Uncertainty propagation in a multiscale model of nanocrystalline plasticity

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Motivation

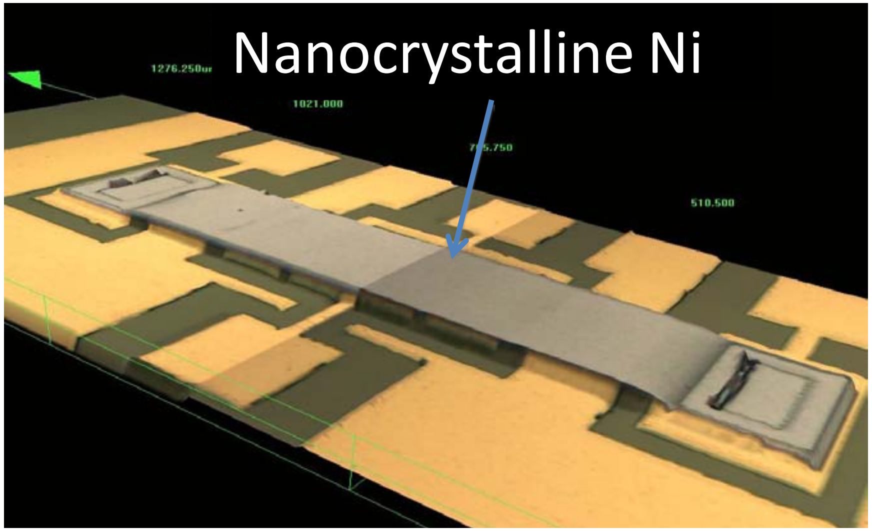
- Quantify how internal stresses that result from the fabrication process affect the the yield stress of the metallic membrane of a MEMS device.
- The model combines molecular dynamics(MD) simulations to characterize atomic level processes that govern dislocation based plastic deformation with a phase field approach to dislocation dynamics (PFDD) that describes how an ensemble of dislocations evolves and interact to determine the mechanical response of the material.
- We apply this approach to a nanocrystalline Ni specimen of interest in micro-electromechanical (MEMS) switches.
- Our predictions show that, for a nanocrystalline sample with small grain size (4 nm), a variation in residual stress of 20 MPa (typical in today's microfabrication techniques) would result in a variation on the critical resolved shear yield stress of approximately 15 Mpa, a very small fraction of the nominal value of approximately 9 GPa.

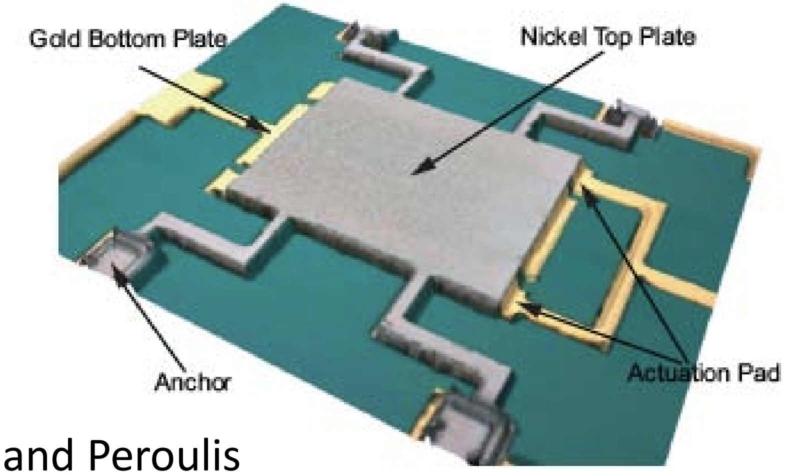
Uncertainty propagation in a multiscale model of nanocrystalline plasticity,
Koslowski and Strachan, in press, RESS, 2010

Outline

- RF MEMS switches
- Plastic deformation in nanocrystalline materials.
- Atomisitc simulations.
- Phase field dislocation dynamics (PFDD) model.
- Uncertainties and propagation across scales.
- Summary.

RF MEMS switch



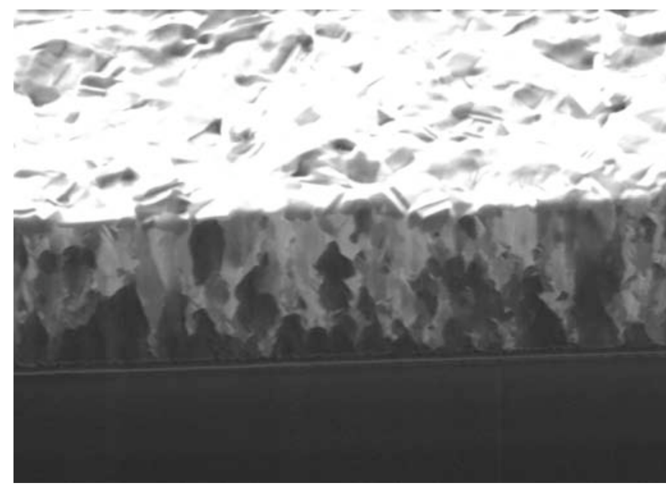


Hsu and Peroulis

Critical issues in design of MEMS:

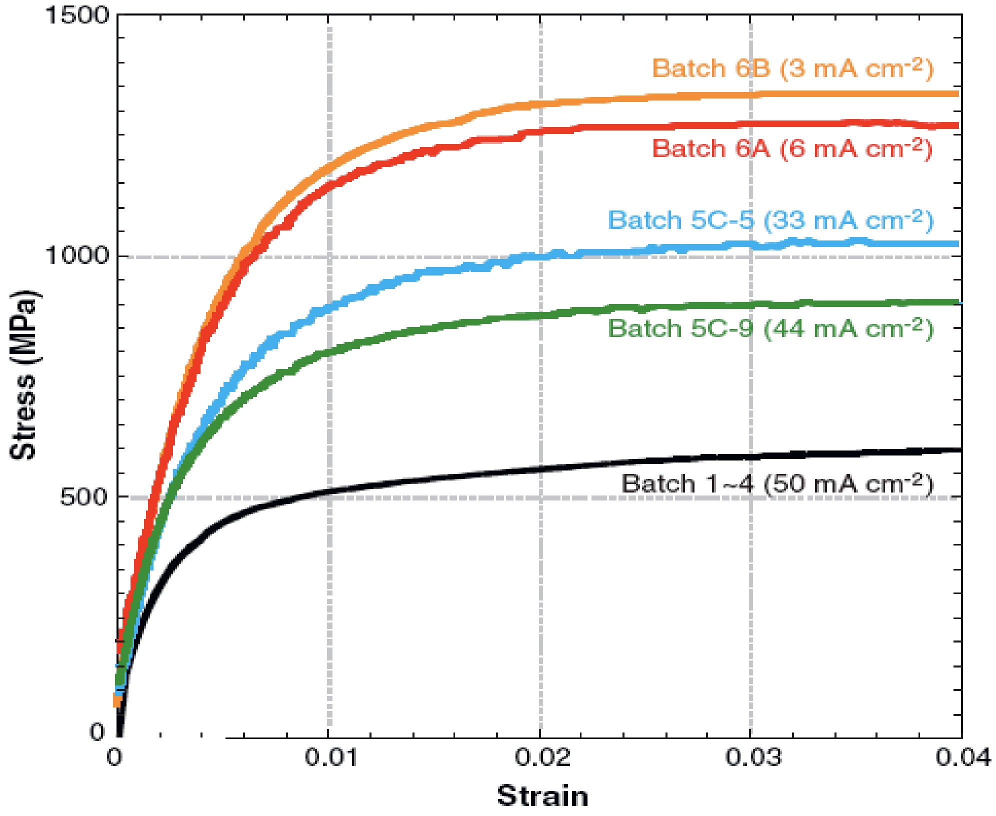
- Dielectric charging
- Contact surfaces, asperity size and geometry.
- Stiction.
- Creep.

Walraven, IEEE, 2007



Cantwell and Stach

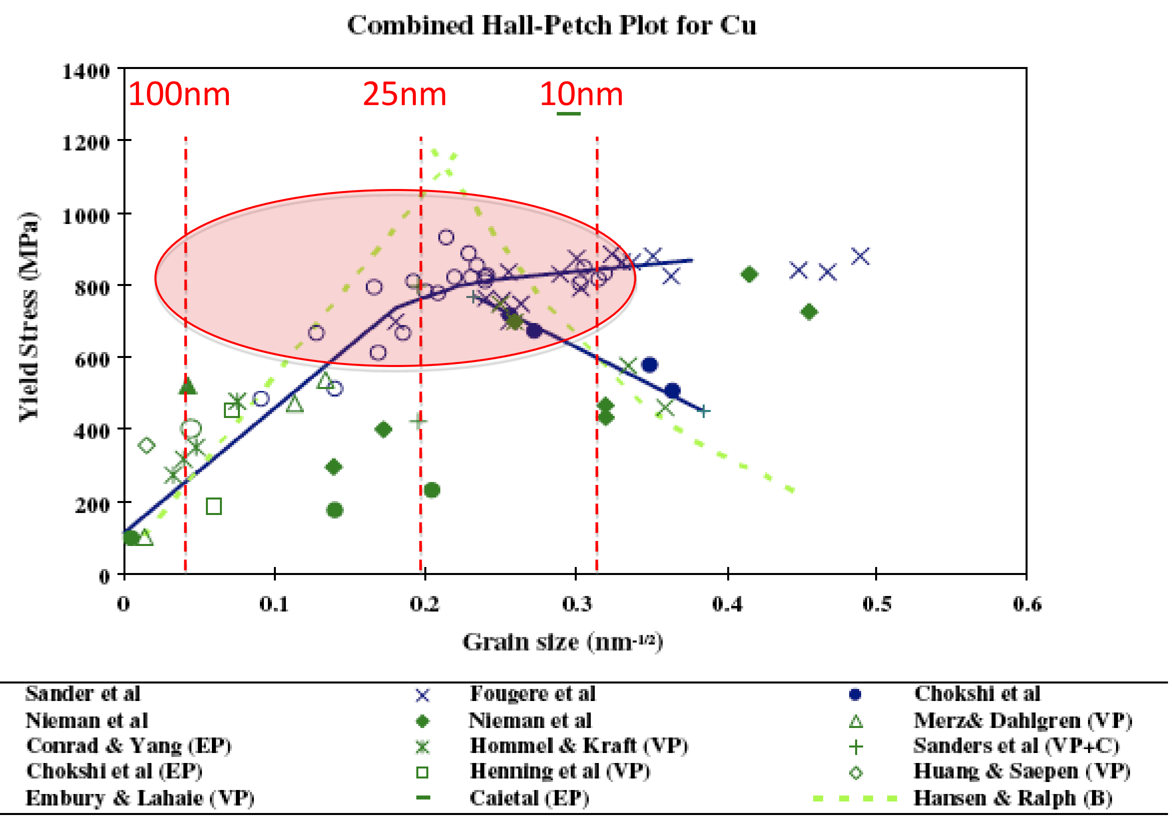
Plastic deformation in nc Ni



Stress/strain curves showing Hall-Petch effect in Liga Ni membranes.

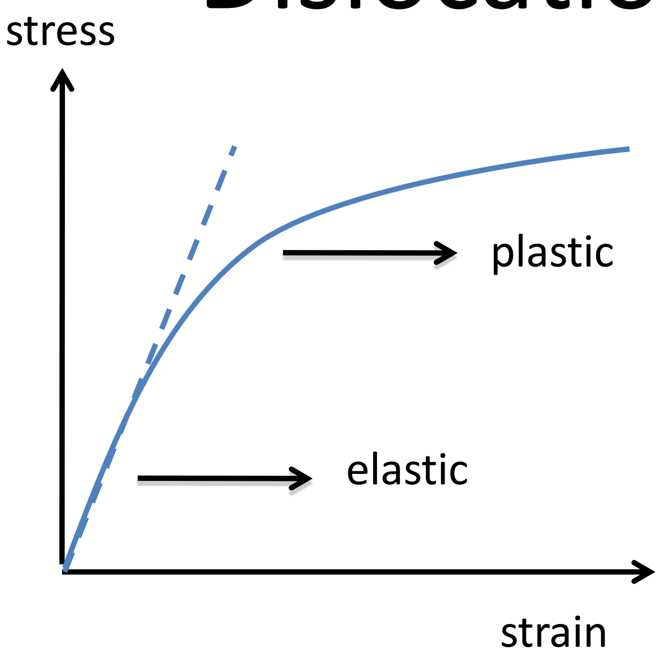
Hemker, 2007

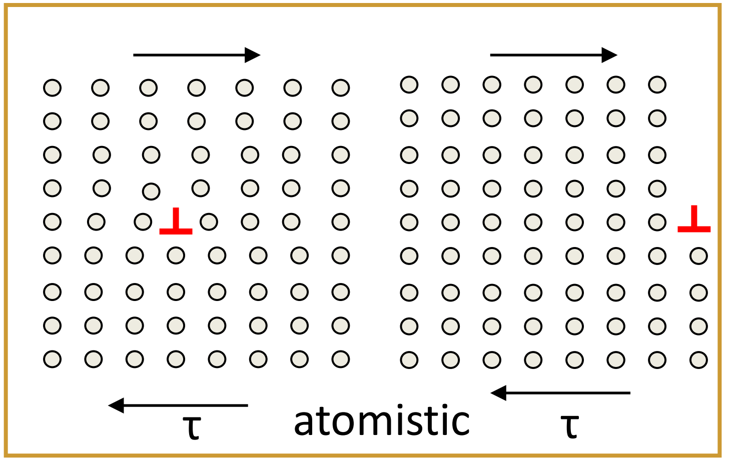
Size effects in plastic deformation: Inverse Hall-Petch

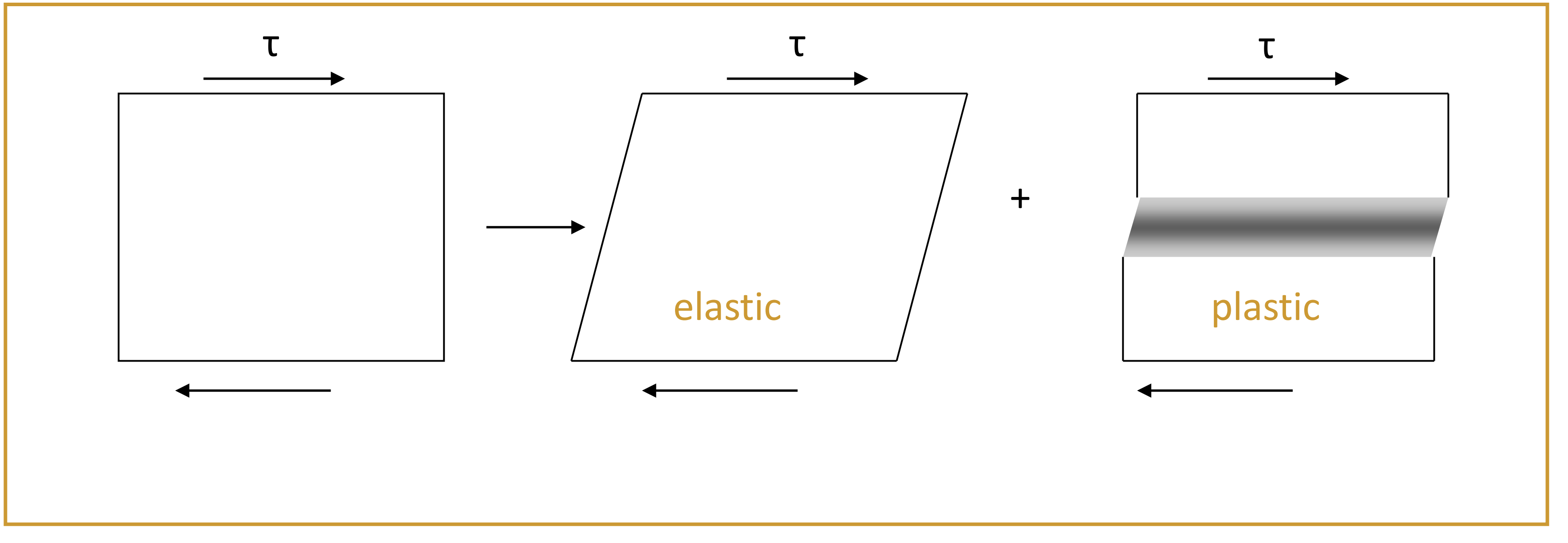


M.A. Meyers et al. / Progress in Materials Science 51 (2006) 427–556

Dislocation-Plasticity in metals

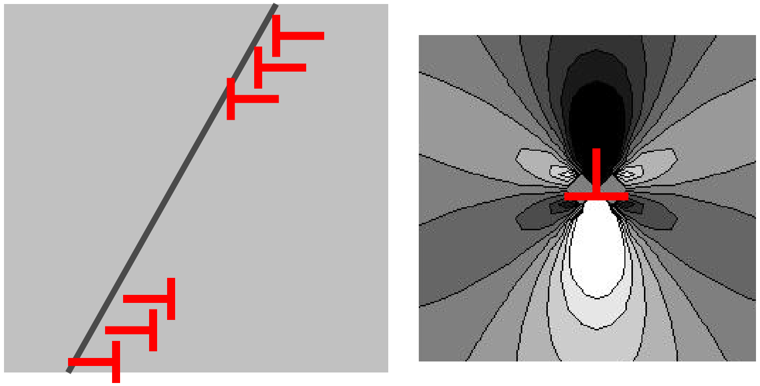




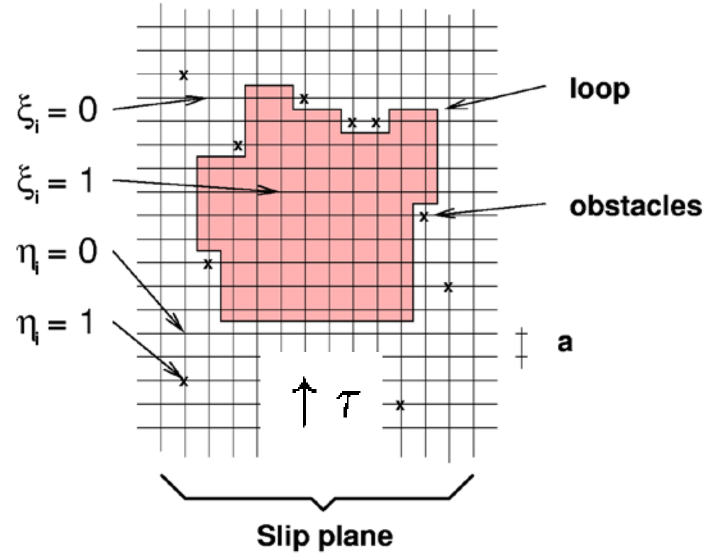


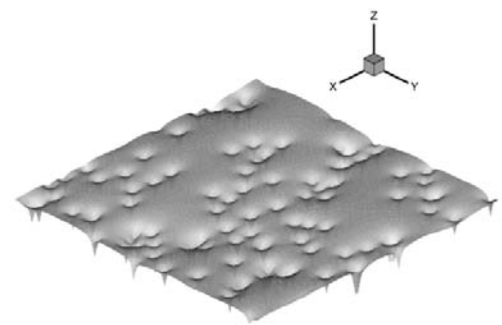
Dislocation dyanmics

dislocation dynamics



Phase field model of dislocations





$$\xi(x_1, x_2)$$

$$\beta_{ij}^{p} = \sum_{\alpha} \xi^{\alpha} s_i^{\alpha} m_j^{\alpha}$$

MD to PFDD

Molecular Dynamics: Individual atoms
Dislocations: explicitly described

Phase field: relative slip between adjacent atomic planes
Dislocations: gradients of phase field

Equations of motion

$$\dot{r}_i = \frac{p_i}{m_i}$$

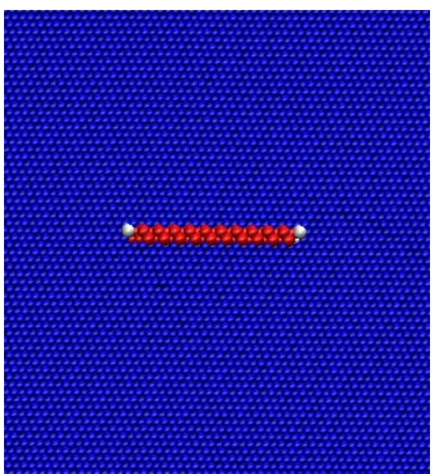
$$\dot{p}_i = -\nabla_{r_i} U(\{r_i\})$$

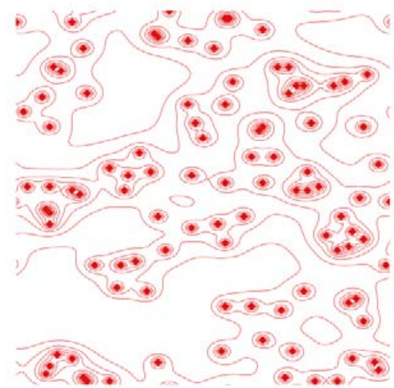
$$\frac{\partial \xi(\alpha, x)}{\partial t} = -L \frac{\partial E}{\partial \xi(\alpha, x)}$$

Energy expression

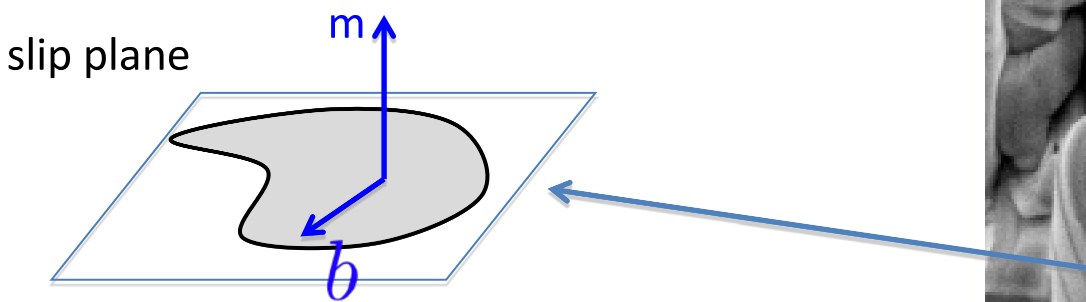
$$U(\{r_i\}) = \sum_{i<j} \phi(r_{ij}) + \sum_i F(\rho_i)$$

$$E = E^{elas} + E^{crys} + E^{grad}$$





Phase field dislocation dynamics

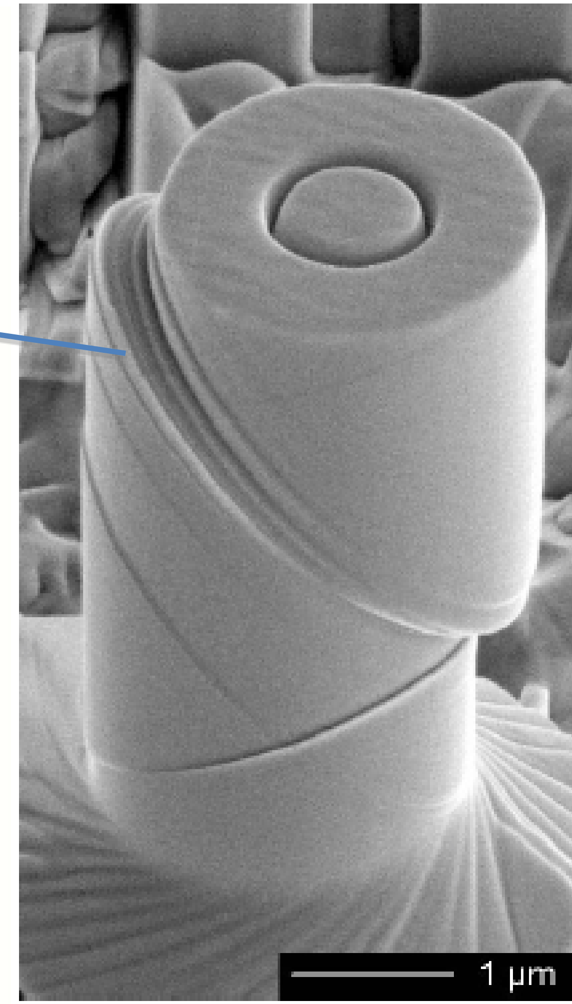


$$\beta^p_{ij}(x) = \sum_{\alpha=1}^{N_s} \sum_{n_\alpha=1}^{N} \xi^\alpha_{n_\alpha}(x)\delta_{n_\alpha} m^\alpha_i b^\alpha_j$$

$$E^{\text{int}} = \frac{1}{2}\int \hat{A}_{mnuv}(k)\hat{\beta}^p_{mn}(k)\hat{\beta}^{p*}_{uv}(k)\frac{d^3k}{(2\pi)^3}$$

$$\hat{A}_{mnuv}(k) = c_{mnuv} - c_{kluv}c_{ijmn}\hat{G}_{ki}(k)k_j k_l$$

Tensor A_{mnuv} depends on elastic constants (from MD)



SEM images of pure Ni micro-crystals (Uchic, Science 2004)

Koslowski, Cuitino and Ortiz, JMPS (2002)
Hunter, Le, Saied and Koslowski, Journal High Performance Computing (2010)

Elastic interaction

- Displacement field: $$u_k = -G_{ki} * \left(c_{ijmn}\beta^p_{mn}\right)_{,j}$$

- Elastic distortion: $$\beta^e_{kl} = -G_{ki,l} * \left(c_{ijmn}\beta^p_{mn}\right)_{,j} - \beta^p_{kl}$$

- Elastic interaction: $$E^{int} = \frac{1}{(2\pi)^3}\int \tfrac{1}{2}\hat{A}_{mnuw}\,\hat{\beta}^p_{mn}\,\hat{\beta}^{p*}_{uw}\,d^3k$$

- Green function for an isotropic crystal: $$G_{ki} = \frac{1}{8\pi\mu}\left(\delta_{ki}\nabla^2 r - \frac{\lambda+\mu}{\lambda+2\mu}\frac{\partial^2 r}{\partial x_i \partial x_k}\right)$$

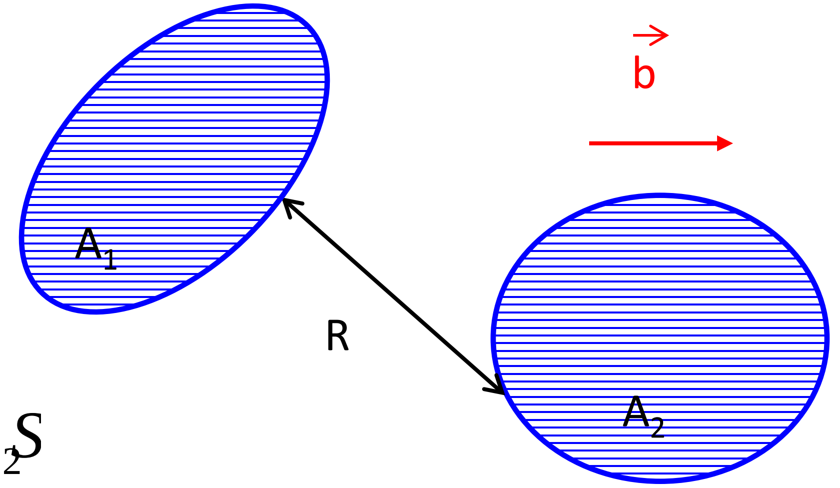
Elastic Interaction

$$E^{int}[\zeta] = \frac{1}{(2\pi)^2}\int \frac{\mu b^2}{4} K(k_1,k_2)\left|\hat{\zeta}\right|^2 d^2k$$

with $$\zeta(x_1,x_2) = \delta(x_1,x_2)/b$$

$$K(k_1,k_2) = \frac{1}{1-\nu}\frac{k_1^{\,2}}{\sqrt{k_1^{\,2}+k_2^{\,2}}} + \frac{k_2^{\,2}}{\sqrt{k_1^{\,2}+k_2^{\,2}}}$$

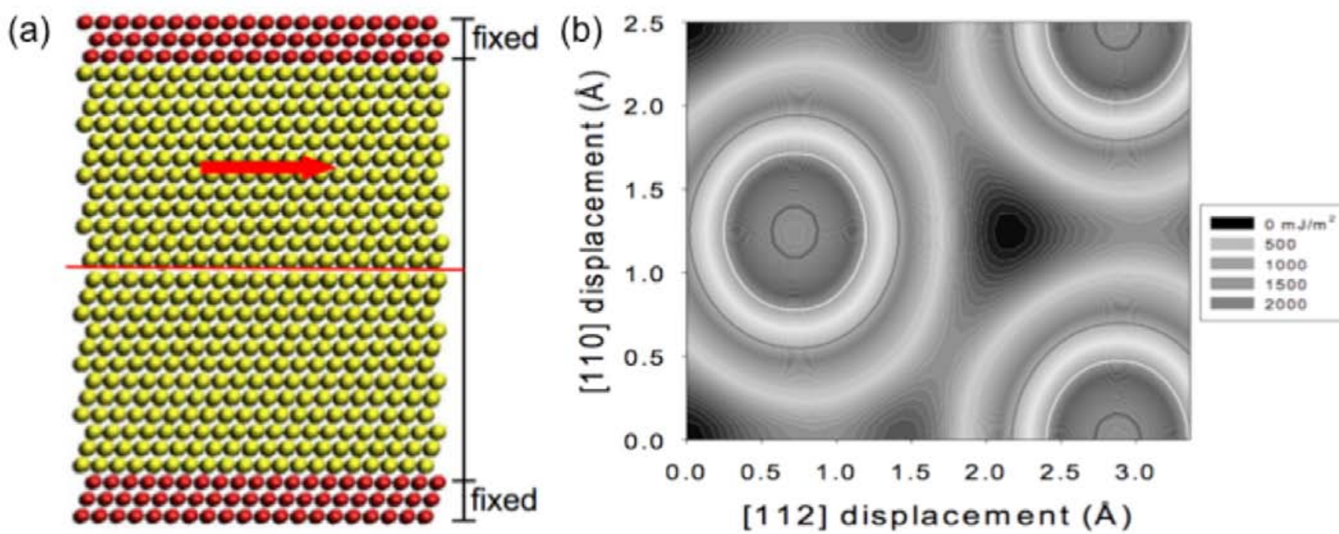
$$E^{int} = \frac{\mu b^2}{8\pi}\int_{A_1}\int_{A_2} \frac{1}{R}\,\overline{\nabla}\zeta_1 \begin{bmatrix} \frac{1}{1-\nu} & 0 \\ 0 & 1 \end{bmatrix} \overline{\nabla}\zeta_2 \, dS_1\, dS_2$$



(Hirth and Lothe,1969)

MD to phase field micromechanics

$$E^{misfit} = \sum_{\alpha=1}^{N_s} \sum_{n_\alpha=1}^{N} \int \phi_{n_\alpha}(x) d^3x$$

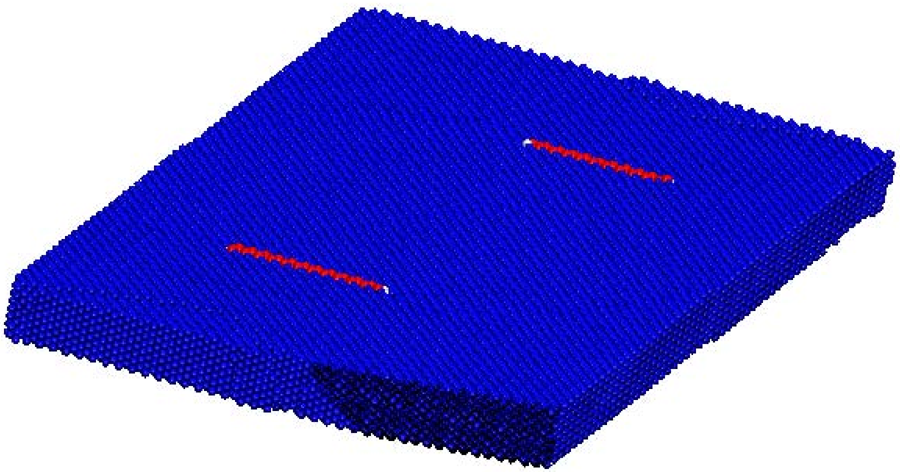


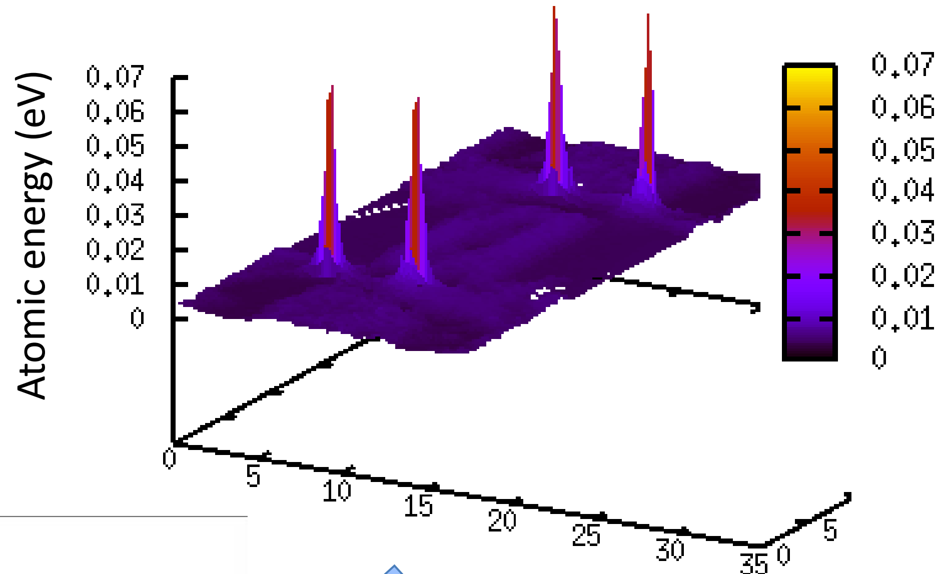
Lee, Kim, Strachan and Koslowski (submitted PRB, 2010)

MD to phase field micromechanics

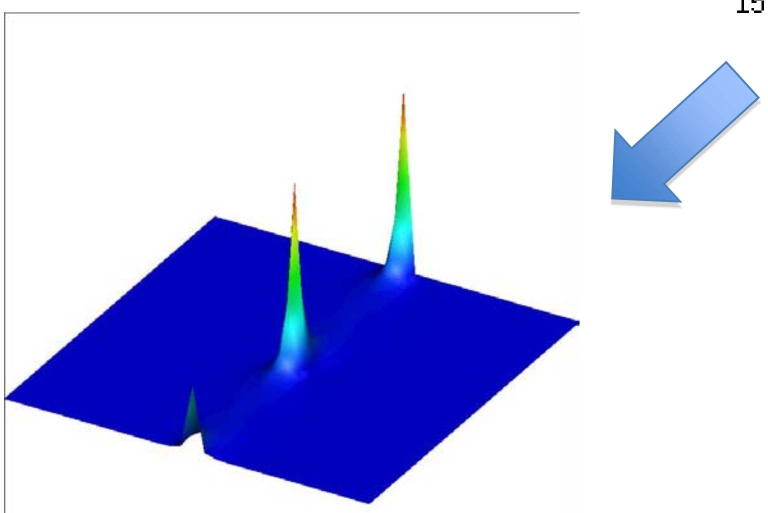
$$E^{grad} = \frac{1}{2}\int \sum_{\alpha\beta} H(\alpha,\beta)_{ijkl} b_i^{\beta} \frac{\partial \xi(\alpha,x)}{\partial x_j} b_k^{\alpha} \frac{\partial \xi(\beta,x)}{\partial x_l} d^3x$$

Tensor *H* associated with dislocation core energies





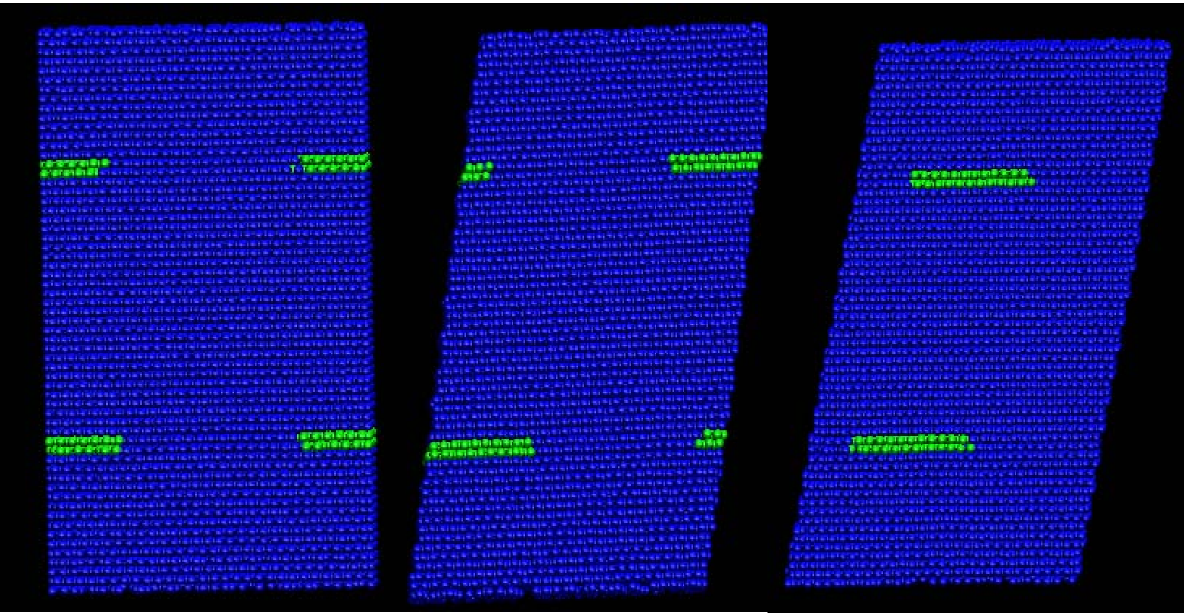
Phase field local energy

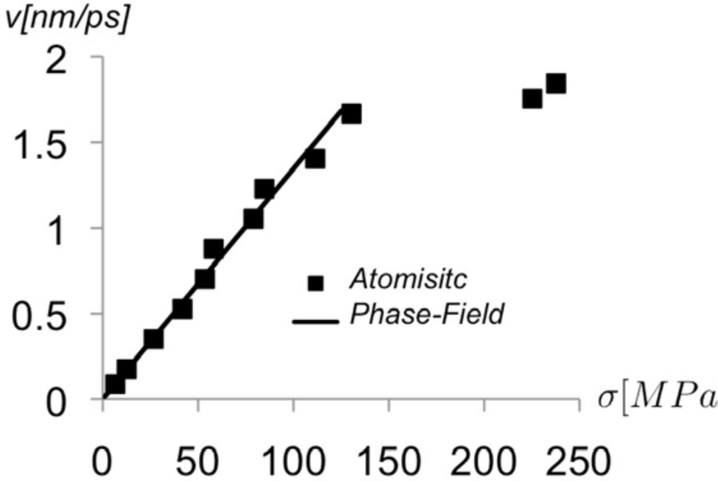


MD to phase field micromechanics

$$\frac{\partial \xi(\alpha, x)}{\partial t} = -L \frac{\partial E}{\partial \xi(\alpha, x)}$$

L governs dislocation mobility



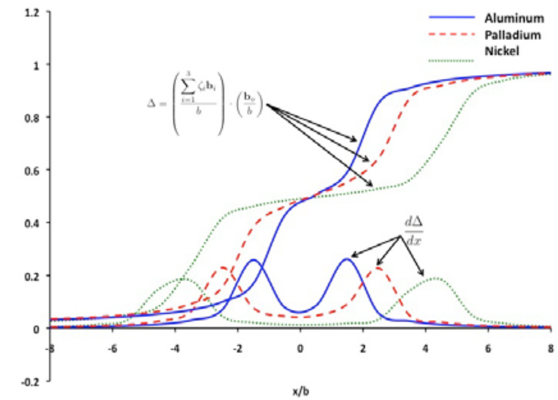


15

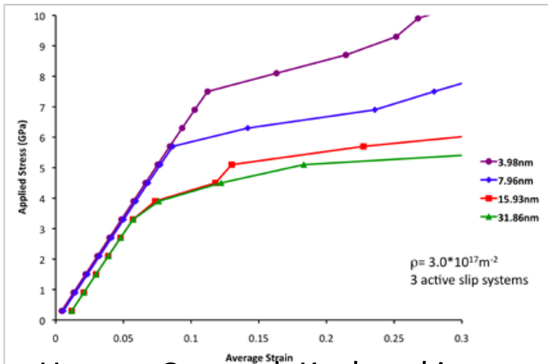
PFDD

Phase field Micro Mechanics

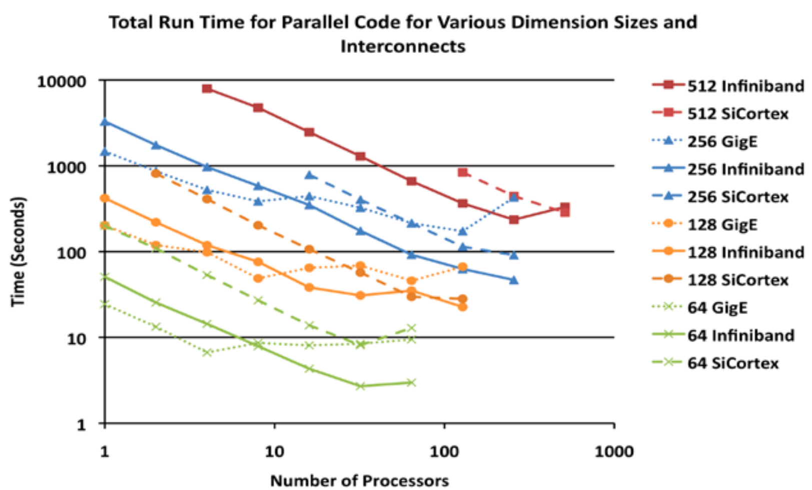
- **3D parallel code**, includes elastic/plastic deformation tracking individual dislocations.
- Scalability on data sets with up to 10^9 degrees of freedom, along with the efficiency on up to 1024 processors.
- Fully informed from atomistic simulations.
- Includes:
  - Interactions of dislocations with interfaces, grain boundaries, passivation and free surfaces.
  - Partial dislocations.
  - Grain boundary sliding



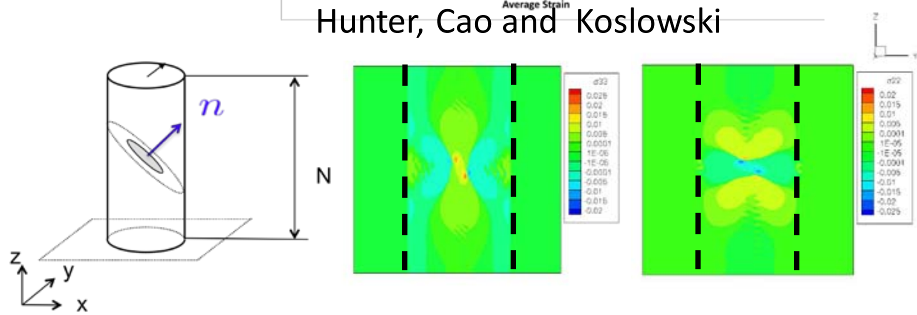
Hunter, Beyerlin, Germann and Koslowski



Hunter, Cao and Koslowski

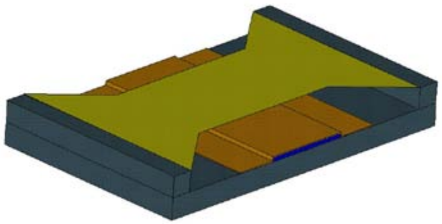


Hunter, Le, Saied and Koslowski, 2010

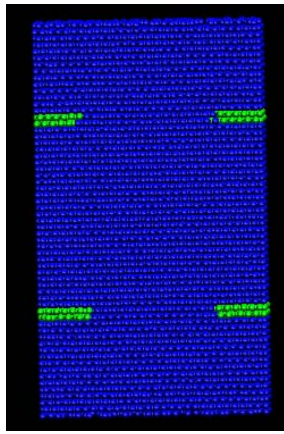


Effect of free surfaces on the stress field of a dislocation loop in a nano-pillar. Lei and Koslowski, 2010.

Uncertainty propagation across the scales

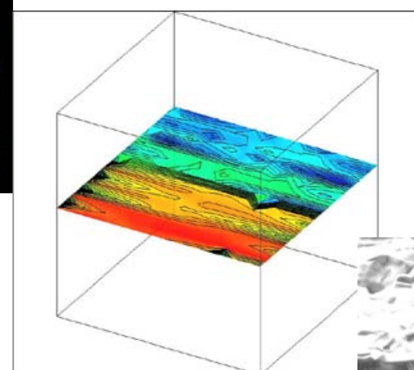


Residual stress



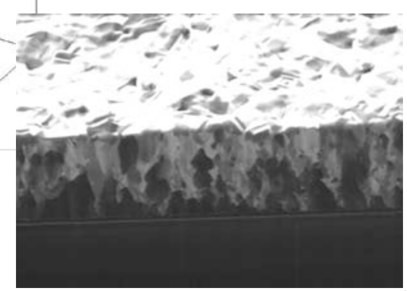
MD

Parameters to PFDD

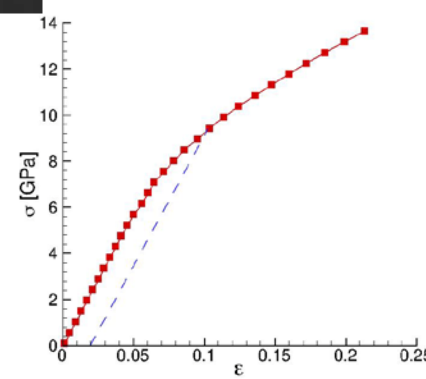


PFDD

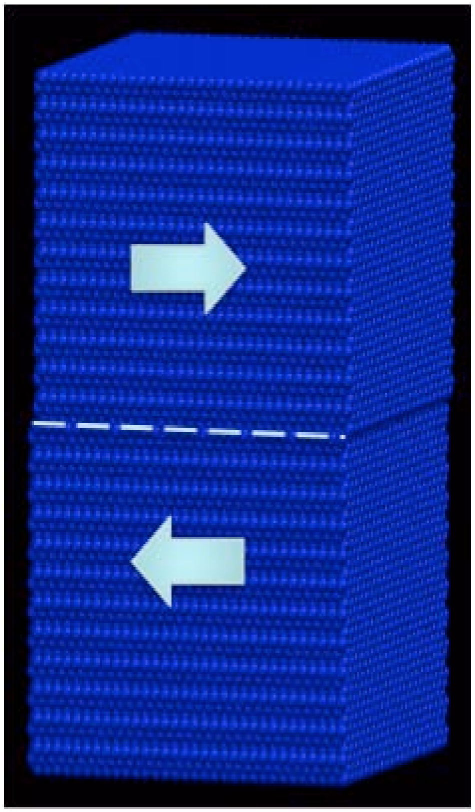
CRSS

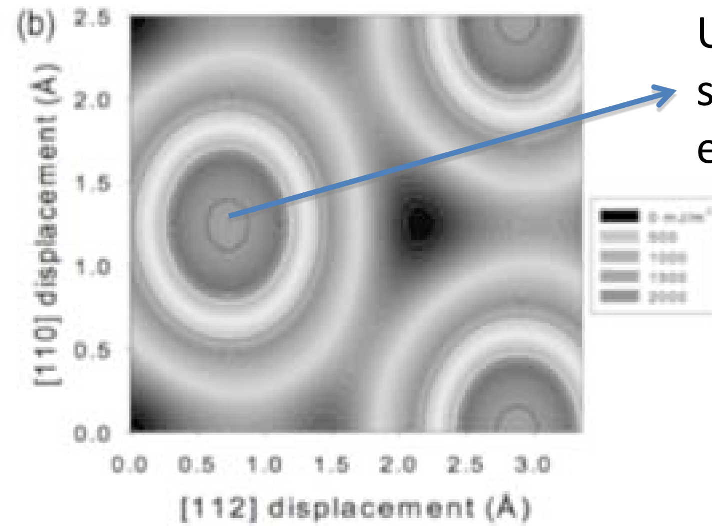


microstructure

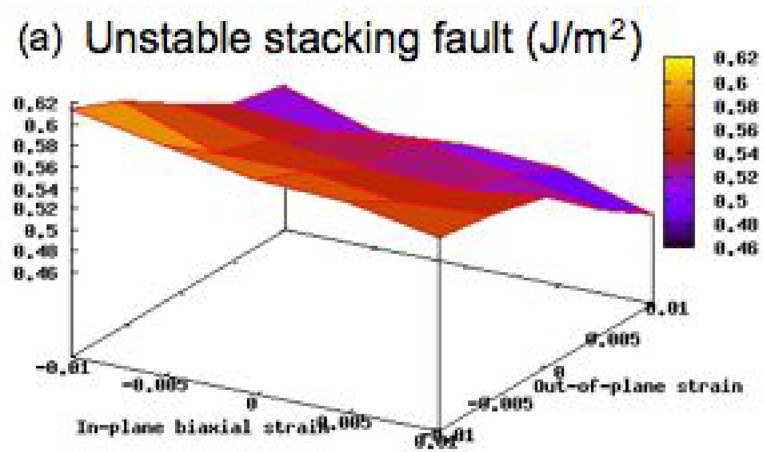


Sensitivity and response functions MD

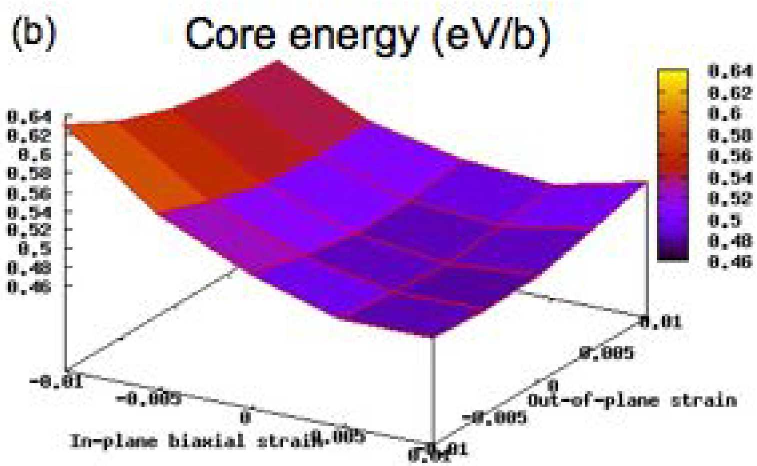


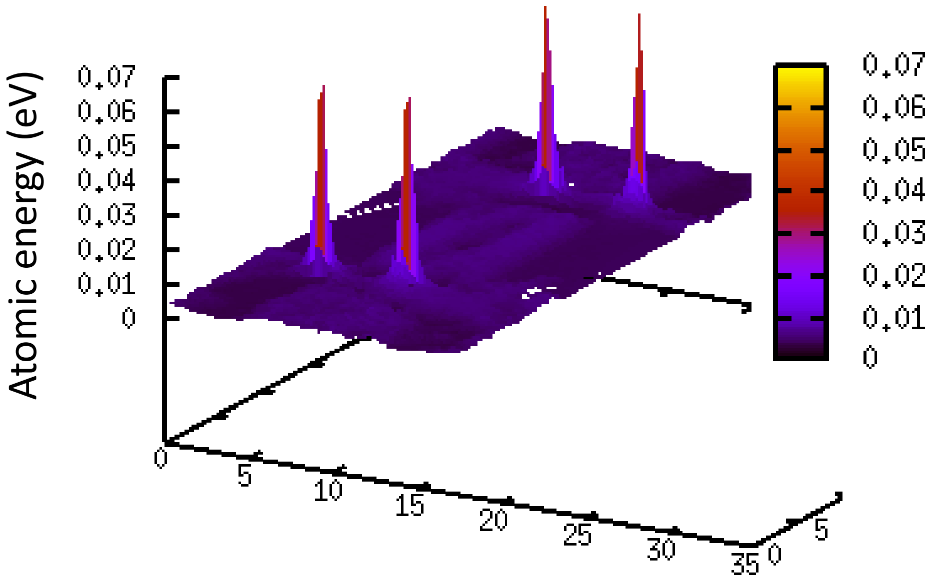


Unstable stacking fault energy

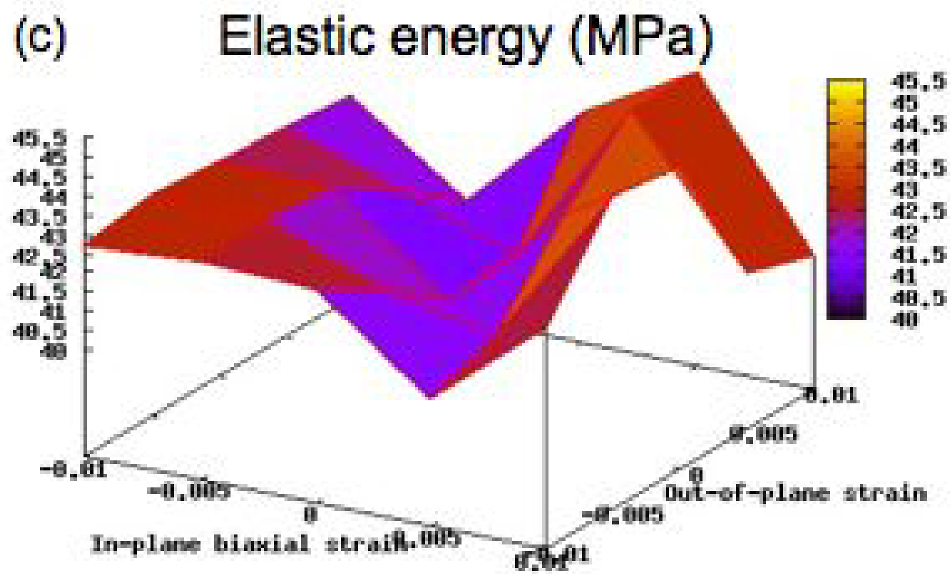


Sensitivity and response functions MD

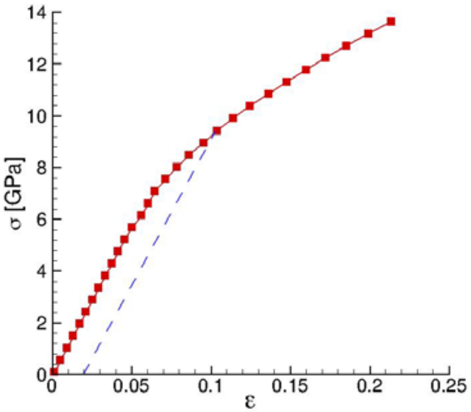




Sensitivity and response functions MD



Sensitivity and response functions FPDD



$$\frac{\partial \xi(\alpha, x)}{\partial t} = -L \frac{\partial E}{\partial \xi(\alpha, x)}$$

$$E = E^{int} + E^{grad} + E^{misfit}$$

$$E^{\text{int}} = \frac{1}{2} \int \hat{A}_{mnuv}(k) \hat{\beta}^{p}_{mn}(k) \hat{\beta}^{p*}_{uv}(k) \frac{d^3 k}{(2\pi)^3}$$

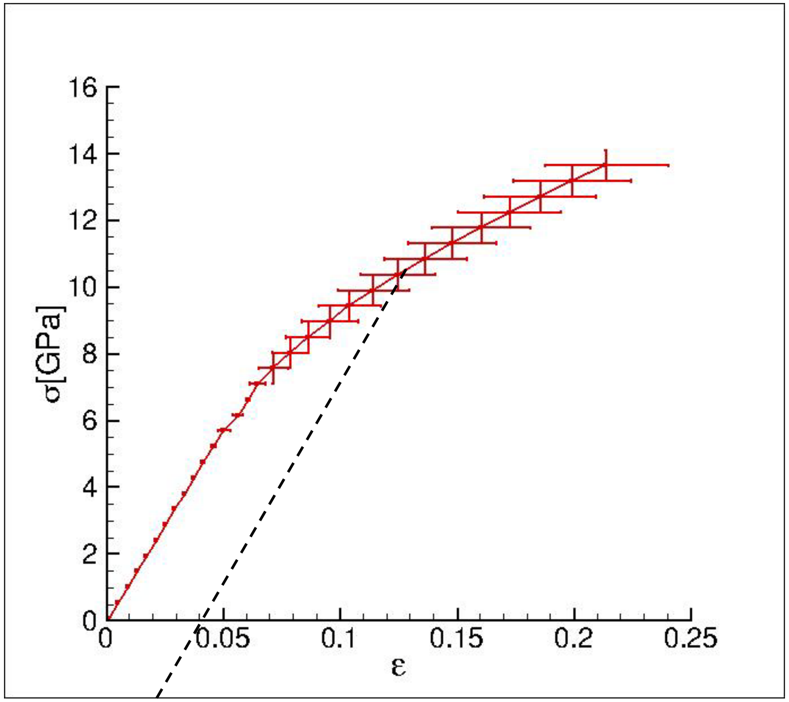
(elastic energy)

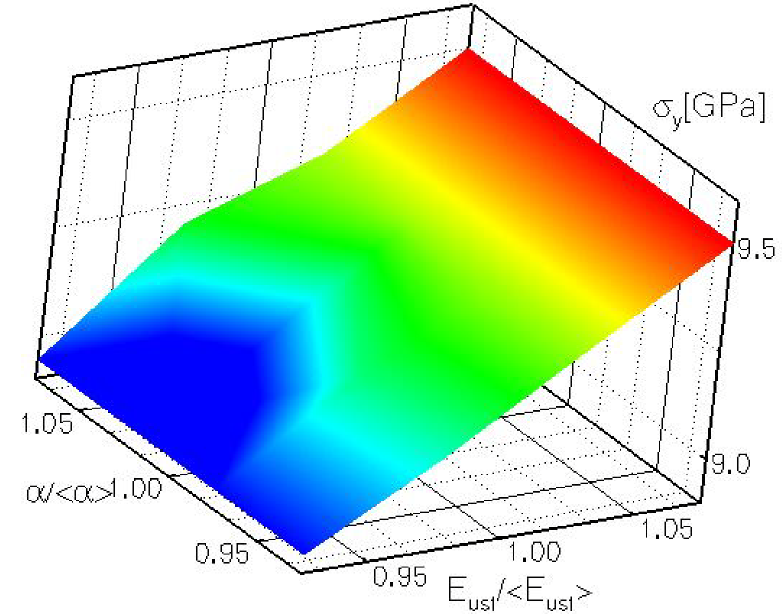
$$E^{grad} = \frac{1}{2} \int \sum_{\alpha\beta} H(\alpha, \beta)_{ijkl} b_i^{\beta} \frac{\partial \xi(\alpha, x)}{\partial x_j} b_k^{\alpha} \frac{\partial \xi(\beta, x)}{\partial x_l} d^3 x$$

$$E^{misfit} = \sum_{\alpha=1}^{N_s} \sum_{n_\alpha=1}^{N} \int \phi_{n_\alpha}(x) d^3 x$$

(unstable stacking fault energy)

Sensitivity and response functions FPDD

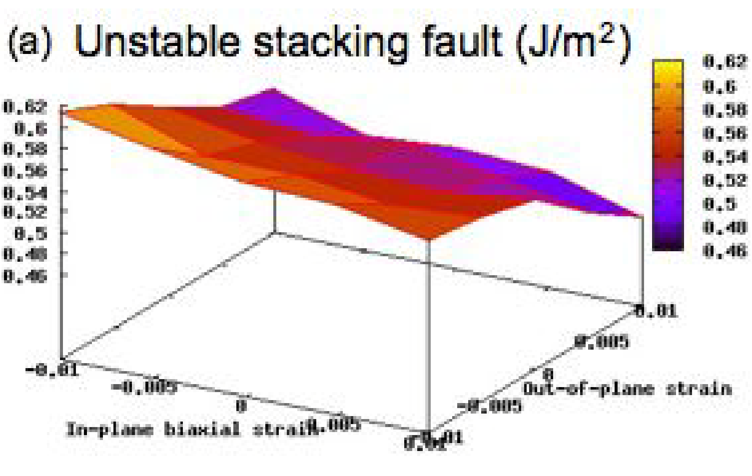


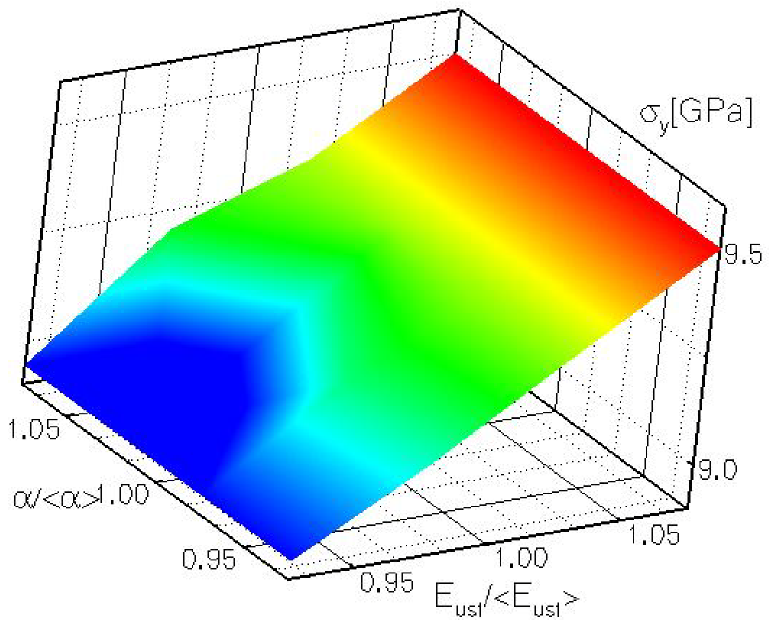


$$< E_{usf} >= 0.56J/m^2,$$

$$\sigma_Y(E_{usf},\alpha) = 9.28GPa + 3.63\left(\frac{E_{usf}}{< E_{usf} >} - 1\right)GPa + 0.07\left(\frac{\alpha}{< \alpha >} - 1\right)GPa$$

UQ across the scales



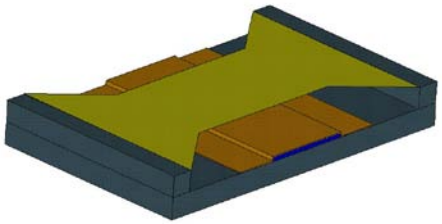


$$E_{USF}(\epsilon_t, \epsilon_l) = 0.541 J/m^2 - 1.67\epsilon_t J/m^2 - 4.75\epsilon_l J/m^2$$

$$\sigma_Y(E_{usf}, \alpha) = 9.28GPa + 3.63\left(\frac{E_{usf}}{< E_{usf} >} - 1\right)GPa + 0.07\left(\frac{\alpha}{< \alpha >} - 1\right)GPa$$

UQ across the scales

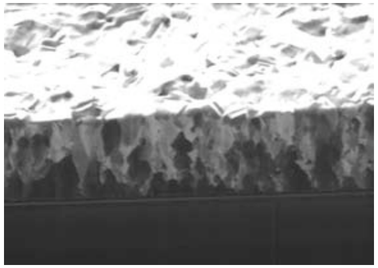
Residual stress



σ_r=25MPa
Standard deviation 19MPa

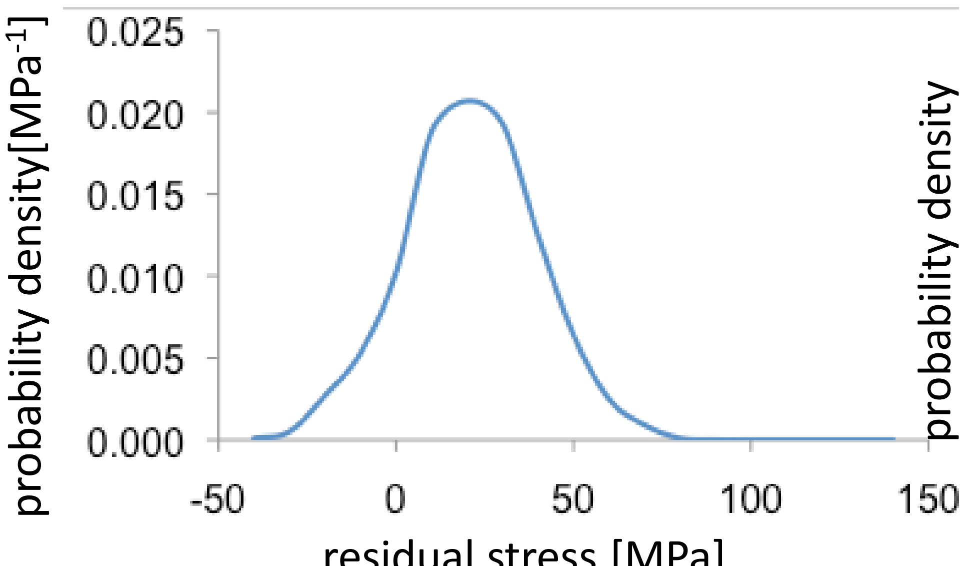
Alexenko, et al., 2010

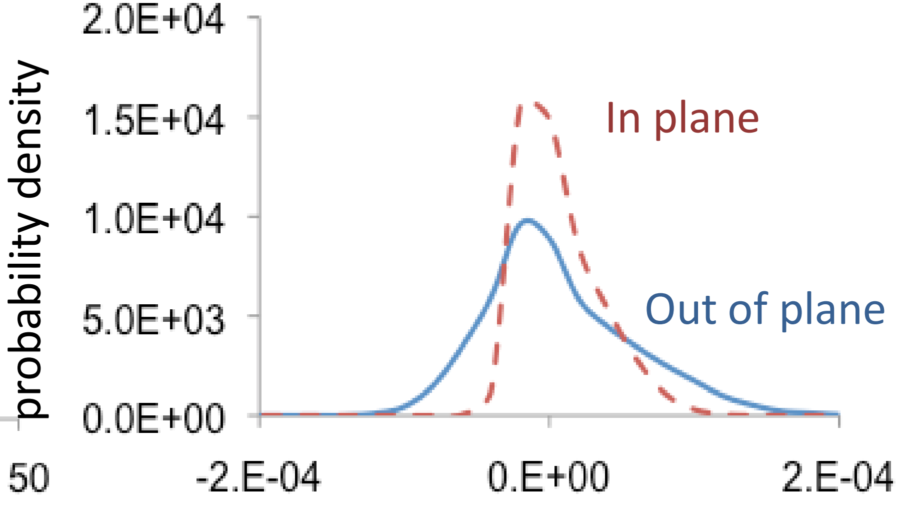
Strain distribution



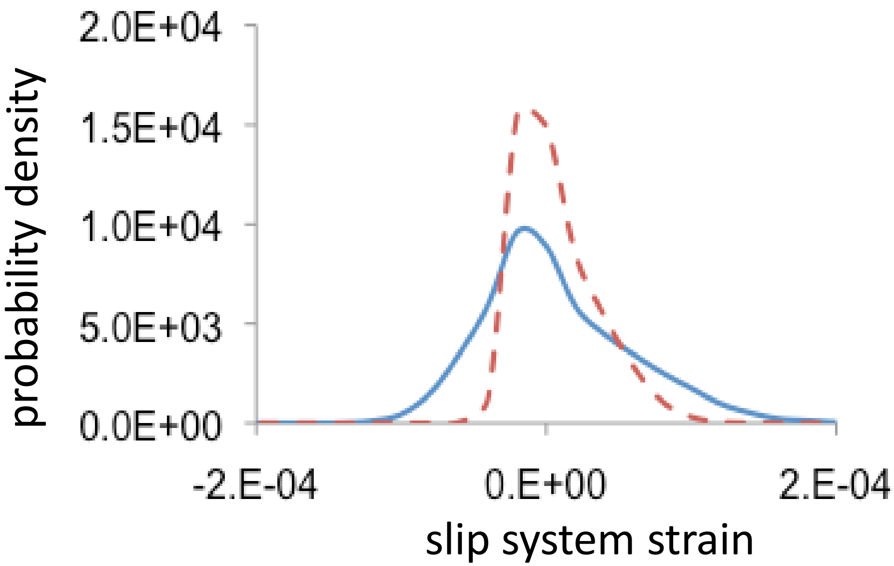
Cantwell and Stach

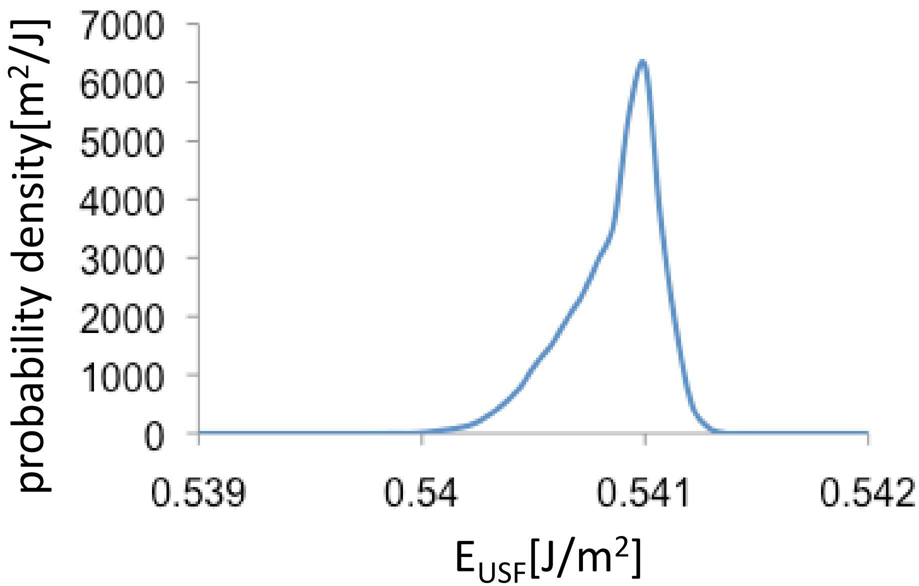
Distribution of grains with [001] orientation and random orientation in xy plane.





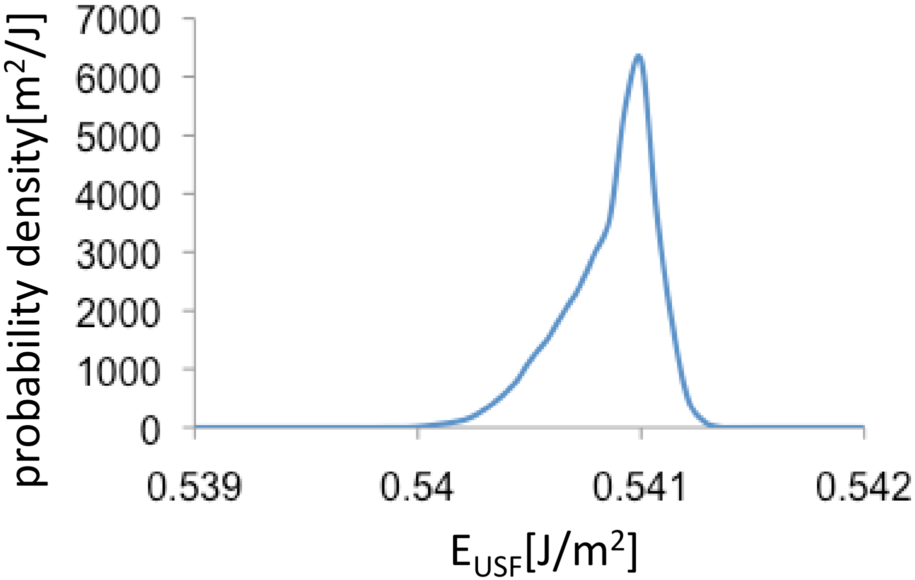
UQ across the scales

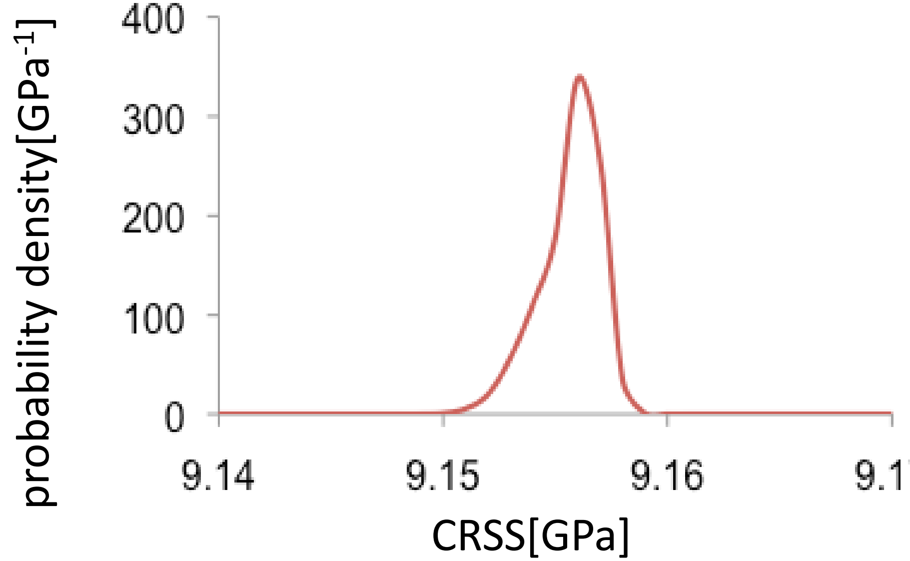




$$E_{USF}(\epsilon_t, \epsilon_l) = 0.541 J/m^2 - 1.67\epsilon_t J/m^2 - 4.75\epsilon_l J/m^2$$

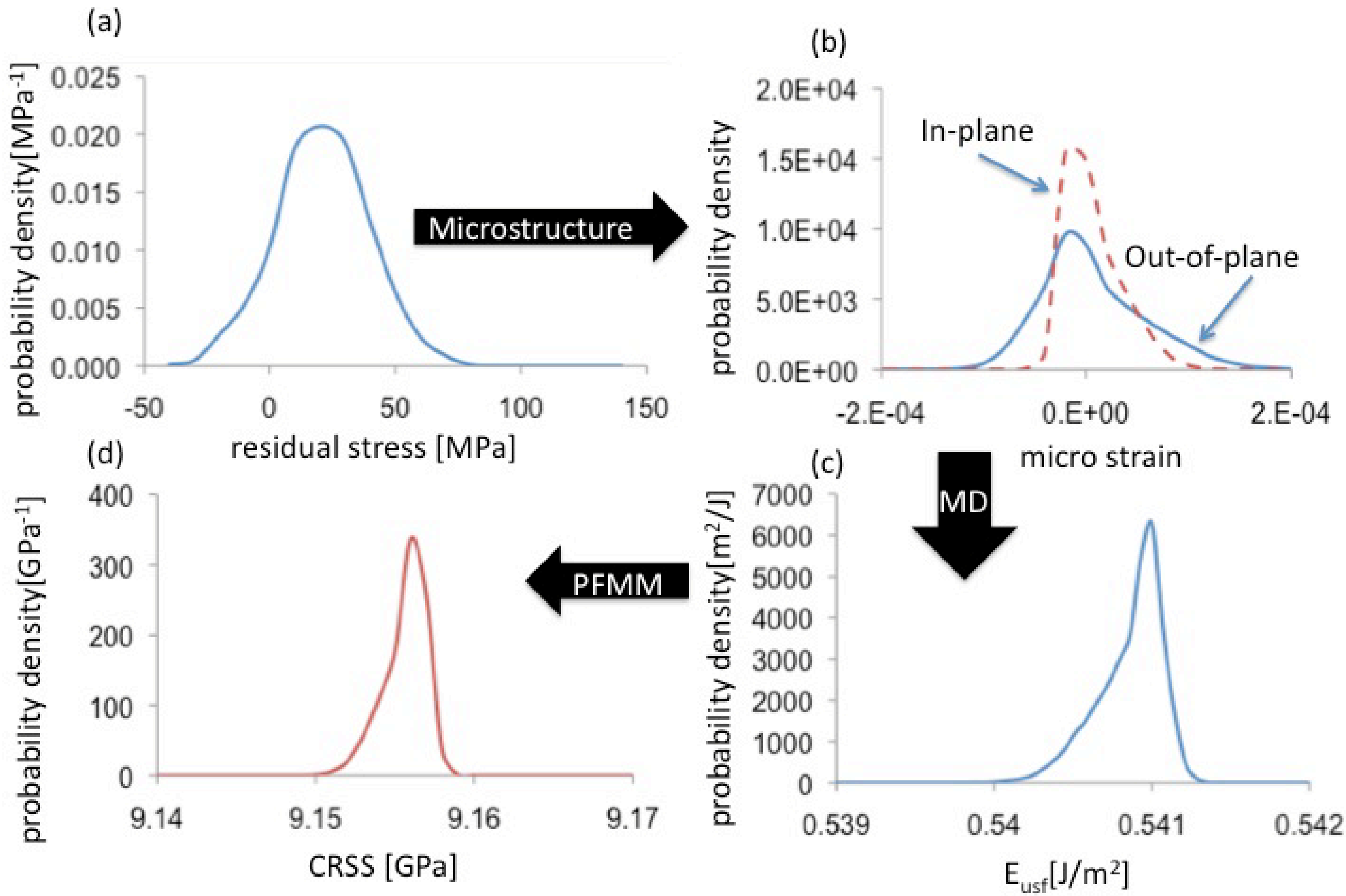
UQ across the scales





$$\sigma_Y(E_{usf}, \alpha) = 9.28GPa + 3.63\left(\frac{E_{usf}}{< E_{usf} >} - 1\right)GPa + 0.07\left(\frac{\alpha}{< \alpha >} - 1\right)GPa$$

UQ across the scales



Summary

- Uncertainties across scales in a multiscale plasticity model
- From atomistics to macroscopic scale.
- For 4nm grains CRSS = 9GPa
- Change in the CRSS is 15MPa