2013 LAMMPS Users' Workshop and Symposium
Albuquerque, New Mexico
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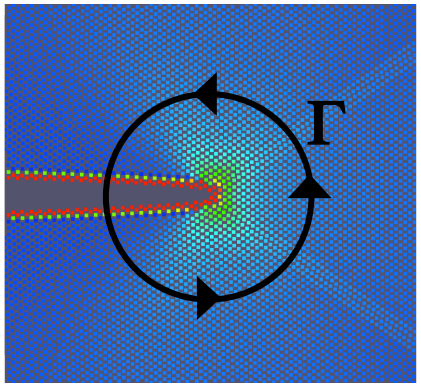

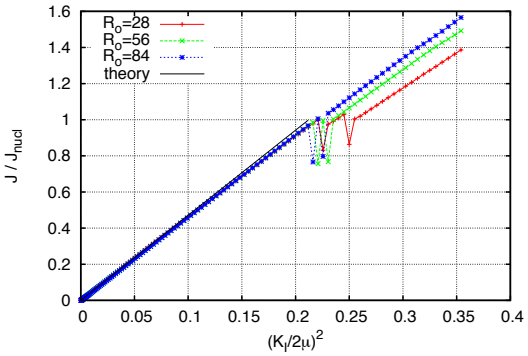

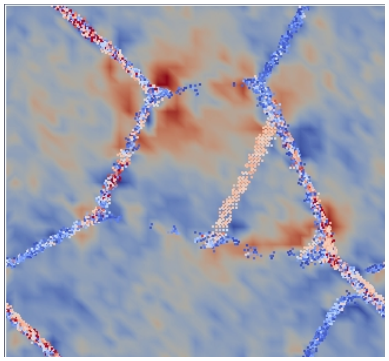

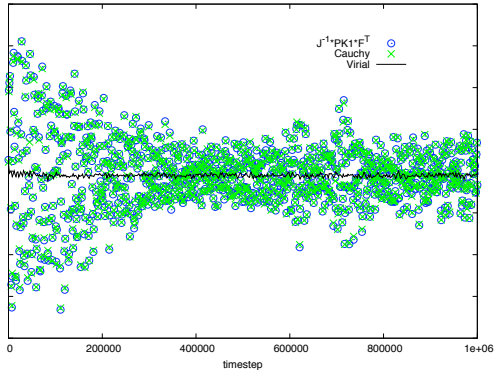

Evaluating Continuum Mechanical Quantities at the Atomic Scale

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NNSA National Nuclear Security Administration

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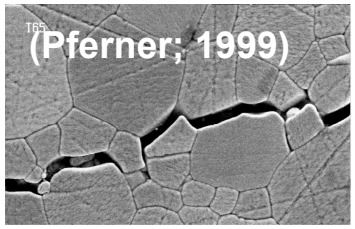
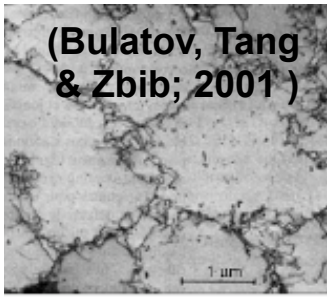
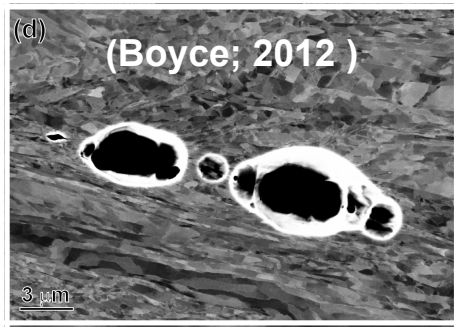
Motivation: Continuum mechanics at the nanoscale

Material deformation and failure occurs at various length scales:

- Brittle and ductile fracture
- Dislocation activity
- Grain boundary sliding
- Stiction, friction and wear







Continuum mechanics-based models to predict failure have been very effective at various length scales (10^{-4} – 10^{2} m) but can/should they work at the nanoscale?

Our premise:

- Define consistent fields from molecular simulation
- Continuum theory

→ nanoscale results

I.e. first connect atomistics to continuum fields in a manner consistent with balance laws, then use continuum theory to analyze the process.

Atomistic-Continuum formulation of R.J. Hardy

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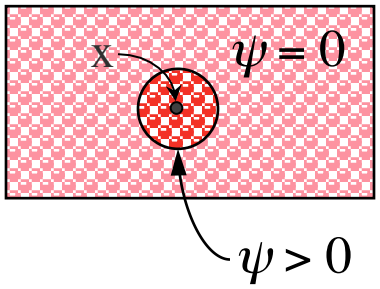
Hardy (*Journal of Chemical Physics*, 1982) -

$$\rho(\mathbf{x},t) = \sum_{\alpha=1}^{N} m^{\alpha}\psi\left(\mathbf{x}^{\alpha}-\mathbf{x}\right) \qquad \mathbf{p}(\mathbf{x},t) = \sum_{\alpha=1}^{N} m^{\alpha}\mathbf{v}^{\alpha}\psi\left(\mathbf{x}^{\alpha}-\mathbf{x}\right)$$

$$E^{0}(\mathbf{x},t) = \sum_{\alpha=1}^{N}\left\{\frac{1}{2}m^{\alpha}\mathbf{v}^{\alpha}\cdot\mathbf{v}^{\alpha}+\phi^{\alpha}\right\}\psi\left(\mathbf{x}^{\alpha}-\mathbf{x}\right) \qquad [\psi] \sim \frac{1}{V_c}$$



Applying these expressions to the spatial forms of the balance laws, *e.g.*

$$\frac{\partial \mathbf{p}}{\partial t} = \frac{\partial}{\partial \mathbf{x}}\cdot\left(\boldsymbol{\sigma} - \rho\mathbf{v}\otimes\mathbf{v}\right) \qquad \text{linear momentum}$$

and separating continuum-scale momentum flux from atomic motion,

$$\hat{\mathbf{v}}^{\alpha}(\mathbf{x},t) = \mathbf{v}^{\alpha}(t) - \mathbf{v}(\mathbf{x},t) \quad \longleftarrow \quad \mathbf{v} \equiv \mathbf{p}/\rho$$

yields an expression for the Cauchy stress tensor:

$$\boldsymbol{\sigma}(\mathbf{x},t) = -\left\{\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{x}^{\alpha\beta}\otimes\mathbf{f}^{\alpha\beta}B^{\alpha\beta}(\mathbf{x}) + \sum_{\alpha=1}^{N} m^{\alpha}\hat{\mathbf{v}}^{\alpha}\otimes\hat{\mathbf{v}}^{\alpha}\psi\left(\mathbf{x}^{\alpha}-\mathbf{x}\right)\right\}$$

Thermal variables (heat flux, temperature) are also part of this formulation.

Now that we have these tools, what can we do with them… ?

Deformation of nanocrystalline Ta

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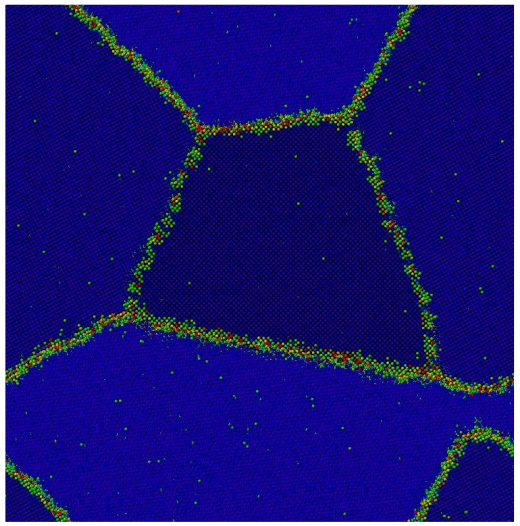
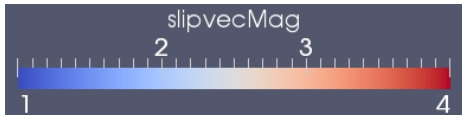
- Objective: Characterize the defects that form during uniaxial tension of a NC-Ta thin film, and use continuum fields to connect their generation to locally "measured" critical stresses.
- Simulation details:
  - EAM by Li *et al.* (Phys. Rev. B, 2003)
  - Simulations done with LAMMPS (http://lammps.sandia.gov)
  - Geometry: thin film of dimensions 34.5 nm x 34.5 nm x 7 nm
  - 3 columnar grains of size 20 nm with random orientations
  - Approximately 464,000 atoms
  - Equilibration via heating to 1700K for 200 ps,
    then cooling to 300K for 200 ps,
    using a Nosé-Hoover thermostat
  - Uniaxial stress applied at strain rates 10^5 to 10^9 sec^{-1}

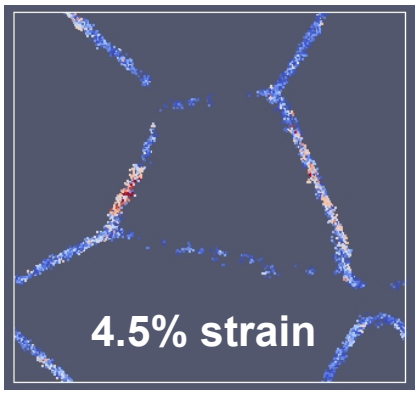


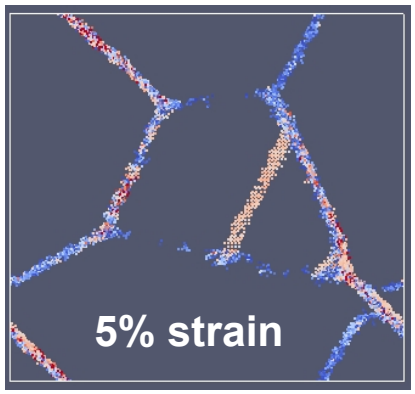
Deformation of nanocrystalline Ta

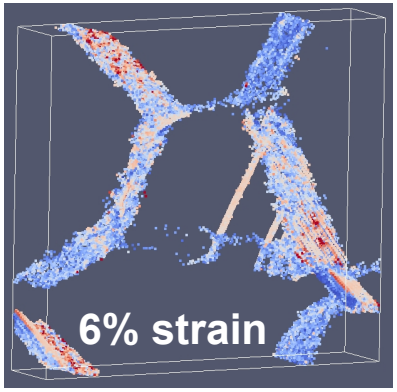
- First active mechanism is dislocation emission from grain boundaries:

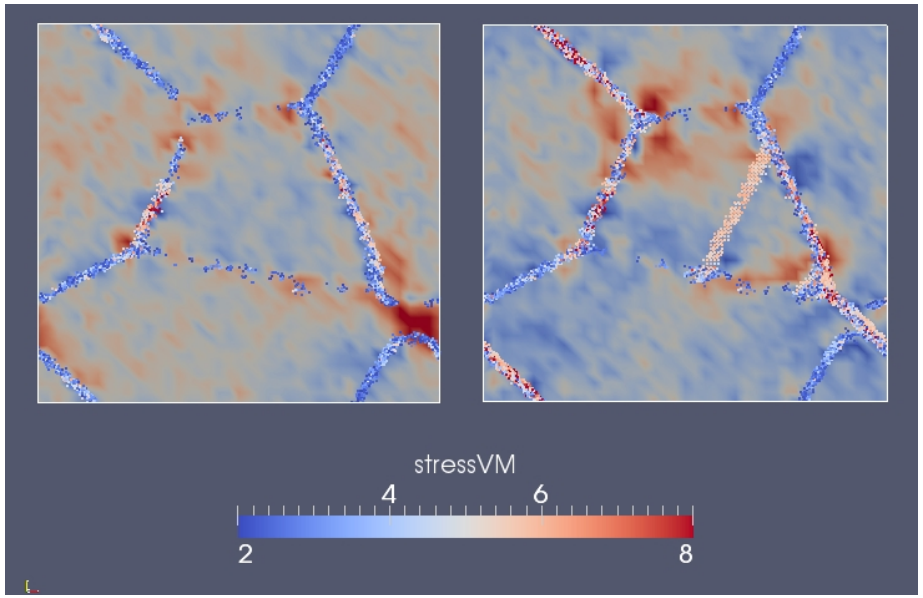
$$\dot{\varepsilon} = 10^{6}\ \text{sec}^{-1}$$











- Cauchy stress expression can be used to correlate local evaluations of stress (Von Mises) with defect nucleation sites.
- Stresses where defects form are significant in some places, but not in others.
- Emission events may indicate ‘weak spots’ on grain boundaries.

Material frame version of Hardy formulation

Material frame balance laws:

$$\frac{d\rho_0}{dt} = 0 \qquad \rho_0 \frac{d\mathbf{v}}{dt} = \frac{d\mathbf{p}_0}{dt} = \mathrm{Div}(\mathbf{P}) + \rho_0 \mathbf{b} \qquad \rho_0 \frac{d\varepsilon}{dt} = \mathbf{P} : \dot{\mathbf{F}} - \mathrm{Div}(\mathbf{Q}) + \rho_0 h$$

Densities:

$$\rho_0(\mathbf{X}) = \sum_{\alpha=1}^{N} m^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X})$$

$$\mathbf{p}_0(\mathbf{X}, t) = \sum_{\alpha=1}^{N} m^\alpha \mathbf{v}^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X})$$

$$\rho_0 e(\mathbf{X}, t) = \sum_{\alpha=1}^{N} \left\{ \frac{1}{2} m^\alpha (v^\alpha)^2 + \phi^\alpha \right\} \psi(\mathbf{X}^\alpha - \mathbf{X}) \qquad e = \varepsilon + \frac{1}{2} v^2$$

Substitute densities into balance laws and do a lot of math…

Resulting variables

$$\mathbf{v} = \frac{\sum_{\alpha=1}^{N} m^{\alpha}\mathbf{v}^{\alpha}\psi(\mathbf{X}^{\alpha}-\mathbf{X})}{\sum_{\alpha=1}^{N} m^{\alpha}\psi(\mathbf{X}^{\alpha}-\mathbf{X})} \longrightarrow \mathbf{u}(\mathbf{X},t) = \frac{\sum_{\alpha=1}^{N} m^{\alpha}\mathbf{u}^{\alpha}\psi(\mathbf{X}^{\alpha}-\mathbf{X})}{\sum_{\alpha=1}^{N} m^{\alpha}\psi(\mathbf{X}^{\alpha}-\mathbf{X})}$$

$$\nabla_{\mathbf{X}}\mathbf{u} = \sum_{I=1}^{M} \nabla_{\mathbf{X}} N_I(\mathbf{X}) \otimes \mathbf{u}(\mathbf{X}_I,t) \qquad \mathbf{F}(\mathbf{X},t) = \mathbf{1} + \nabla_{\mathbf{X}}\mathbf{u}$$

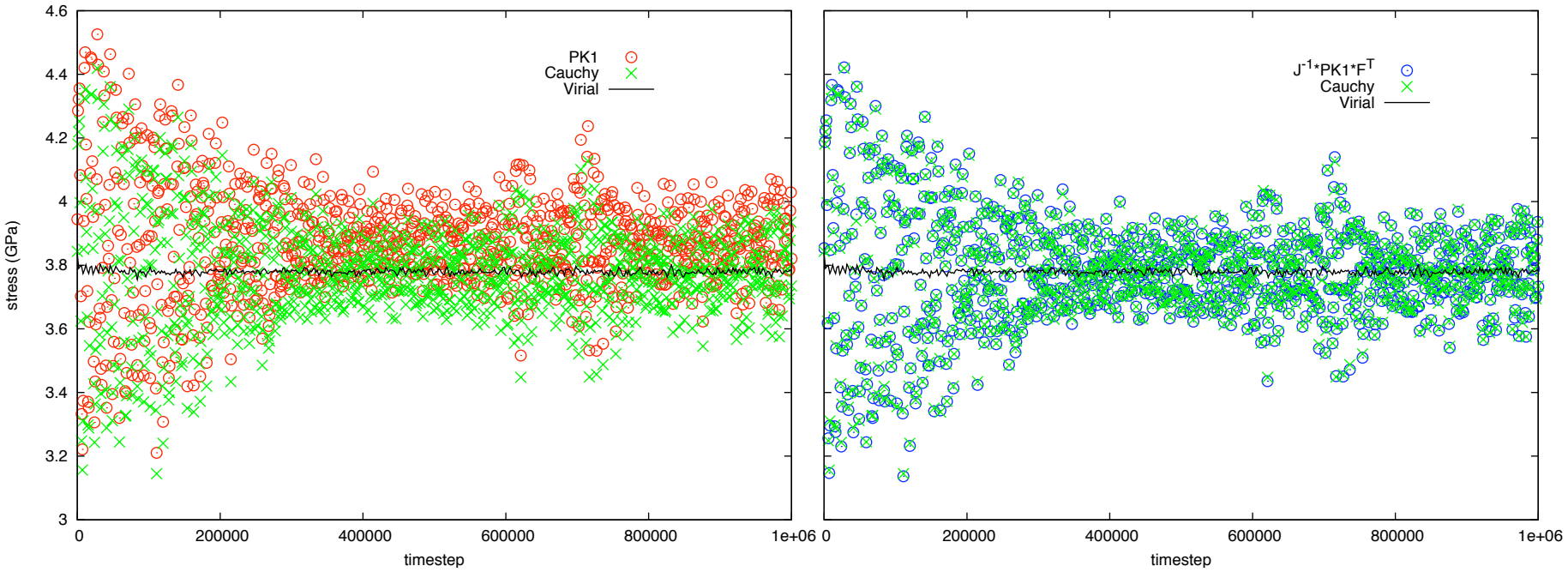
$$\mathbf{P} = -\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \mathbf{X}^{\alpha\beta} B^{\alpha\beta}(\mathbf{X}) \qquad \mathbf{b} = \frac{\sum_{\alpha=1}^{N} m^{\alpha}\mathbf{b}^{\alpha}\psi(\mathbf{X}^{\alpha}-\mathbf{X})}{\sum_{\alpha=1}^{N} m^{\alpha}\psi(\mathbf{X}^{\alpha}-\mathbf{X})}$$

$$\mathbf{Q} = -\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N} \left(\frac{\partial \phi^{\beta}}{\partial x^{\alpha\beta}} \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} \cdot \hat{\mathbf{v}}^{\alpha} \right) \mathbf{X}^{\alpha\beta} B^{\alpha\beta}(\mathbf{X}) \qquad h = \frac{\sum_{\alpha=1}^{N} m^{\alpha}\mathbf{b}^{\alpha}\cdot\hat{\mathbf{v}}^{\alpha}\psi(\mathbf{X}^{\alpha}-\mathbf{X})}{\sum_{\alpha=1}^{N} m^{\alpha}\psi(\mathbf{X}^{\alpha}-\mathbf{X})}$$

$$\mathbf{f}^{\alpha\beta} \equiv \left(\frac{\partial \phi^{\alpha}}{\partial x^{\alpha\beta}} + \frac{\partial \phi^{\beta}}{\partial x^{\alpha\beta}} \right) \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}$$

Is P consistent with Hardy's Cauchy stress?

Volume expansion of 1% at 100K and zero pressure



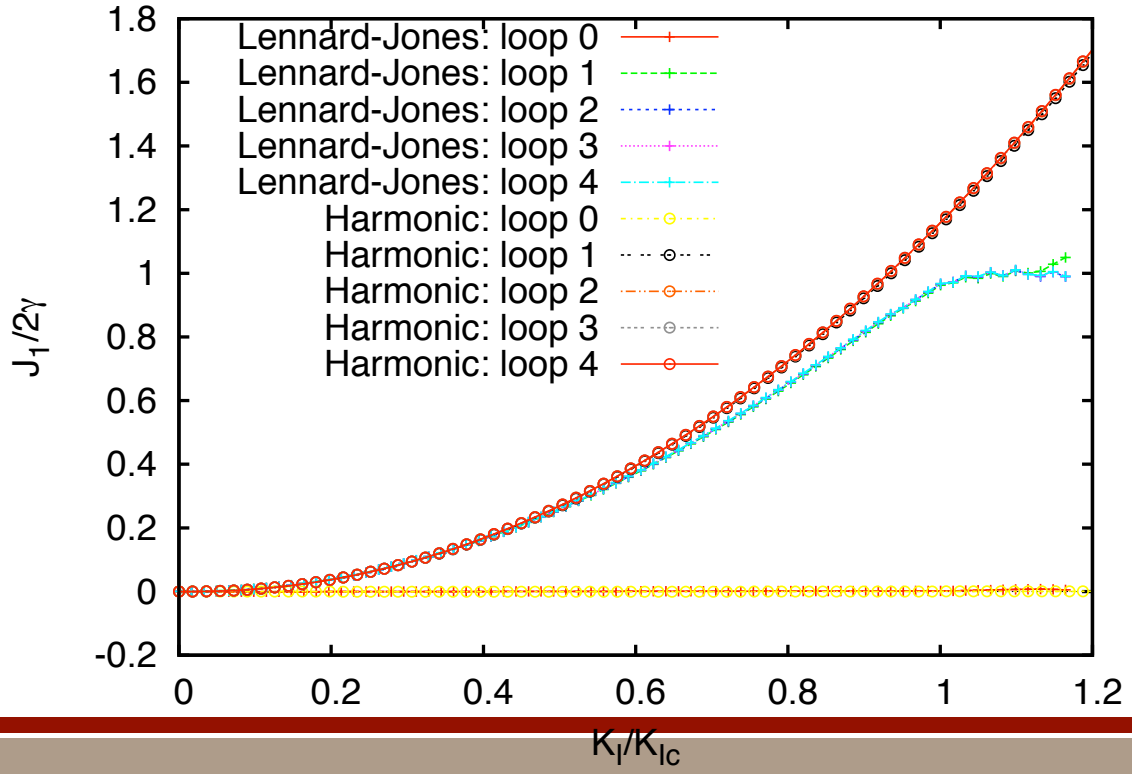
- Simulations show consistency between σ and **P** instantaneously in time.
- Both σ and transformed **P** show consistency with system virial, but display a larger range of variation (± 0.3 GPa after 300,000 timesteps [300 ps] of equilibration).

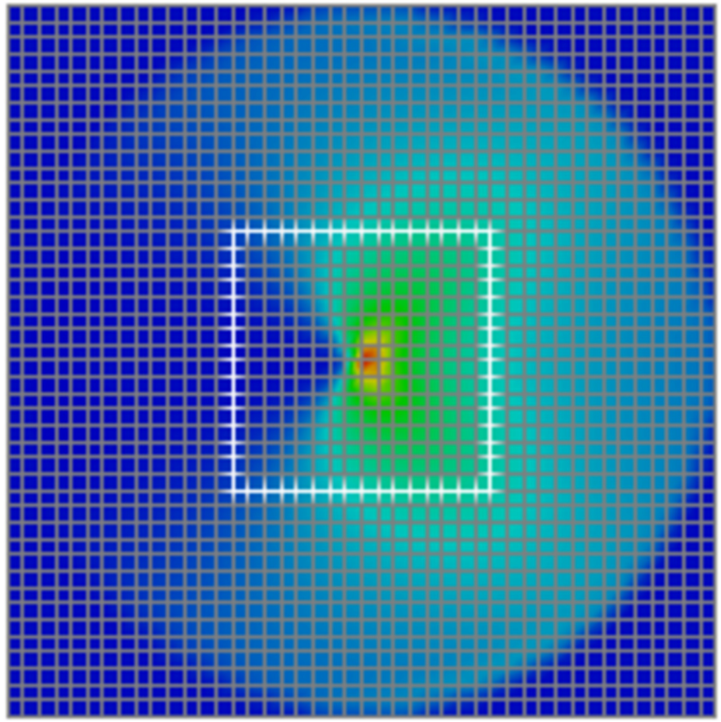
J-integral analysis for quasi-static crack initiation

Quasi-static analysis shows:

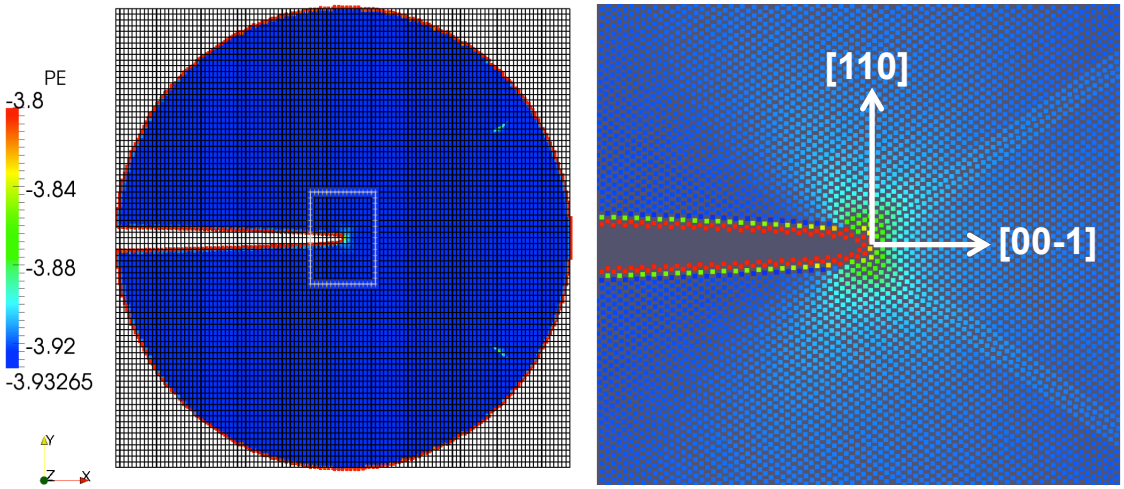
- path independency of J integral
- agreement with LEFM for Harmonic material
- fracture occurs when J = 2γ for materials of finite strength

$$\mathbf{J} = \int_{\Gamma_0} \mathcal{S} \cdot \mathbf{N} ds = \int_{\Gamma_0} \left(W_0 \mathbf{N} - \mathbf{F}^T \cdot \mathbf{P} \cdot \mathbf{N} \right) ds$$



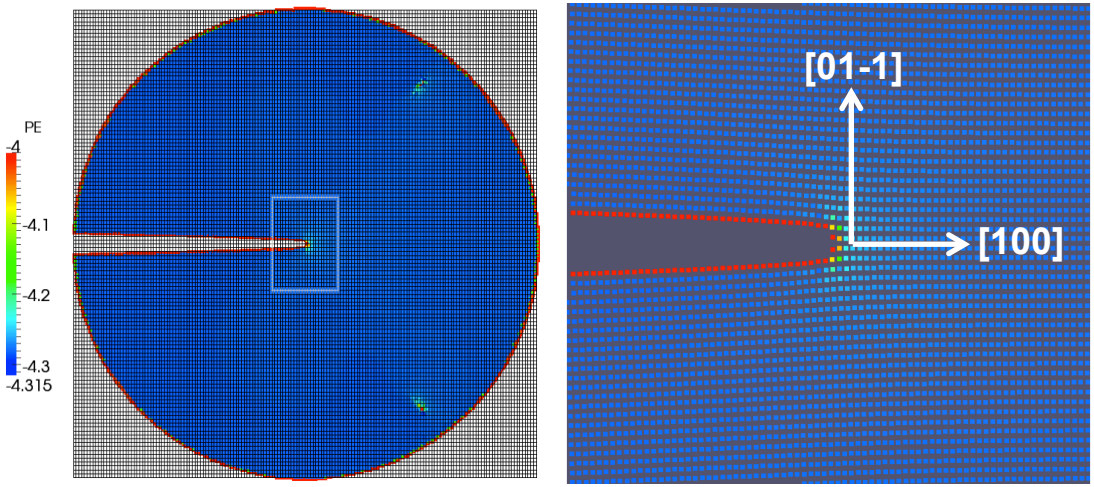


J-integral for ductile crack propagation



FCC Au

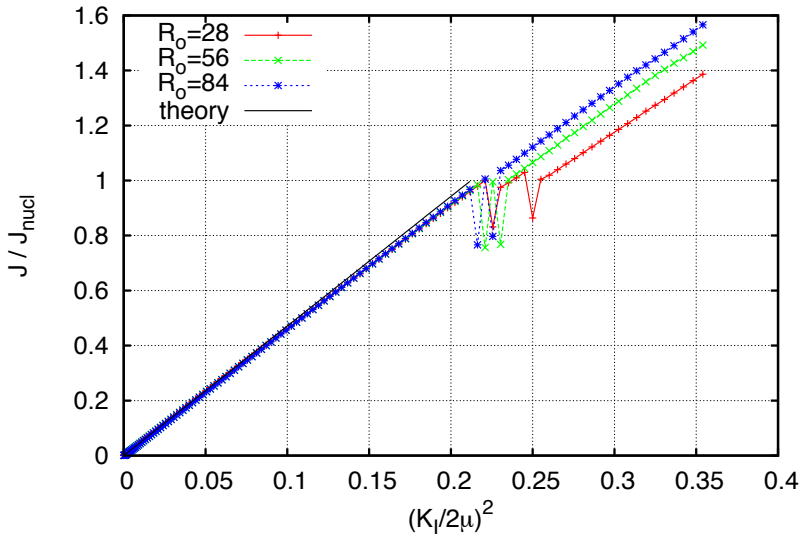
- EAM potential by Foiles et al. (1986)
- Emission of <112> type partial edge dislocations along {111} planes
- Formation of stacking faults
- $J_{Rice} = 1.27 < J_c = 1.95$ [J/m^2]



BCC Fe

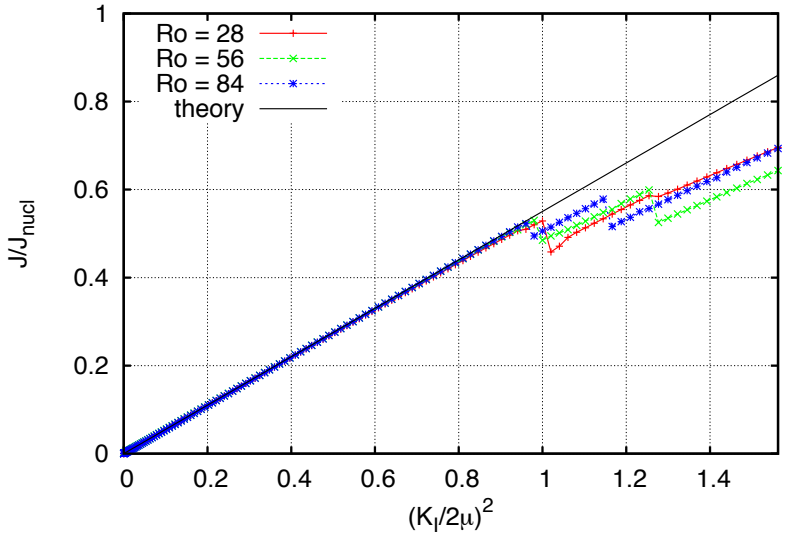
- EAM potential by Simonelli et al. (1993)
- Emission of <111> type full edge dislocations along {211} planes
- No stacking faults
- $J_{Rice} = 6.56 > J_c = 2.87$ [J/m^2]

J-integral for ductile crack propagation



FCC Au

- Dislocation emission occurs at J = 1.25 J/m^2
- After emission, J-integral exhibits a jump of 0.29 J/m^2, then recovers.
- Second dislocation emission occurs at a marginally higher J and also displays near-immediate recovery.



BCC Fe

- Dislocation emission occurs at J = 3.42 J/m^2
- After emission, J-integral exhibits a jump of 0.20 J/m^2; J remains at it's new, lower level.
- Second dislocation emission occurs at a significantly higher value of J = 3.78 J/m^2.

J-integral formulation at finite temperature

At finite temperatures, stress and deformation are conjugates of the free energy. Thus, the J-integral must be defined as…

$$\mathbf{J} = \int_{\Gamma_0} \left(\langle \Psi \rangle \mathbf{N} - \left\langle \mathbf{F}^T \cdot \mathbf{P} \right\rangle \cdot \mathbf{N} \right) ds = \mathbf{J} = \int_{\Gamma_0} \left(\langle \Psi \rangle \mathbf{N} - \left\langle \mathbf{H}^T \cdot \mathbf{P} \right\rangle \cdot \mathbf{N} \right) ds$$

Free energy Ψ is difficult to calculate directly. Instead, we choose to approximate it with the Quasi-Harmonic (QH) approach:

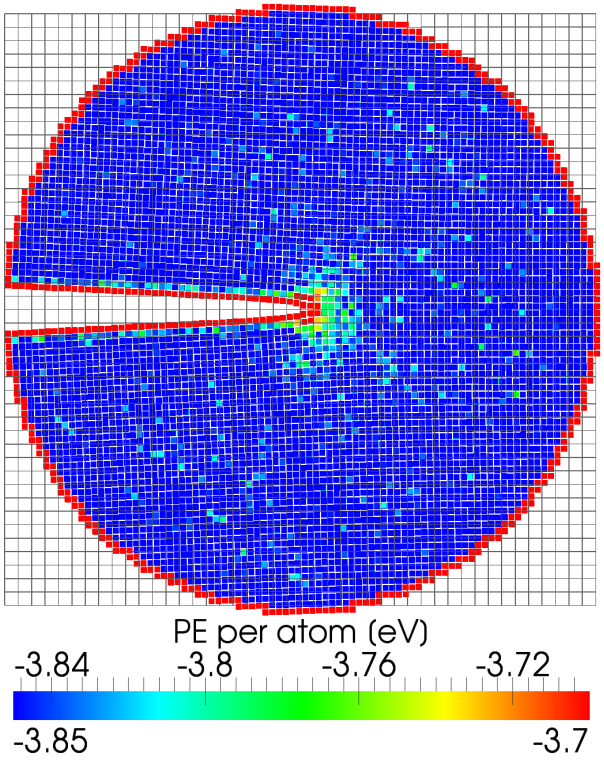
$$\Psi \approx \Psi_{QH} = \Phi_0 + \frac{k_B T}{V} \log \left(\prod_{i=1}^{n} \frac{\hbar \omega_i}{k_B T} \right)$$

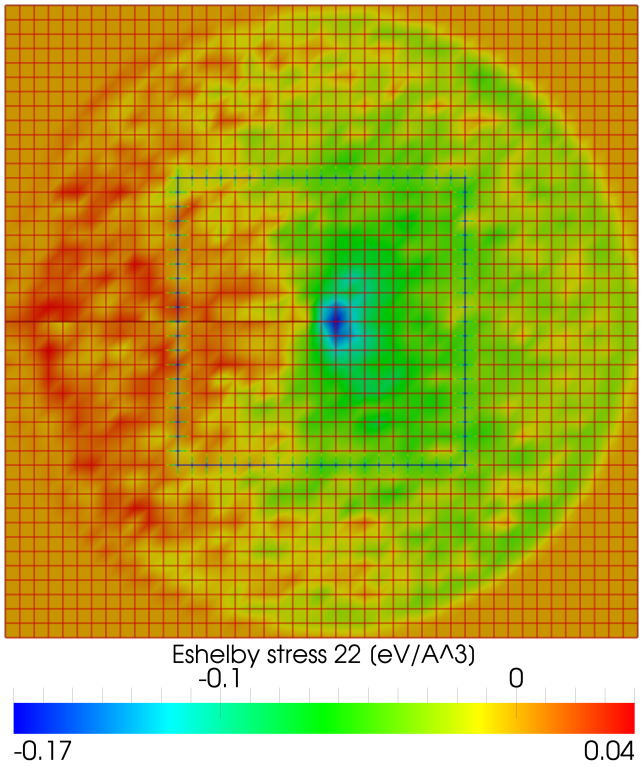
We further use the Local-Harmonic (LH) simplification of QH that depends on a localized (diagonal) version of the dynamical matrix:

$$\Psi_{LH} = \Phi_0 + \frac{k_B T}{V_\alpha} \log \left(\left(\frac{\hbar}{k_B T} \right)^3 \sqrt{\det \left(\mathbb{D}_{LH} \right)} \right) \qquad \mathbb{D}_{LH} = \frac{1}{m} \frac{\partial^2 \Phi}{\partial \mathbf{u}_0 \partial \mathbf{u}_0}$$

J-Integral analysis for finite temperature crack initiation

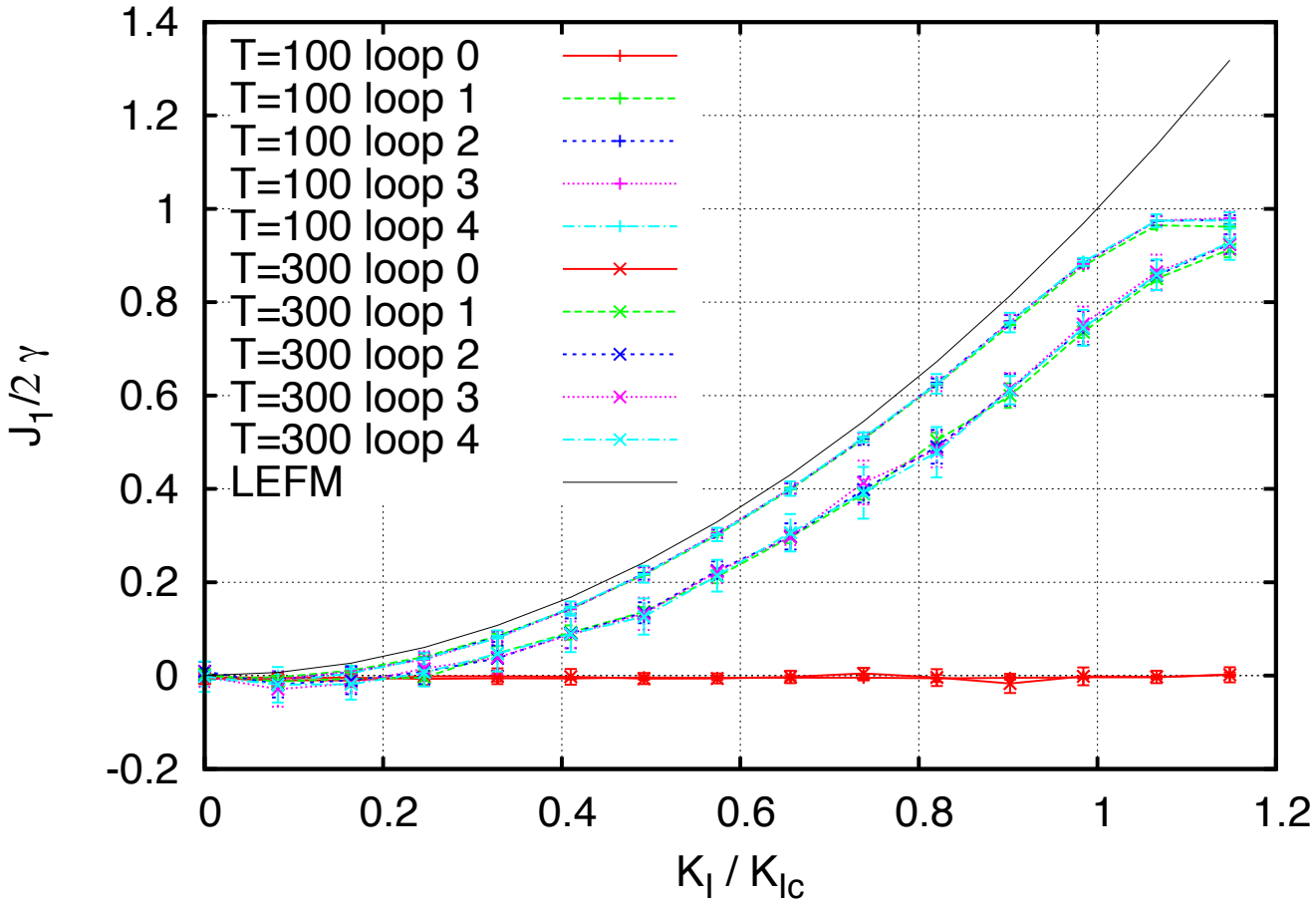
Using thermalization of a sequence of minimized states with far field loading, we obtain fields that show localization together with thermal noise:





- Zero temperature annulus of atoms used to enforce LEFM BCs.
- Fields are time-averaged over a period of 40 ps (10^5 samples).

J-Integral retains path independence



- Path independence at both 100 and 300K.
- J decreases with increasing T due to thermal compression reducing effective stress intensity factor.

Concluding remarks

Thank you to:

- Reese Jones*, Jeremy Templeton*
- Jay Foulk, Alejandro Mota
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- Jeff Rickman (Lehigh)

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