

Multi-scale modeling of ultra-hard nanoparticles deformation

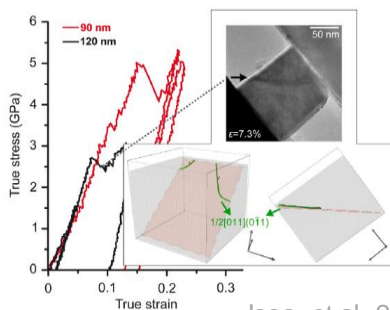
Context

MgO:

- Model ceramics material
- Refractory agent in the construction of crucibles
- Excellent insulator
- Stable nanocrystal

Problematics:

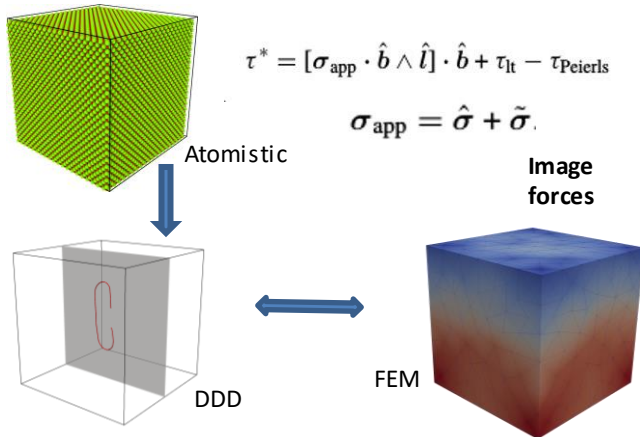
- Understanding of ceramic nanoparticle plasticity.
- Scale transition from atomistic to meso-scale
- Size vs strain-rate deformation properties



Issa, et al. 2015

Method and tools

Multiscale coupling:



DDD:

Numodis, Laurent Dupuy(collaborator)
CEA Saclay.



FEM:

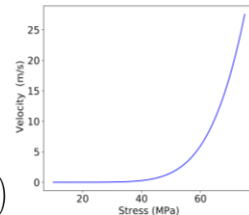
Elmer, CSC, Finland



Results

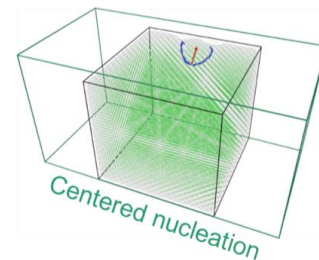
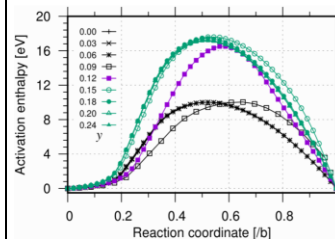
Implementation of MgO mobility law

$$v(\tau, T) = a' v_D b \frac{L}{w_c^2} \exp\left(\frac{-\Delta H_0}{kT}\right) \times \sinh\left(\frac{\Delta H_0}{kT} \left(1 - \left(1 - \left(\frac{\tau}{\tau_p}\right)^p\right)^q\right)\right)$$



Amedeo, et al. 2011

Dislocation nucleation



DDD/FEM

