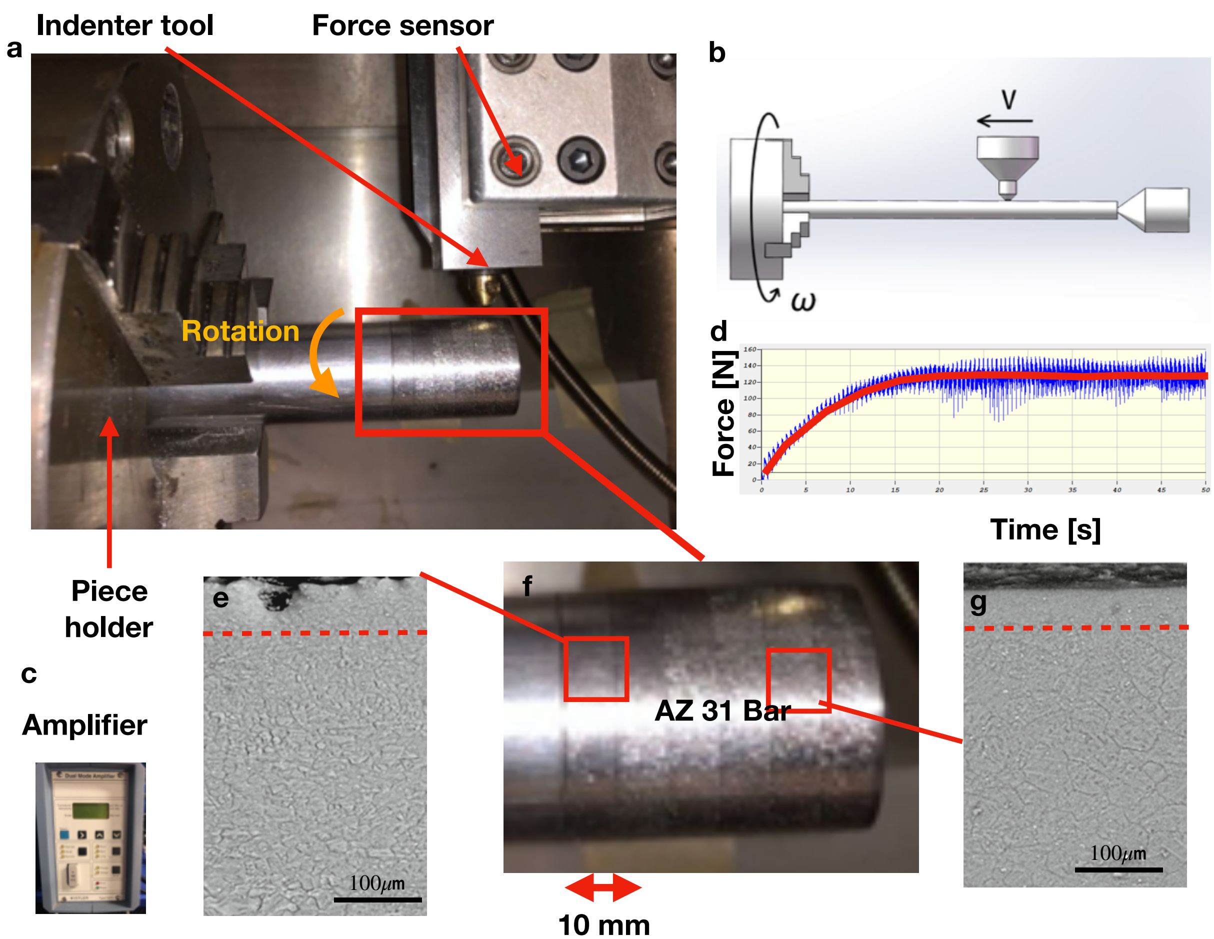




"Imparting high strength without conceding too much ductility is one of the major challenges in nano-structuring metals"

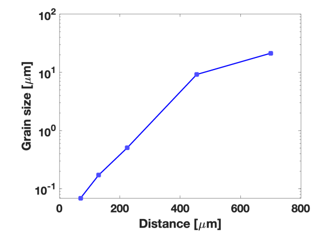
Surface mechanical grinding in Mg alloys

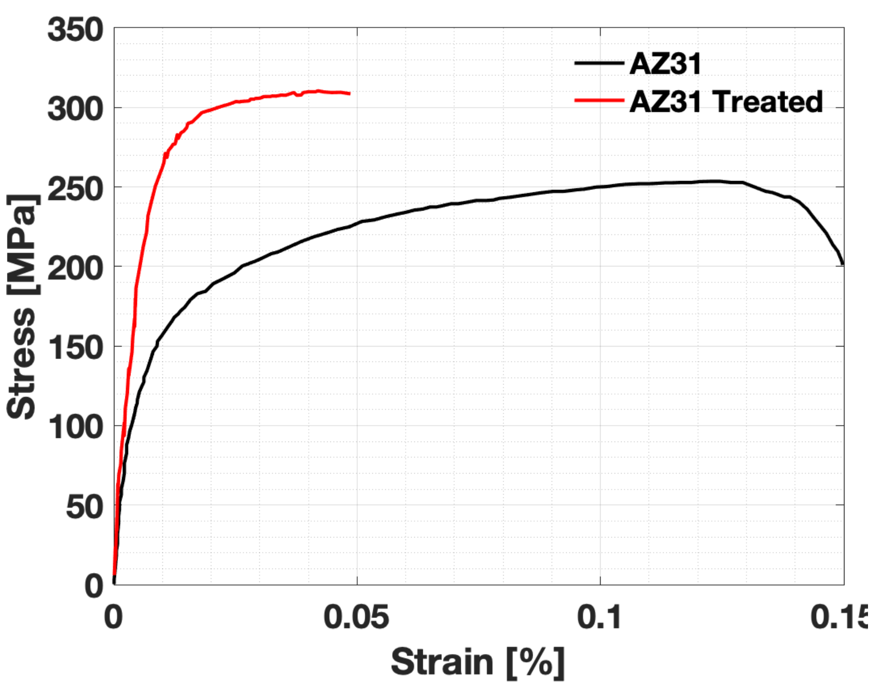
Other ways to achieve GNG in (soft) metals

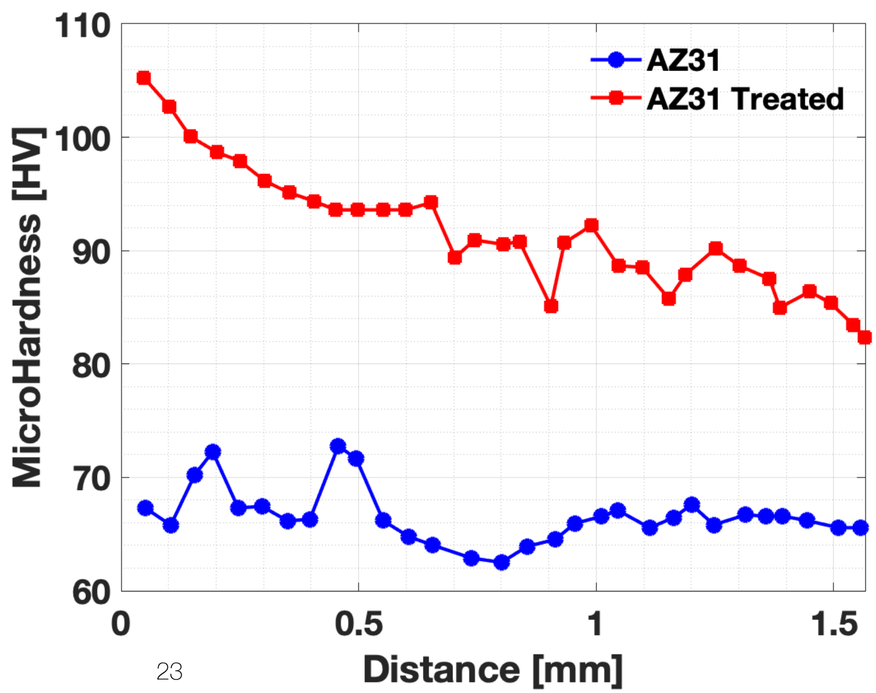


Surface mechanical grinding in Mg alloys

Mechanical properties of treated Mg AZ31

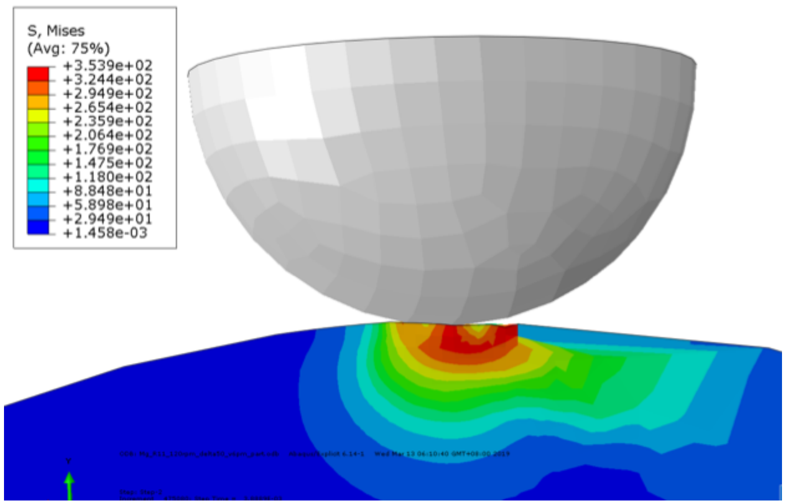


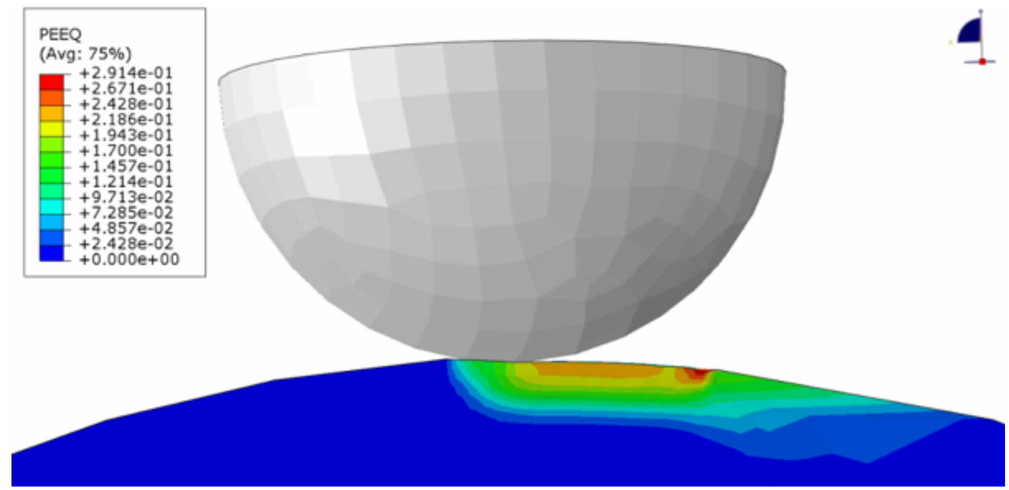




Surface mechanical grinding in Mg alloys

Simulations reveal a plastic stress and strain under the indenter





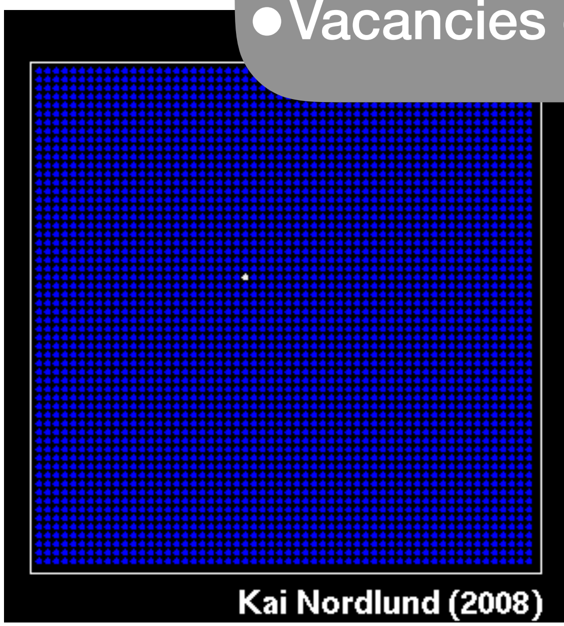
This generate an avalanche of twins, recrystallizing the material near the surface

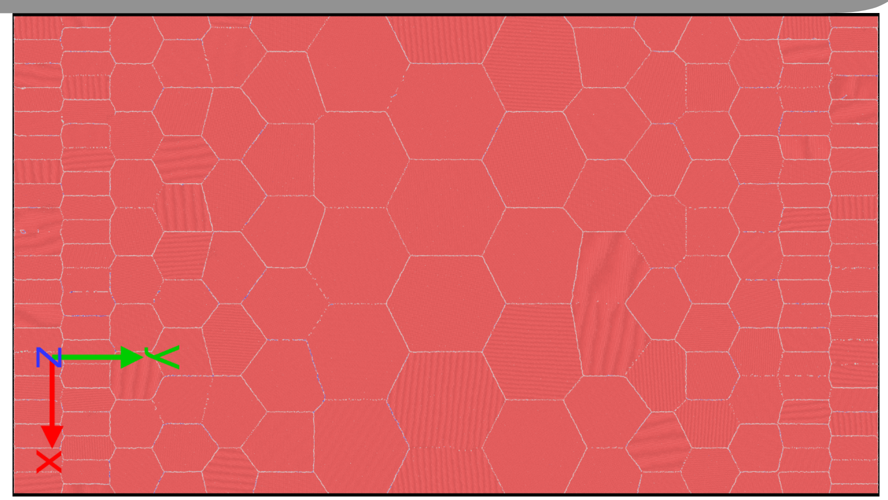
GNG use as a shield for radiation

- Large number of interfaces per volume (near the surface).
- Good mechanical properties and toughness.
- Good th

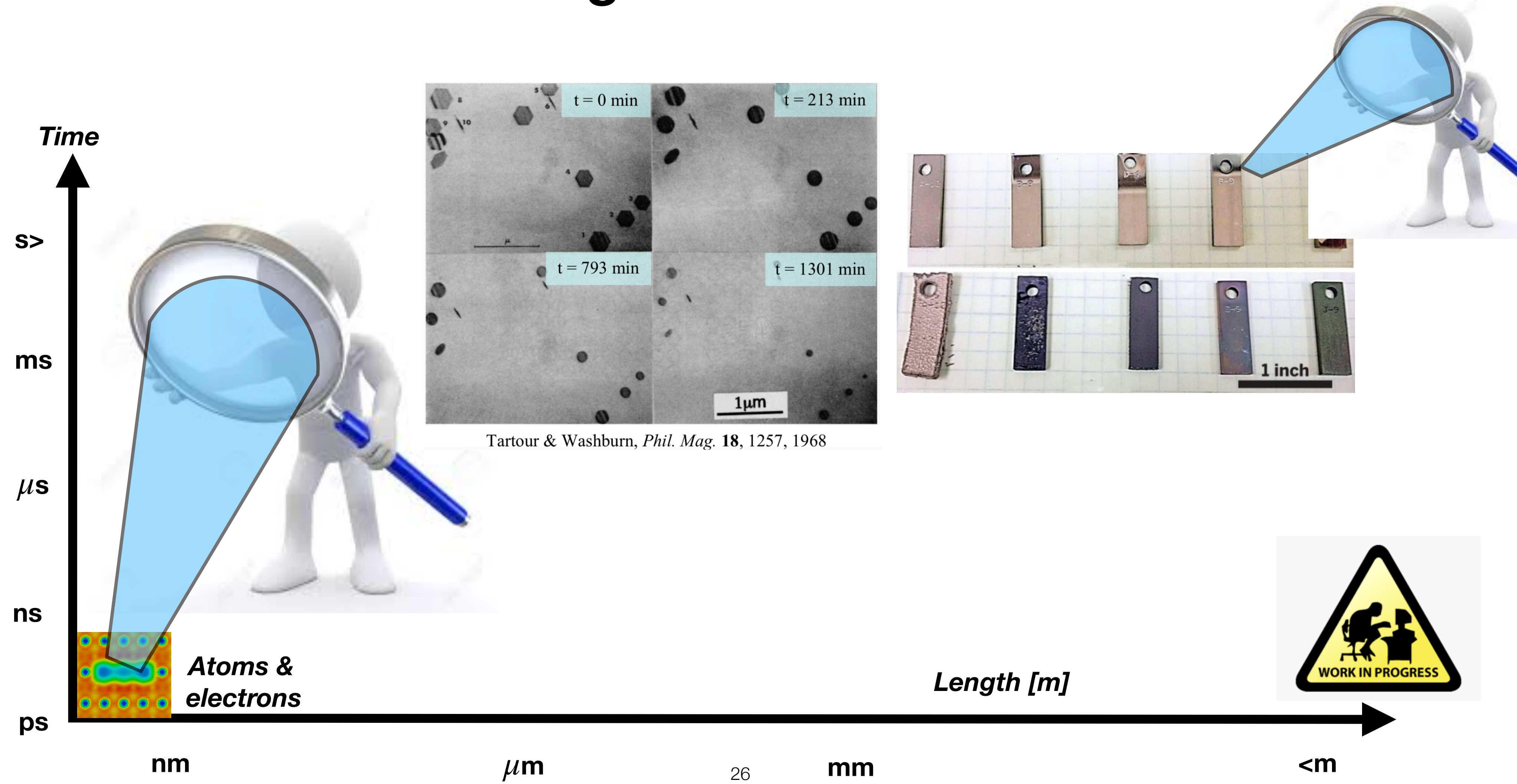
- Warning! Ions move very quickly! (>50KeV).
- Their interaction with radiation shield is very fast (20 ps).
- Requires coupling of phonons and electrons.
- Vacancies diffuse in a long (min and hours) scale.

Thus, GN … iour with radiation s

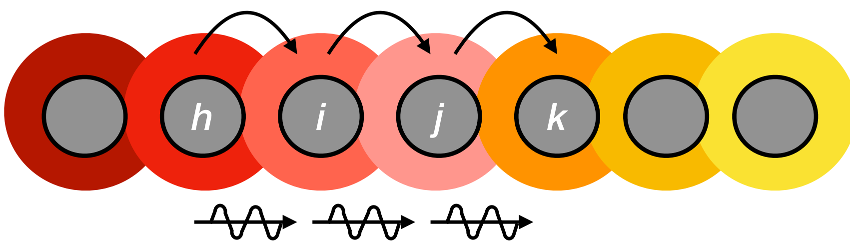




Multiscale modelling of materials radiation damage



Coupling phonons and electrons in MD systems



$$T_i^{lat} = \sum_{j=1}^{N_j} \frac{\frac{1}{2} m_j \mathbf{v}_j \cdot \mathbf{v}_j}{\frac{3}{2} k_B N_j}$$

$$\frac{\partial T_i^e}{\partial t} = T_{max}^e \sum_{\substack{j=1 \\ j \neq i}}^{N_n} K_{ij} \{ \theta_j^e (1 - \theta_i^e) \exp[\Delta e_{ji}] - \theta_i^e (1 - \theta_j^e) \exp[\Delta e_{ij}] \} - \frac{G}{C_e} (T_i^e - T_i^{lat}),$$

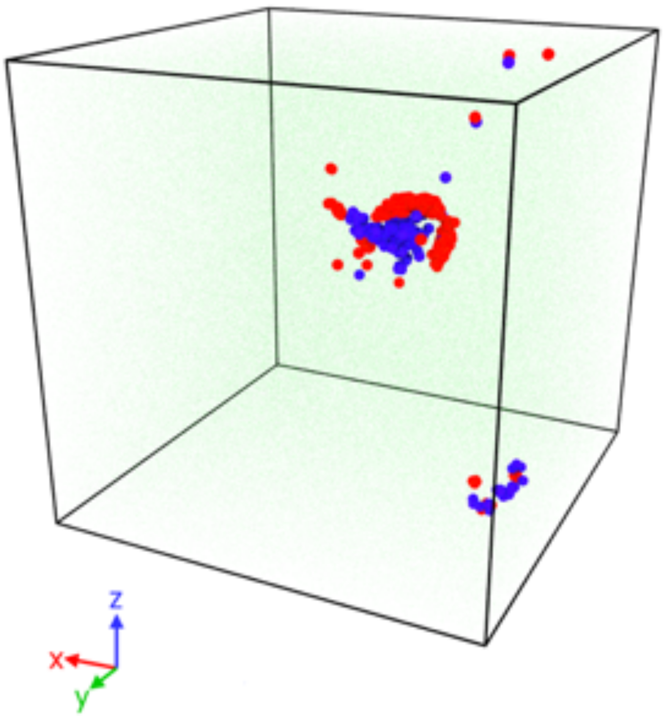
$$m_i \dot{\mathbf{v}}_i = \mathbf{F}_i + \mathbf{F}_i^{damp} = \mathbf{F}_i + \xi_i m_i \mathbf{v}_i$$

$$\xi_i = \frac{G V_{atom} (T_i^e - T_i^{lat})}{2 K_i},$$

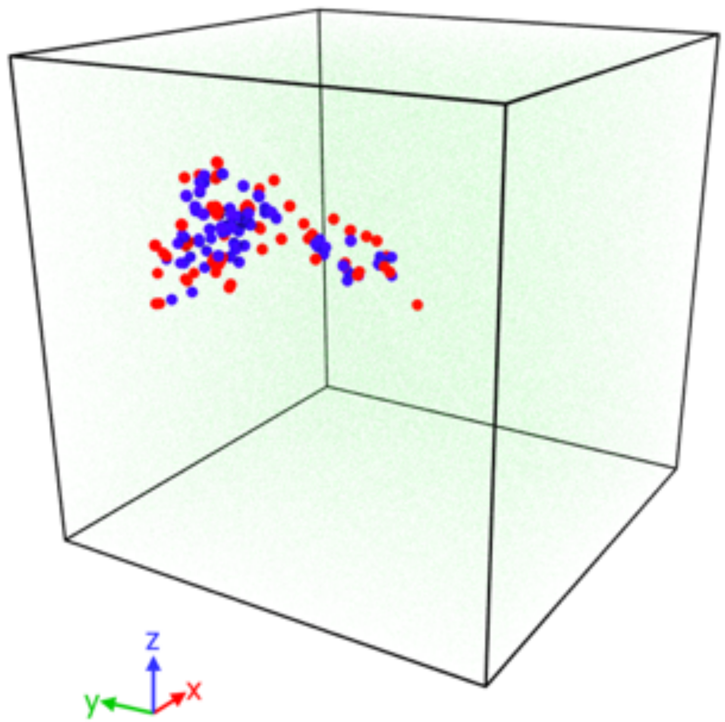
M. Ullah and M. Ponga. MSMSE 27 (2019) 75008.
M. Ponga, D. Sun, MSMSE 26 (2018) 035014.
D. M. Duffy, A. M. Rutherford, JPCM 19 (2007) 016207.
D. S. Ivanov, L. V. Zhigilei, PRB 68 (2003) 064114.

50 KeV PKA simulations in Nickel

Classical MD



I2T-MD



Defect (FPs) Statistics

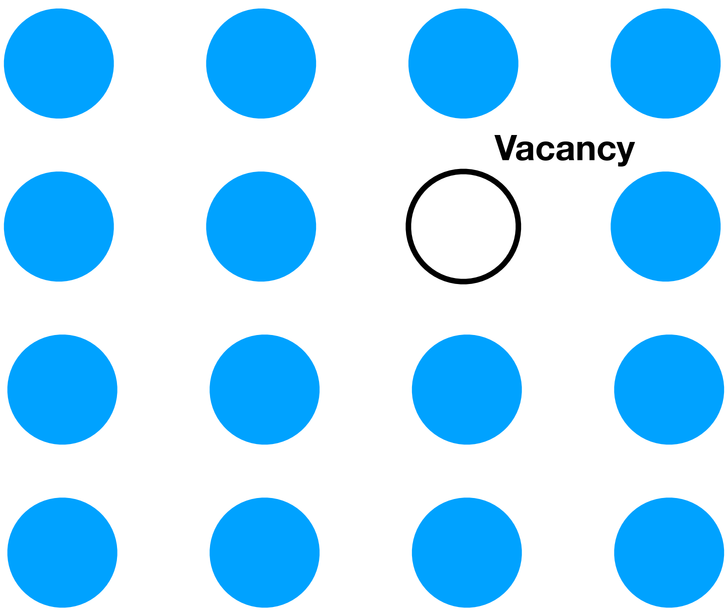
2T-MD : 102 ± 7
MD : 144 ± 14

Electrons increase their heat capacity and thermal conductivity at large temperatures.

M. Ullah and M. Ponga. MSMSE 27 (2019) 75008.
M. Ponga, D. Sun, MSMSE 26 (2018) 035014.
D. M. Duffy, A. M. Rutherford, JPCM 19 (2007) 016207.
D. S. Ivanov, L. V. Zhigilei, PRB 68 (2003) 064114.

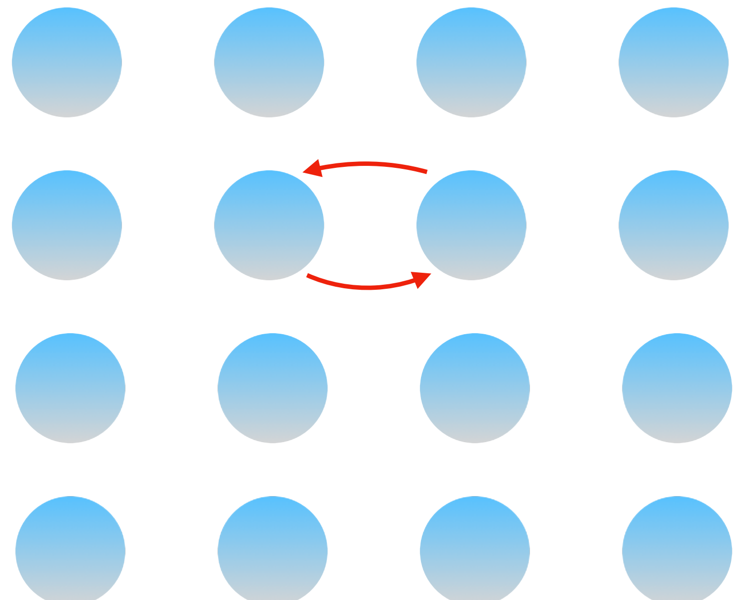
Simulating long-term diffusion of vacancies in GNG

Traditional MD



Restriction: Time step very small (1 fs max!)

Diffusive MD ✓



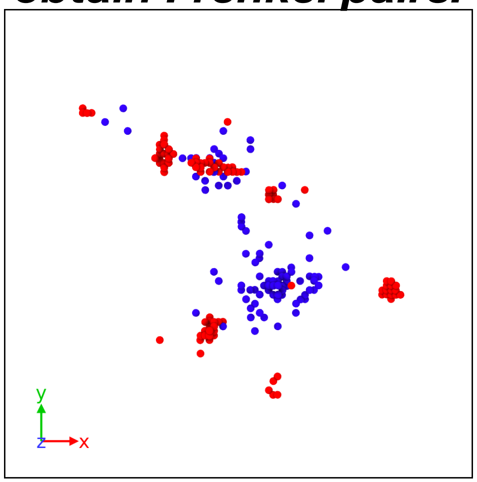
Concentration of vacancies same everywhere

Time step very large (1 ms max!)

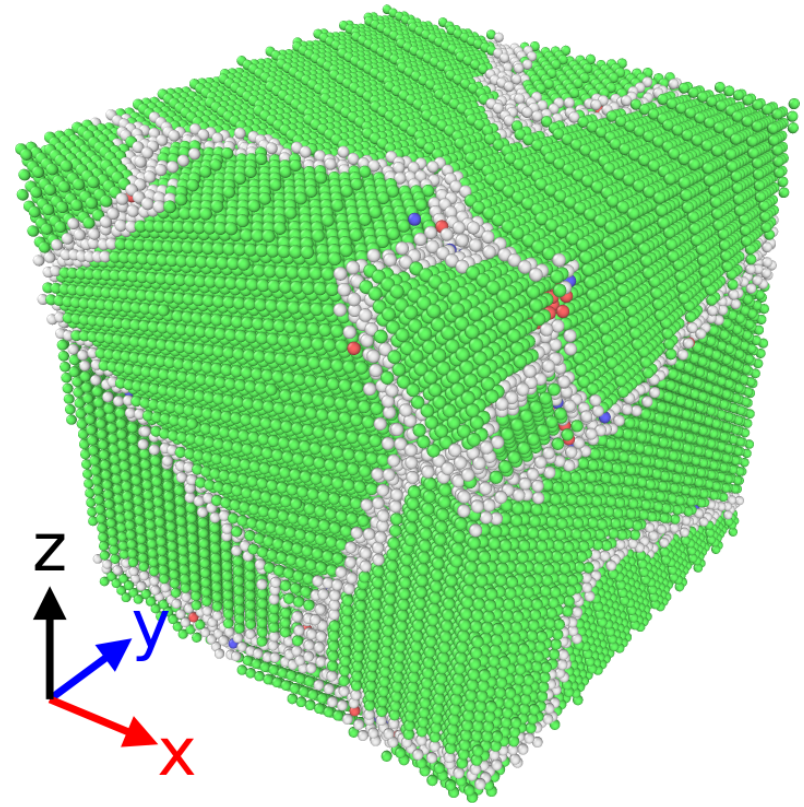
M. Ponga, D. Sun, MSMSE 26 (2018) 035014.
J.P. Mendez & Ponga, CPC, Under review (2019).

Self-healing of GNG materials

Realistic doses can be simulated (<50KeV) to obtain Frenkel pairs.



Simulate long term diffusion (< t=500 s) to investigate the behaviour of GNG materials

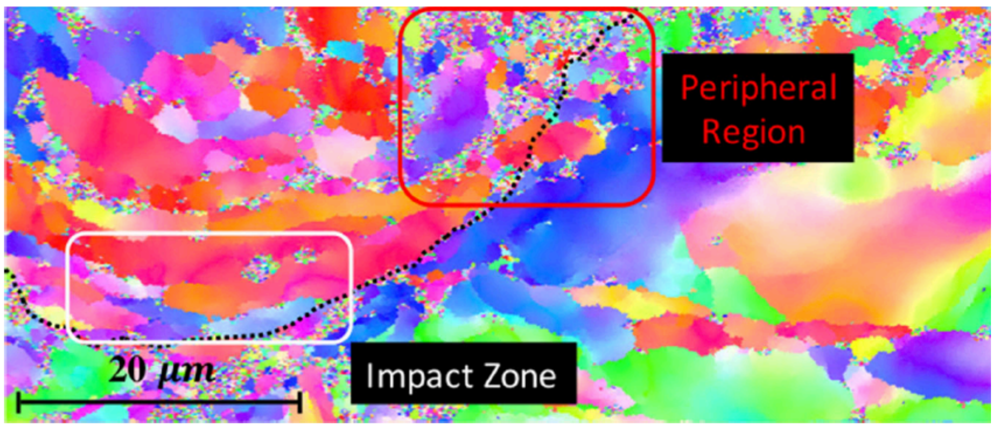


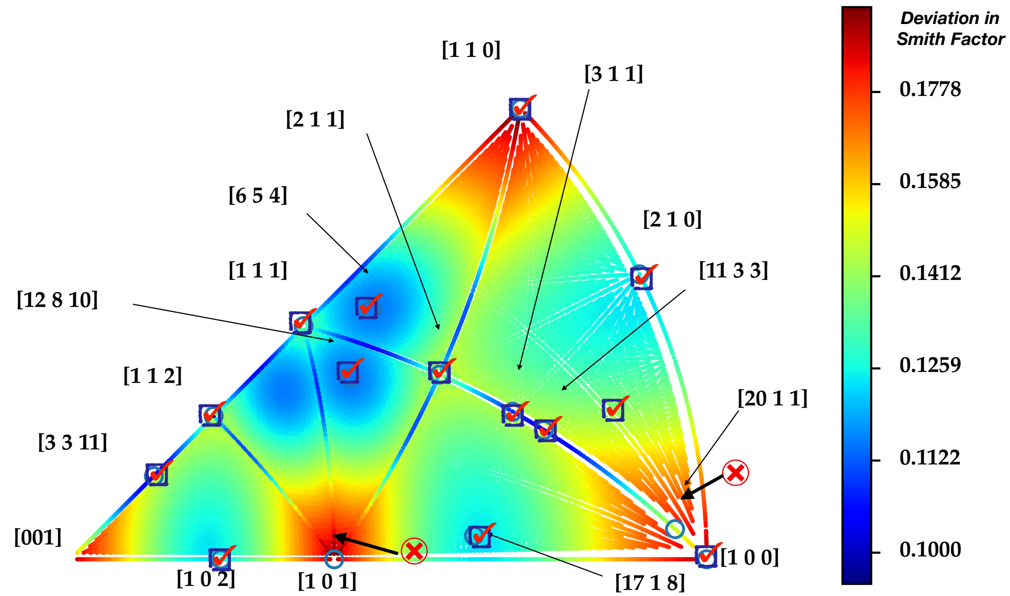
After t = 500 s, GNG absorbs 66% of vacancies reducing porosity.

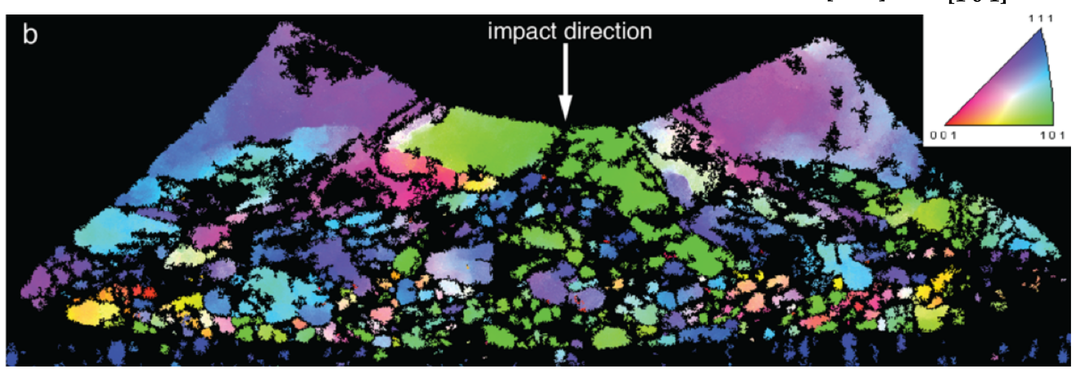
Concluding remarks and future directions

- **GNG materials is a promising avenue to tailor mechanical properties in a broad sense.**
- **Several techniques are available to develop such a rich microstructure.**
- **This can be combined with alloying and other techniques.**
- **GNG arise as promising materials against radiation damage.**
- **Controlling particle orientation during impact a the key to manipulate microstructural features during cold spray.**
- **High entropy alloys and lightweight materials, are ideally candidates to generate GNG.**

Thank you!


Peripheral Region
20 μm
Impact Zone


Deviation in Smith Factor
0.1778
0.1585
0.1412
0.1259
0.1122
0.1000
[1 1 0]
[3 1 1]
[2 1 1]
[6 5 4]
[2 1 0]
[1 1 1]
[11 3 3]
[12 8 10]
[1 1 2]
[20 1 1]
[3 3 11]
[001]
[1 0 0]
[1 0 2]
[1 0 1]
[17 1 8]


b
impact direction