# Simulation of plastic deformation of surfaces under high electric field

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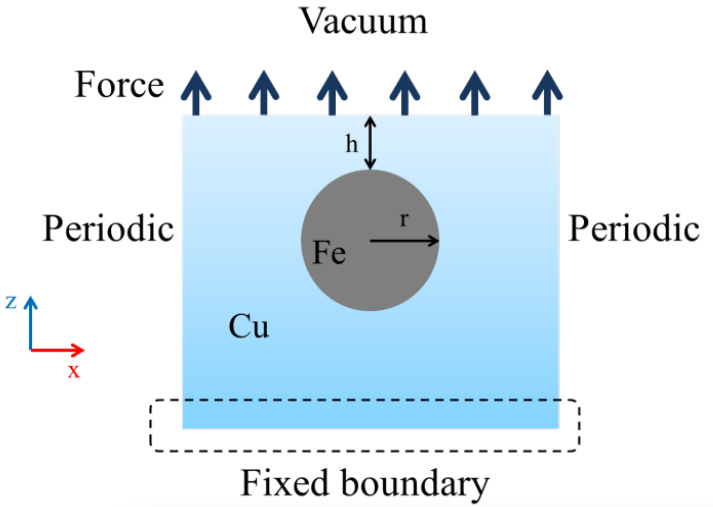
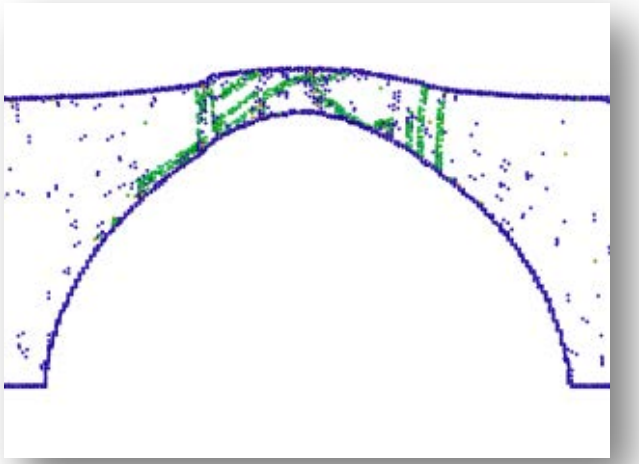
# Outline

- Introduction and motivation
- Fe precipitate effect on surface geometry
  - Void formation near precipitate
  - Internal stress distribution
- Dynamic rising tip simulations in FEM and MD
- Stress near surfaces in FEM
  - Validation of FEM surface stress model

# MD simulations with voids and precipitates

- Near-surface voids are dislocation nucleation sites under external stress.
- Dislocations propagate to the surface and result in surface modification and protrusion growth.
- Study dislocation nucleation and surface geometry modification with other defects.
  - Dislocations on precipitates
  - Stress distribution around voids

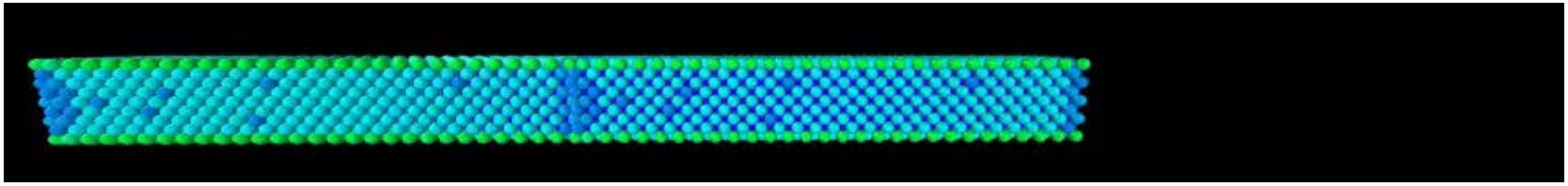


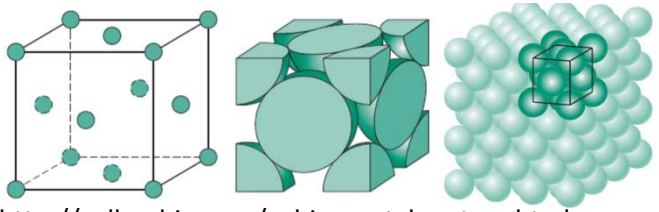


Pohjonen et al. 2013 *J. Appl. Phys.* **114** 033519

# Method - molecular dynamics



- Classical molecular dynamics with LAMMPS, PARCAS and HELMOD
- Interactions between atoms governed by Newton's equations
- Exaggerated external forces are often needed to achieve reasonable calculation time
- EAM potentials for Cu

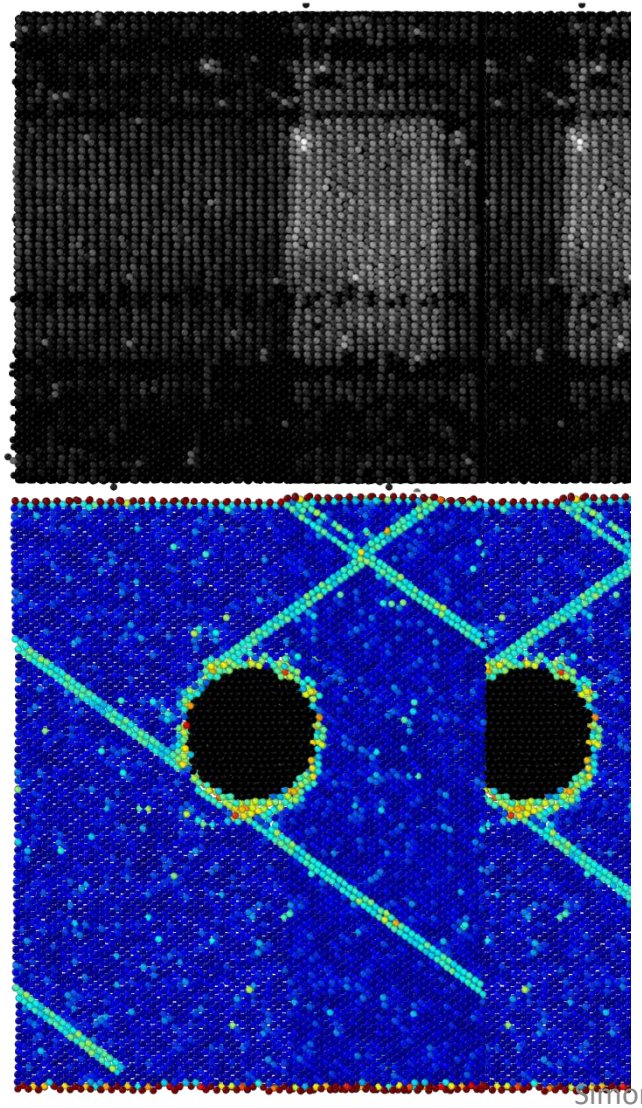


http://galleryhip.com/cubic-crystal-system.html

Anisotropic properties due to FCC crystal structure of Cu

$$E = \frac{1}{2}\sum_{\substack{i,j=1 \\ j\neq i}}^{N} V_{t_i t_j}(r_{ij}) + \sum_{i=1}^{N} F_{t_i}(\rho_i)$$

# Fe precipitate - plateau formation



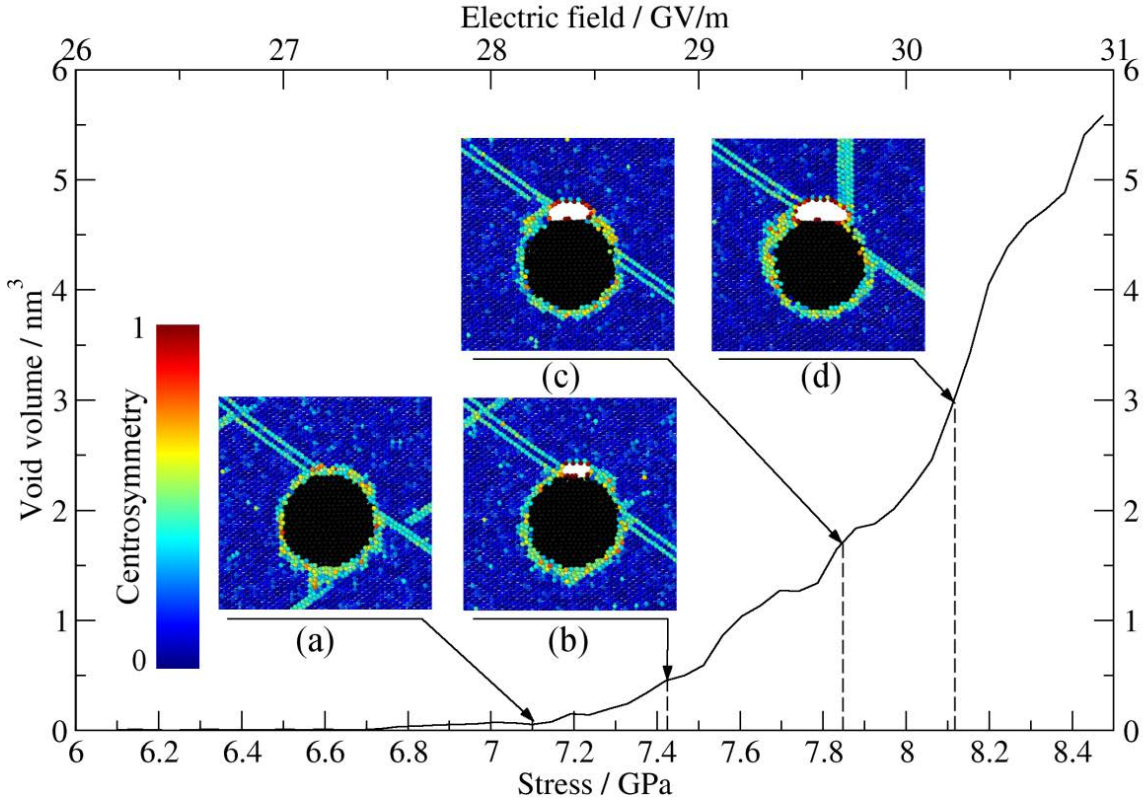
- Dislocations nucleate around the precipitate at relatively high external stress.
- Plateau forms on the surface from the interaction of two precipitates (here periodic images)
- The plateau can grow with increasing stress.

7.15 GPa (28.4 GV/m) 7.15 GPa (28.4 GV/



S. Vigonski *et al.*, *Modelling Simul. Mater. Sci. Eng.*, vol. 23, no. 2, p. 025009, Mar. 2015.

# Fe precipitate - void formation

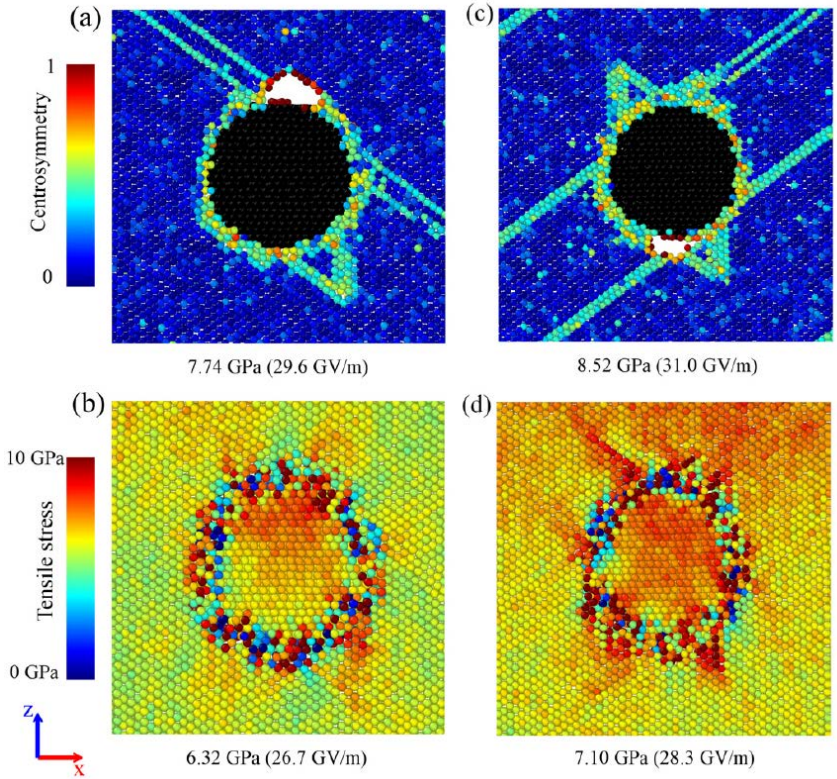



- At high stresses voids appear at the Fe-Cu interface.
- The volume grows until material failure



S. Vigonski *et al.*, *Modelling Simul. Mater. Sci. Eng.*, vol. 23, no. 2, p. 025009, Mar. 2015.

# Fe precipitate – internal stress distribution

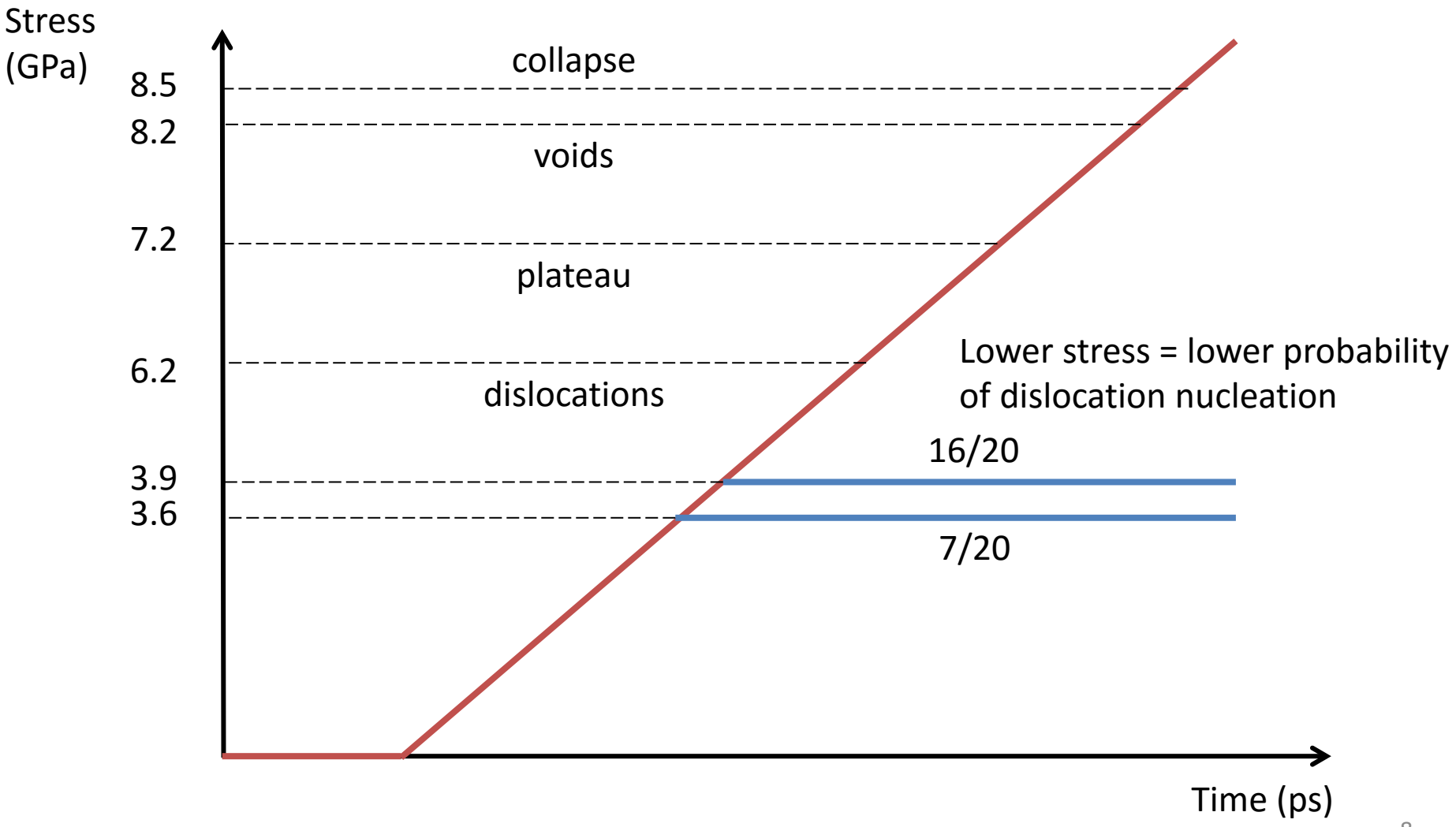



- Stress is concentrated around the precipitate.
- Stress concentrations result in dislocation nucleation and voids.
- Noise due to thermal motion of atoms.

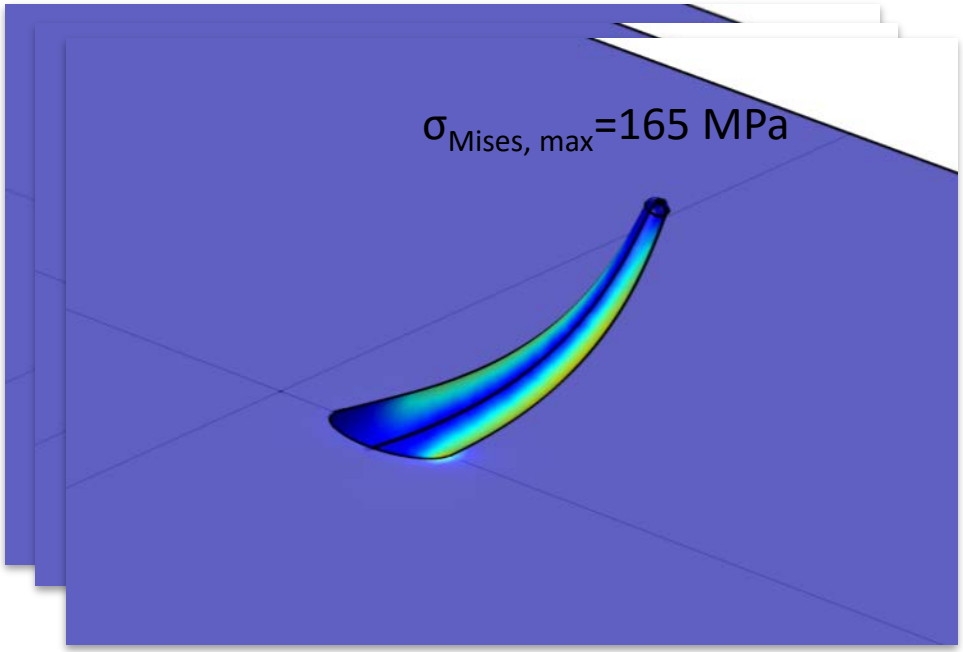


S. Vigonski *et al.*, *Modelling Simul. Mater. Sci. Eng.*, vol. 23, no. 2, p. 025009, Mar. 2015.

# Fe precipitate – effects of external stress

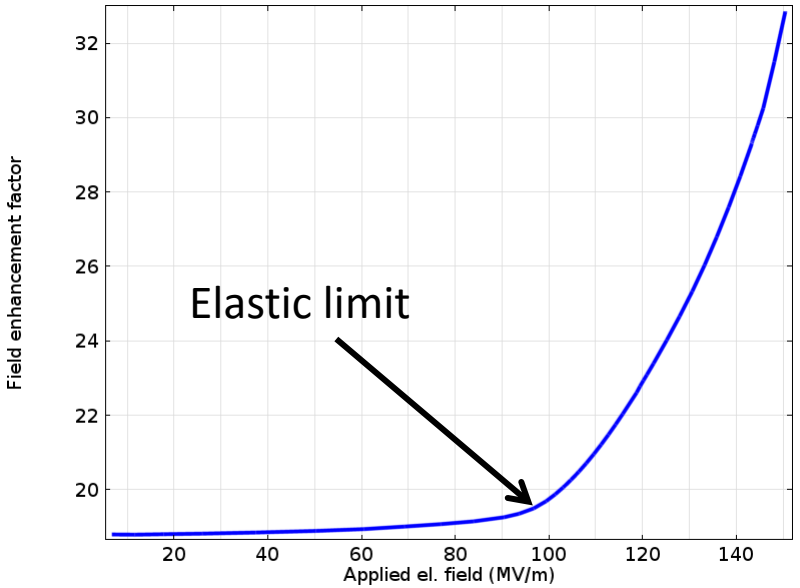


# Rising tip in electric field




- Field emitting tip, rising from the surface is assumed
- Simulation starts when the emitter angle is ~40°
- Simulation ends when fast increase of field enhancement factor starts

- Dynamic behavior of field enhancement factor
- Elastic deformation up to ~90MV/m
- Corresponding field enhancement factor ~20
- Field enhancement factor increases as the tip curves upwards

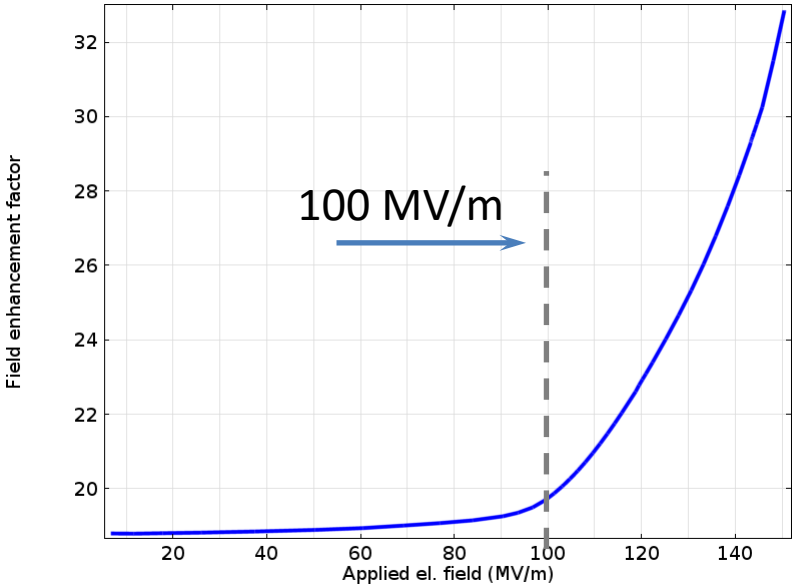


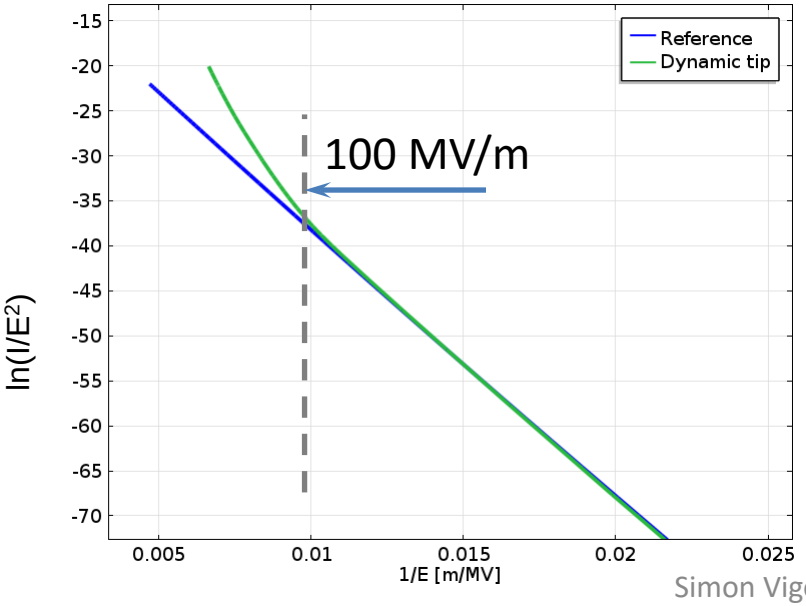
# Field enhancement by „dynamic tip“

- Comparison of static (reference) and dynamic emitters
  - Static emitter does not change shape during the simulation
  - Dynamic emitter deforms elastoplastically

$\gamma$ - slope

$$\beta = \frac{6.53x10^3 \cdot \phi^{3/2}}{\gamma}$$



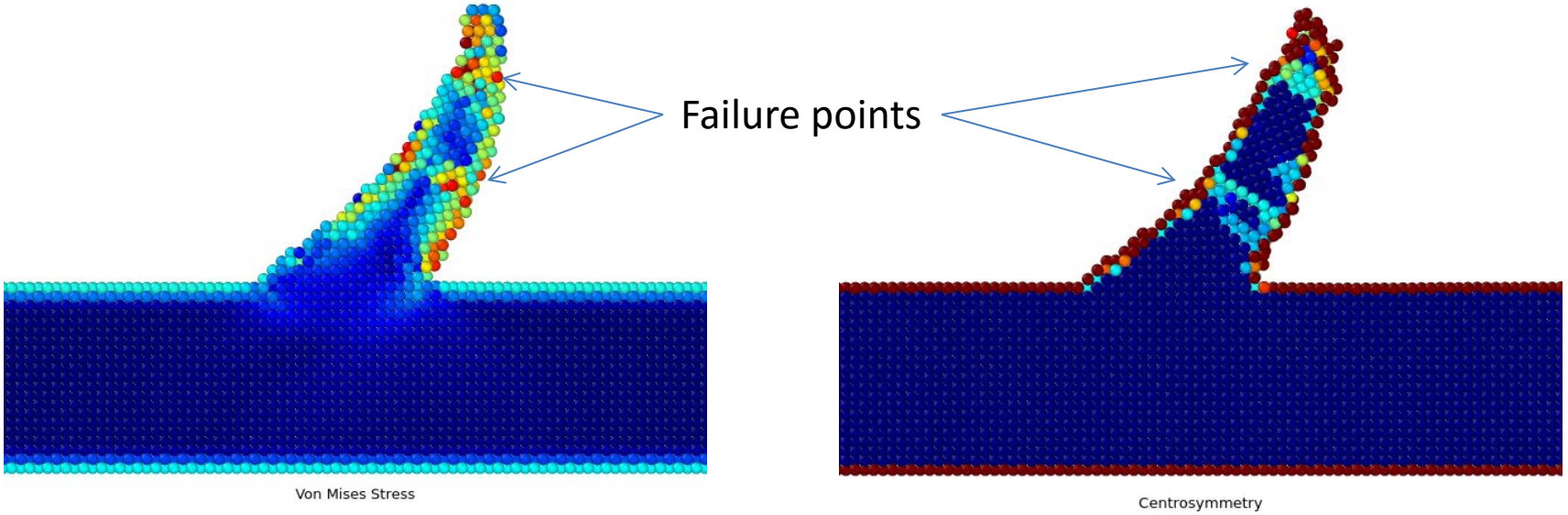

| | Direct calculation from simulation | From FN plot |
|---|---|---|
| Beta from static tip | 18 | 22 |
| Beta from dynamic tip | 18-33 | 11.5 |

- Apparent beta decreases 2-3 times during dynamic deformation of emitter
- Instead of growing emitters, we have decreasing emitters?
- Evaporation of surface protrusions?

# MD simulations of rising tip

Molecular statics with LAMMPS – applied strain + stress calculation

PARCAS + HELMOD – dynamic field calculation



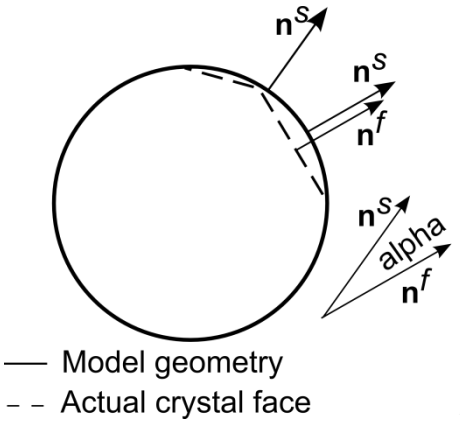

- Nanoscale material behaviour in MD
- Thermal motion problematic in dynamic field calculations
- Similar results for low-temperature dynamic field and energy minimization-based strain simulation

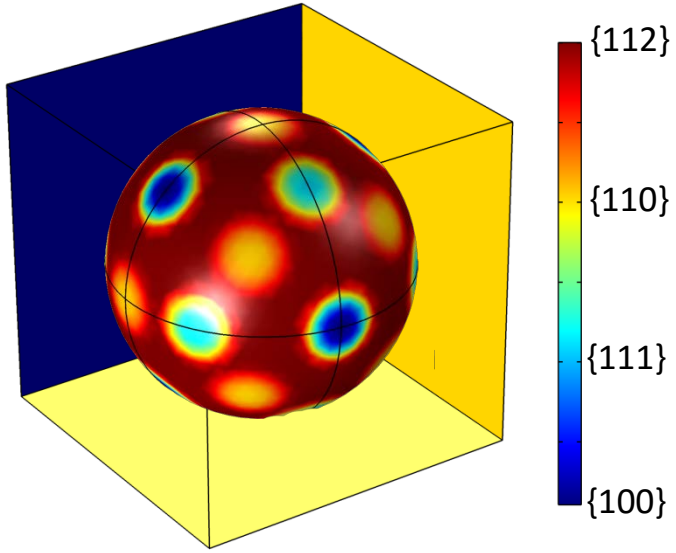
# Surface stress using FEM

- Elastic deformation of material, simulation of large strains:
  - Anisotropic bulk material model
  - Surface stess is calculated using thin layer aproximation in boundary layers
  - Surface parameters are isotropic but crystal face dependent
- Crystal faces detected algorithmically:
  - Ability to simulate arbitrary shapes
  - Only crystal orientation is needed to intialize the simulation
- Initial surface stress and elastic parameters of surface from MD simulations
- Fully copled surface and bulk stress model

| | Stress | Strain |
|---|---|---|
| Bulk model | $S = C : \varepsilon^b$ | $\varepsilon = \frac{1}{2}(F^T F - I)$ |
| Surface model | $\tau_{ij} = \tau_{ij}^0 + S_{ijkl}\varepsilon_{kl}^s$ | |

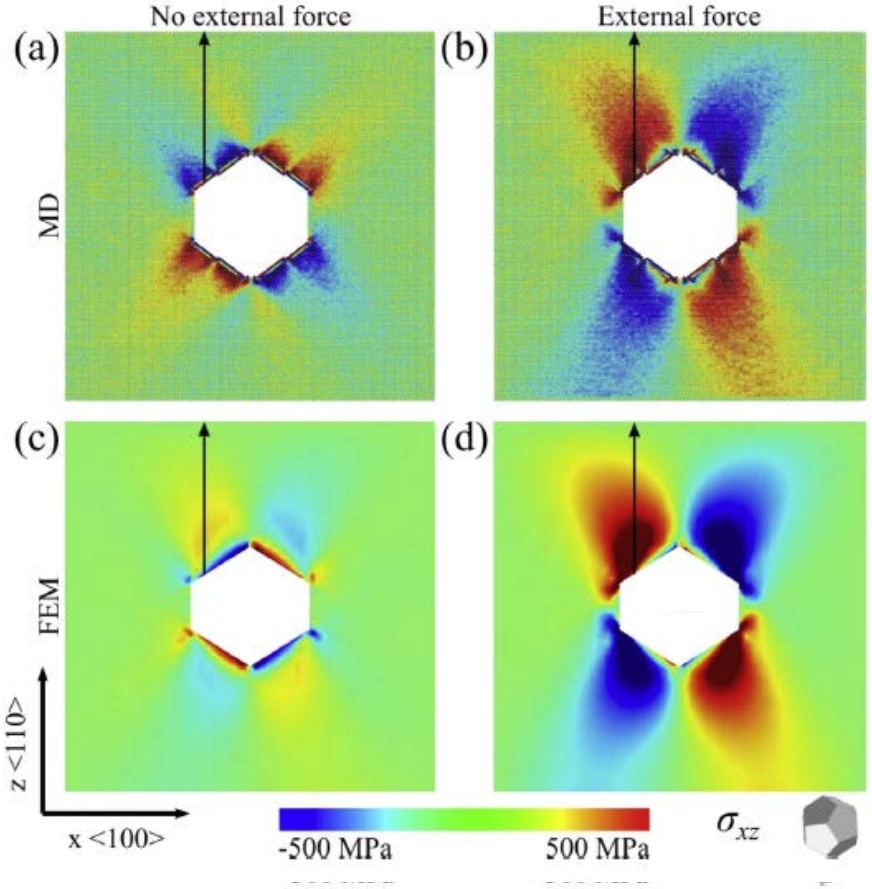
Crystal face detection



# Surface stress model for FEM

- Finite element method is useful for calculating stress, but doesn't take into account nanoscale effects.
- We add a surface stress component to increase accuracy

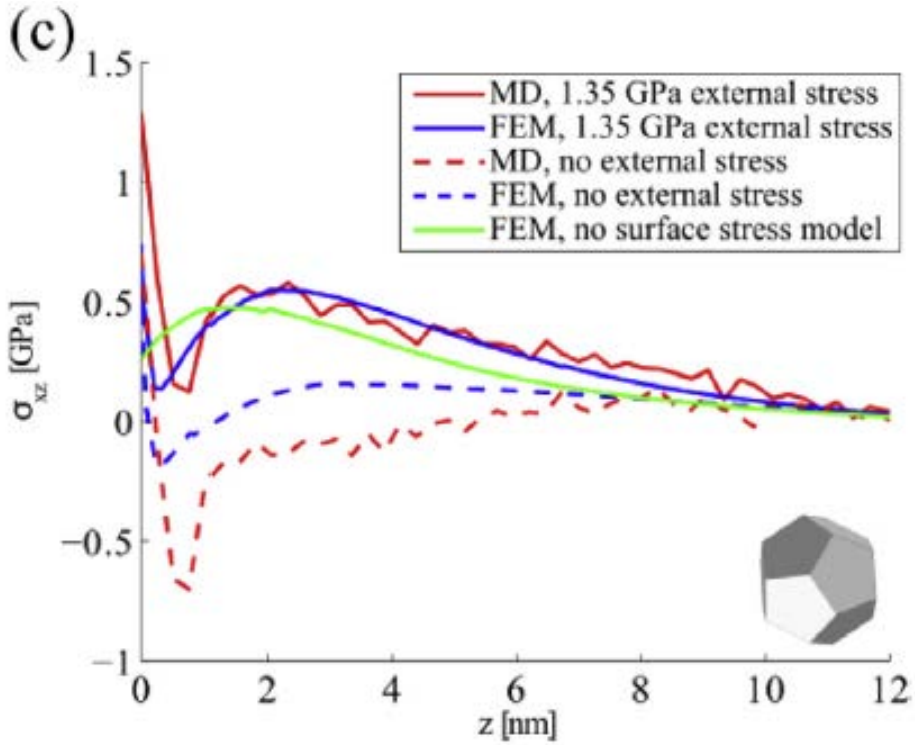



- Comparison with MD under controlled conditions
- Stress changes sign rapidly near the surface
- This effect is accurately captured in FEM model
- Imperfections due to model limitations – only {100}, {110}, {111} and {112} surfaces implemented.



S. Vigonski *et al.*, *Applied Mathematics and Computation, 2015*.

# Surface stress model – quantitative validation



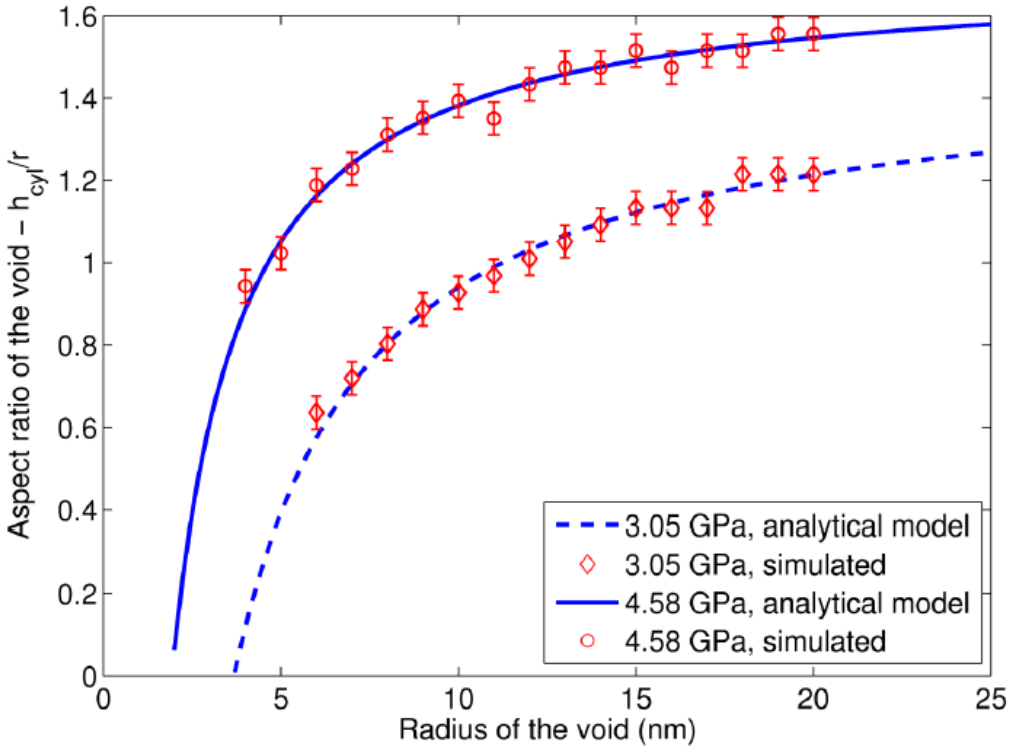

- Stress as a function of the distance from the void surface
- Good agreement between FEM and MD results
- Significant improvement over regular calculation (green line) very close to the void



S. Vigonski *et al.*, *Applied Mathematics and Computation, 2015*.

# Finite size effects in dislocation nucleation

- We use the FEM surface stress model to calculate dislocation nucleation stress.
- Graph: aspect ratio necessary for nucleation vs size of the void
- Aspect ratio = depth of void / radius of void
- At large void sizes independent of radius
- At small sizes strong radius dependence – finite size effects




Analytical model: A.S. Pohjonen *et al.*, Philos. Mag. 92 (2012) 3994.

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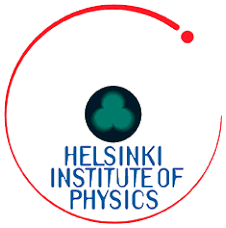

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