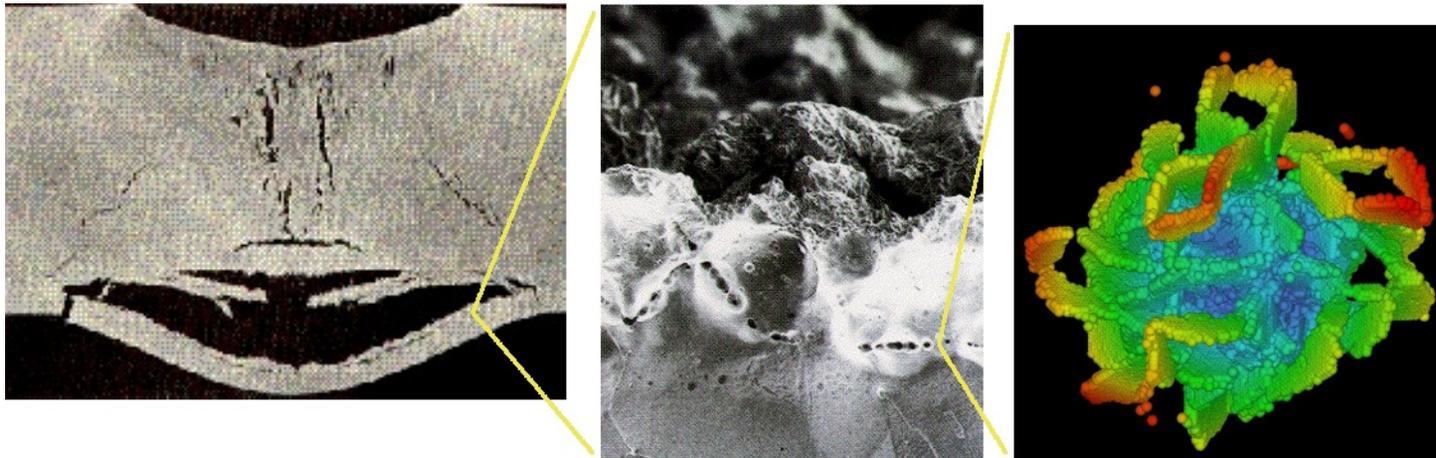


# Concurrent Multiscale Modeling of Solids: CLS and CGMD methodologies

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Voids in collab. with:

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- E. Seppälä (LLNL)
- M. Fivel (INP-Grenoble)
- M. Tang (LLNL)

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**CASC Multiscale Workshop: 15 Jan 2004**

# Motivation and Overview

**Focus: Void nucleation, growth and coalescence play an important role in fracture at high strain rates.**

The efficiency of simulations of cavitation dynamics may be increased through the coarse-graining of the elastic (and plastic) fields surrounding the voids.

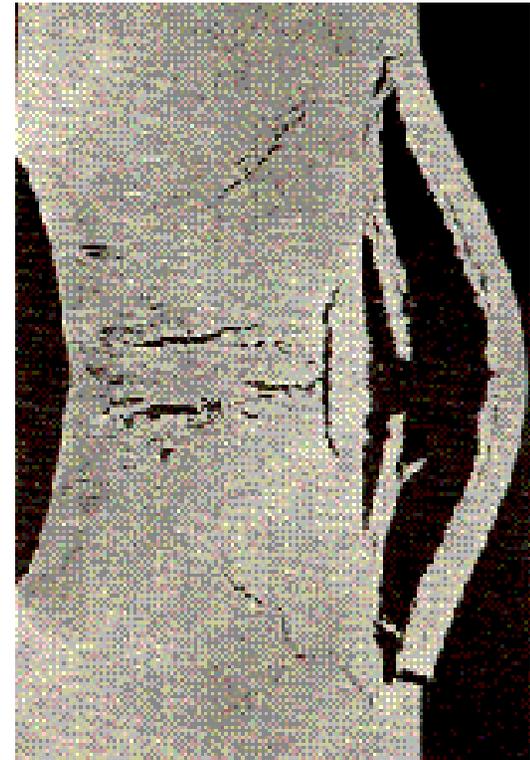
## Outline:

### 1. Atomistic Simulations of Voids

- (a) Void growth in FCC & BCC metals
- (b) Finite temperature
- (c) High strain rate:  $\geq 10^6 \text{ s}^{-1}$
- (d) Stress-strain
- (e) Plasticity
- (f) Dislocation dynamics
- (g) Void linking

### 2. Hybrid modeling: CLS

### 3. Effective modeling: CGMD

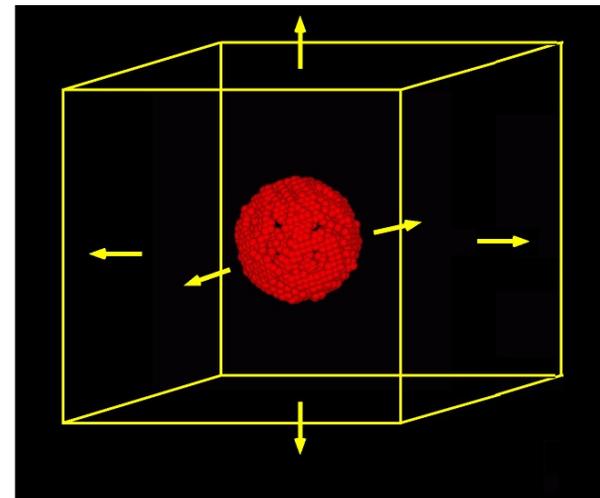


**Dynamic Fracture:  
Spallation**

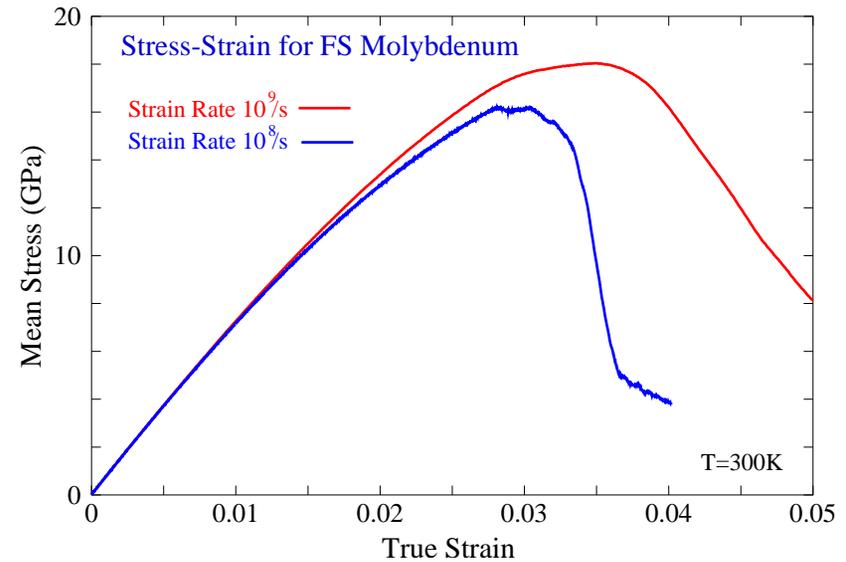
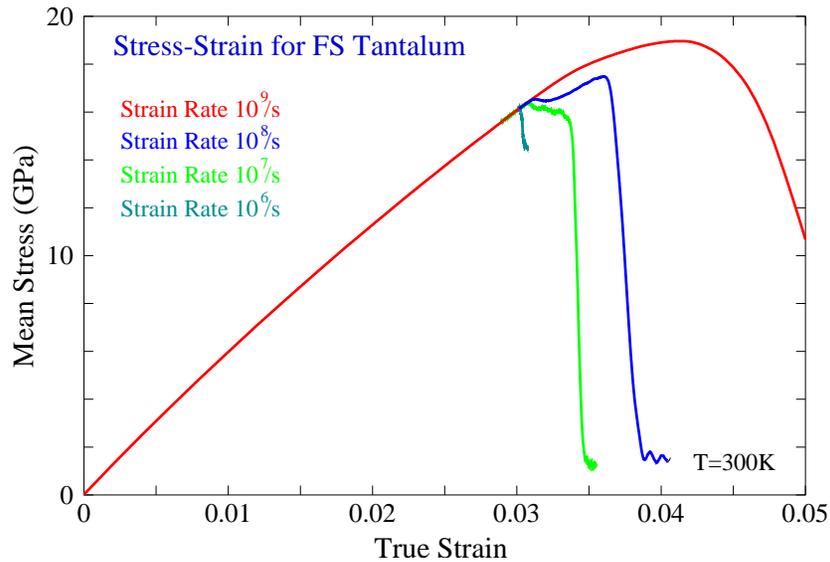
# Atomistic Simulation of Voids

## MD void simulation framework developed by Belak

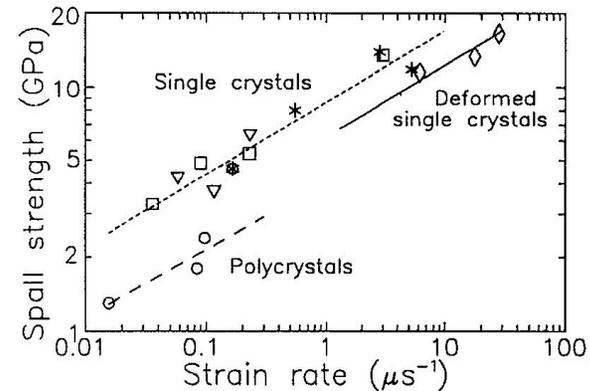
- Procedure for void growth in single crystal:
  - Lattice generated in periodic simulation box
  - Atoms within a sphere (or other region) are removed
  - Tensile stress is applied through box expansion at fixed strain rate in NVE
  - Various properties are monitored during simulation:
    - \* Stress, Temperature
    - \* Void size and shape
    - \* Dislocation activity
- About 1 million atoms for serial code, more in parallel
- Many-body empirical potentials used:
  - Oh-Johnson EAM for Cu
  - Finnis-Sinclair for BCC's
  - Implementing MGPT for BCC Ta
- Initial  $T=300\text{K}$ ,  $\dot{\epsilon} \sim 10^6\text{-}10^9/\text{sec}$



# BCC Stress-Strain Behavior

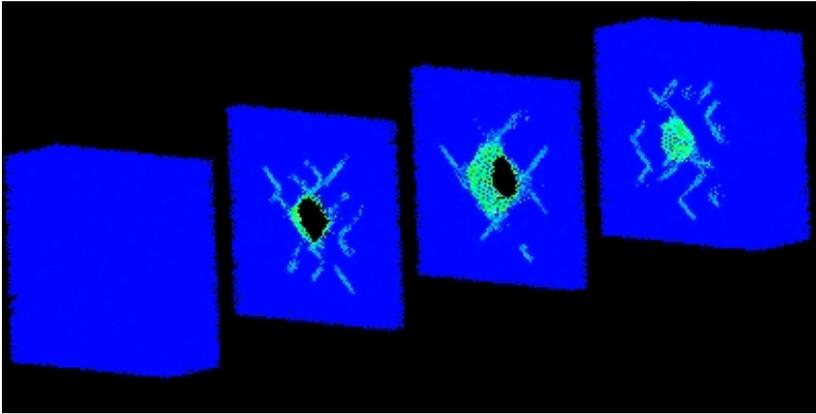


- Stress-strain for BCC metals at two strain rates
- Triaxial expansion of box
- Distinct phases of response
  - Elastic (hyperelastic) stretching
  - Void growth accompanied by stress drop
- Stress at initiation of void growth in reasonable agreement with experimental spall strength



Kanel, et al. APL (1993): Mo

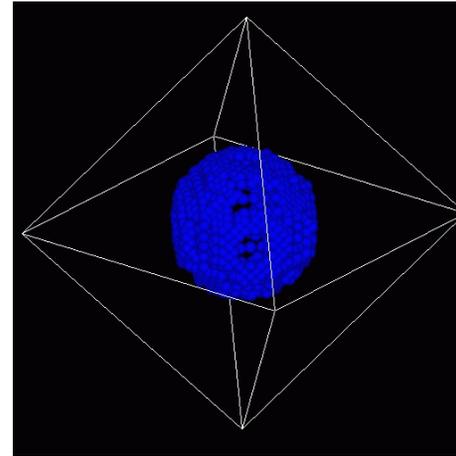
## Visualization of Voids



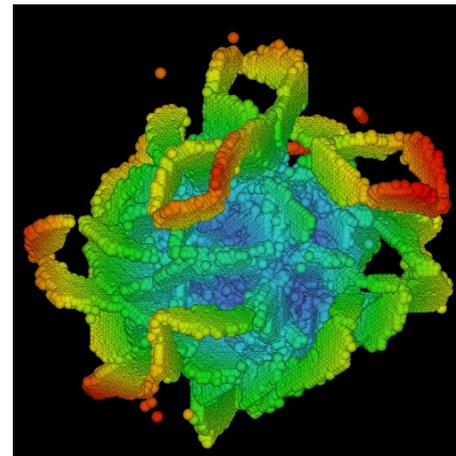
Expanded View of Simulation

Throughout this talk, only the **interesting** atoms will be shown—i.e. those on surfaces, dislocations, stacking faults, grain boundaries, etc., as the case may be.

Dislocations are located using a suite of point group deviation parameters suitable for **finite temperature**.



Surface Atoms

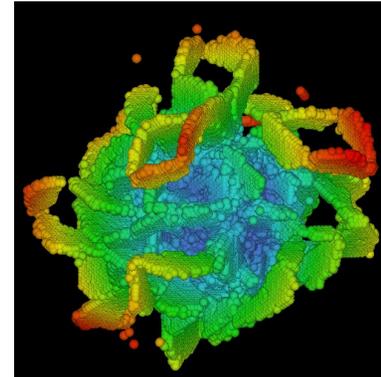


Dislocations

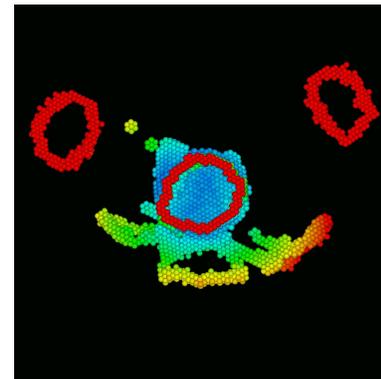
## Comparison of BCC & FCC Loops

Prismatic loops dominate the far-field dislocation activity around a growing void in both FCC and BCC metals.

- FCC loops are parallelgrams, well confined to  $\{111\}$  planes with few jogs.
- BCC loops are much more rounded, ranging from rounded hexagons to triangles with frequent jogs. The loop shape and the glide planes depend on the specific BCC metal and strain rate.
- Both FCC and BCC loops climb toward their equilibrium shapes leaving point defects (principally single vacancies) behind, but the effect is much more common in the BCC metals.

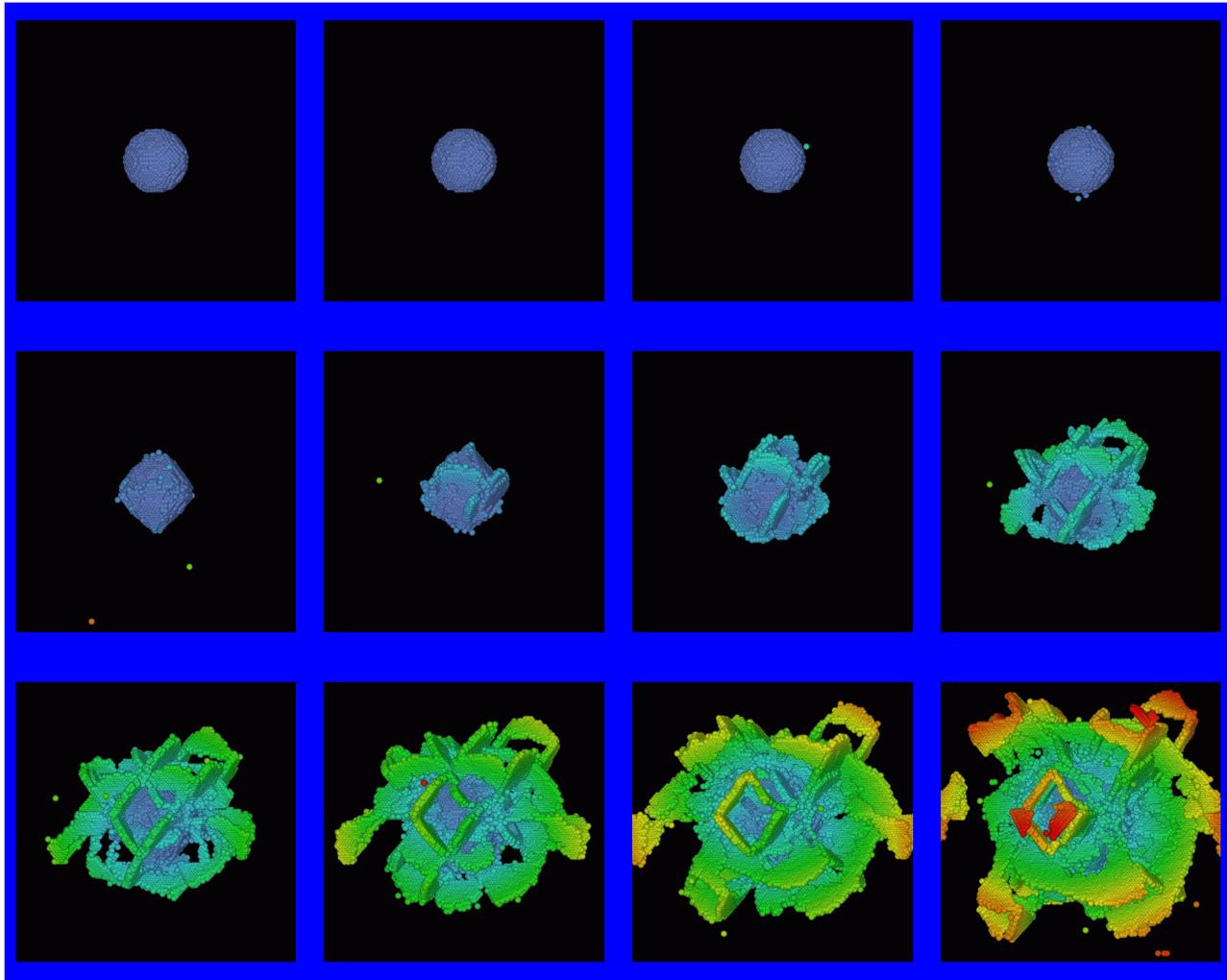


Prismatic Loops in  
Copper (FCC)



Prismatic Loops in  
Molybdenum (BCC)

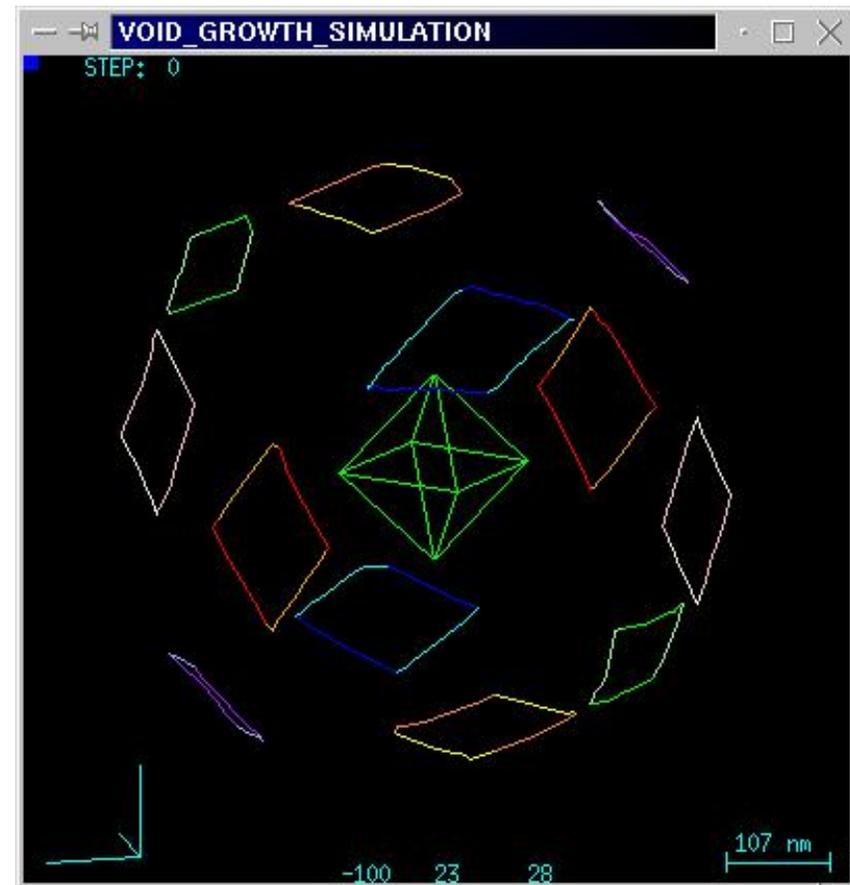
# Void Growth Sequence—Spherical Void



## Linking with Mesoscale Modeling

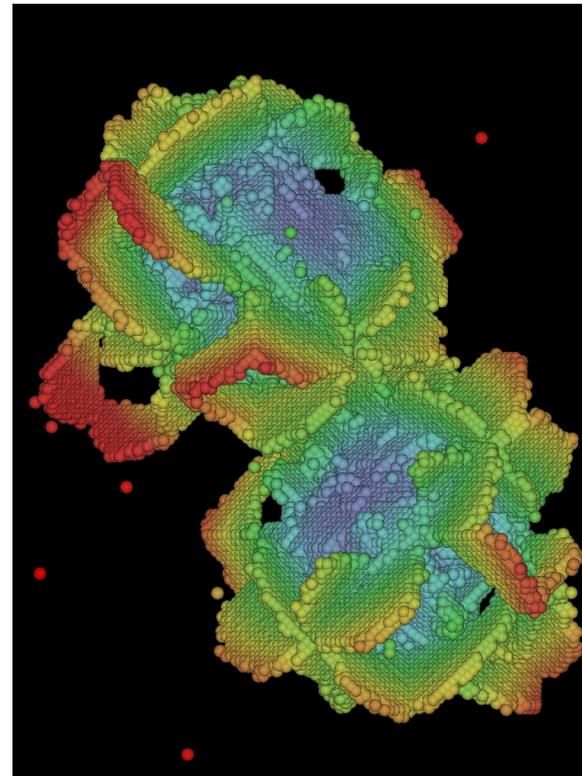
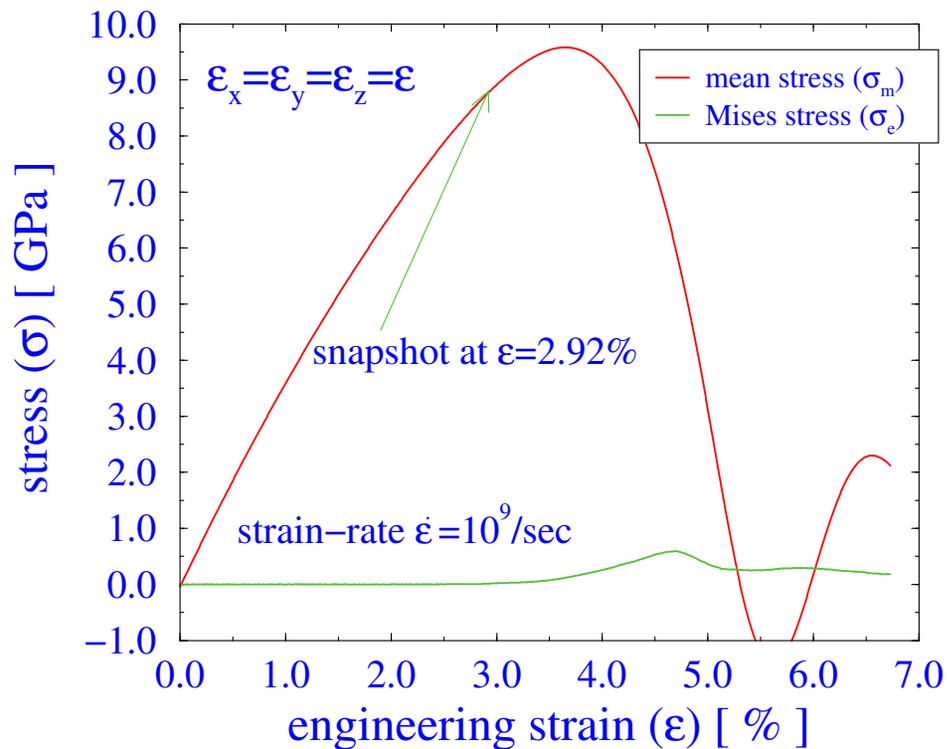
The MD findings (nucleation criteria and plastic zone characterization) are used to define a dislocation dynamics/finite element model (DD/FEM):

- Far-field dislocation activity dominated by glissile prismatic loops.
- No active Frank-Read sources or other multiplication.
- Critical resolved shear stress computed in MD.
- Void volume growth dominated by plastic deformation.
- Rigid matrix void growth law relates loop size to volume increment.
- MD loop sequence is used.



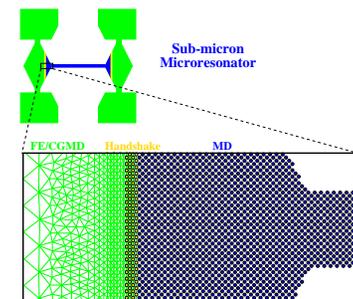
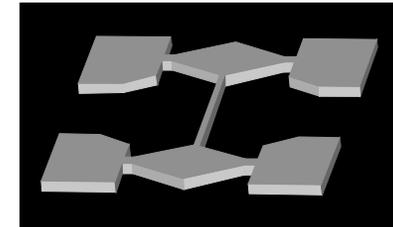
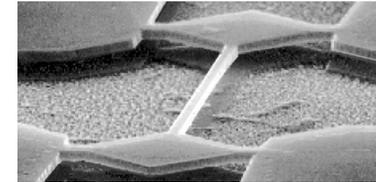
# Void-Void Interactions

- Void-void interactions govern coalescence
- Here two pre-existing voids: radius 2.2 nm with distance 12.2 nm.
- Equilibrium system size at  $T = 300$  K:  $[43.3 \text{ nm}]^3$  of FCC copper; about 7 million atoms using parallel MD3d simulations with 64 CPUs.



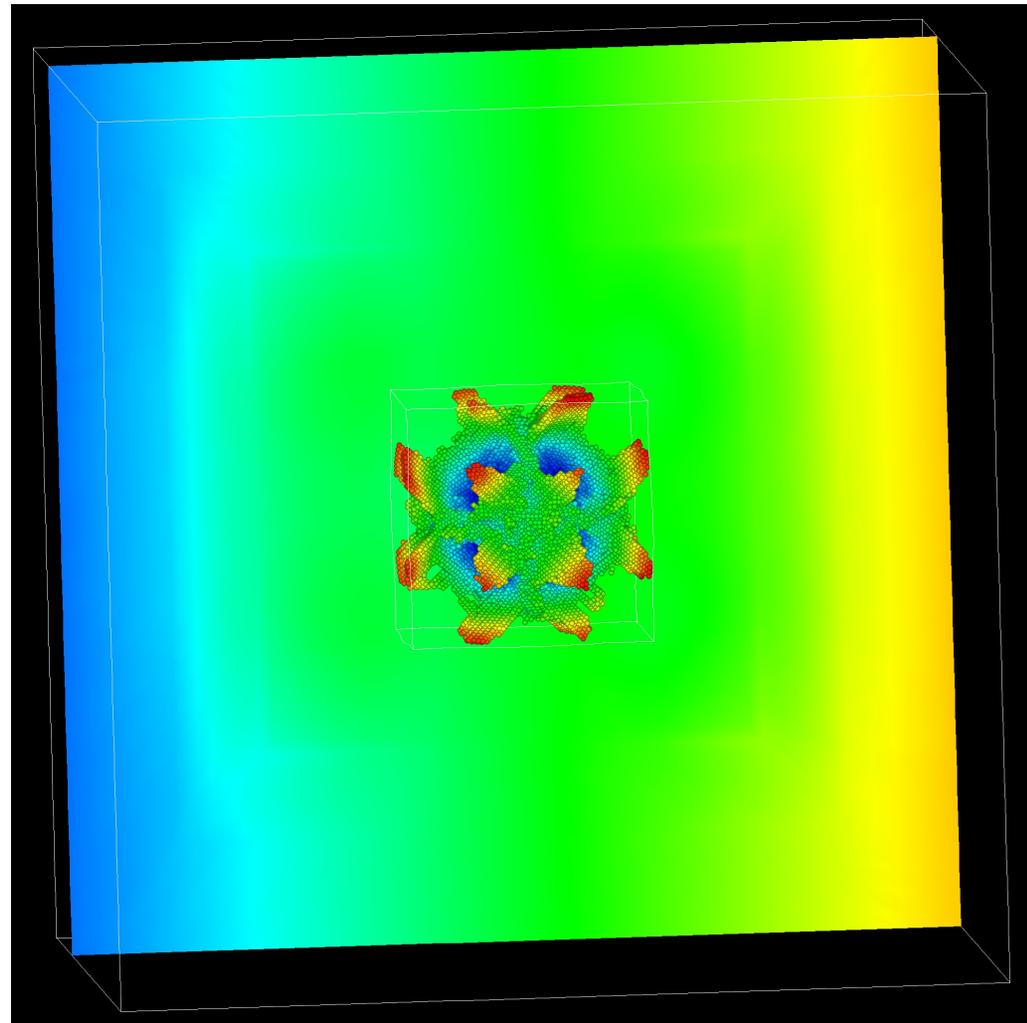
# Concurrent Multiscale Modeling

- MD Void growth modeling restricted to nanoscale
- Need a way to mitigate finite size effects
  - Void sees its periodic image 21 nm away (in Cu)
  - Elastic waves traverse box in  $\{100\}$  direction in 9 ps.
  - Prismatic loops traverse box in  $\{110\}$  direction in 21 ps.
- Concurrent multiscale methodologies concentrate computational power in those regions where it is needed most.
- FEM/MD CLS is a hybrid technique which has demonstrated the validity and utility of concurrent multiscale modeling.
- It is a means to delay the elastic wave recurrence.
- FEM/FEM+DD/MD CLS would be even more desirable.
- It would forestall the prismatic loop recurrence.
- Most of the required elements are now in place . . .



# Hybrid Coupling of Length Scales (CLS)

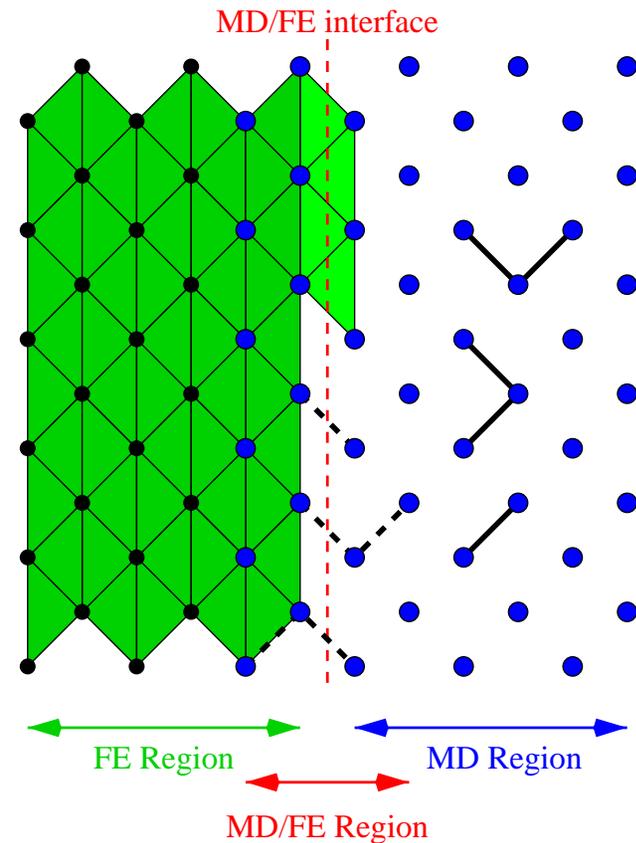
- **Basic Idea:** Take two models suitable for different length scales, well tested and optimized, and combine them to run concurrently in a single simulation.
- **Molecular dynamics (MD)** is used for the atomistic scale; **Finite element modeling (FEM)** for the microscale.
- Each couples to the other at every timestep, effectively providing the requisite boundary conditions on the fly.



Void growth in Ta with FEM/MD at  $T=300\text{K}$

# Original CLS Handshake: SW Si

- FE/MD handshaking at interface
- linear tet/tri FEM implementation
- Matching Degrees of Freedom:
  - FE mesh nodes located at equilibrium lattice sites at interface
  - Initial atomic displacements = initial FE nodal displacements
- $H_{FE/MD}$  Couplings – Mean force:
  - Each cell crossing interface counted with 1/2 weight
  - Each 2- and 3-body bond crossing counted with 1/2 weight

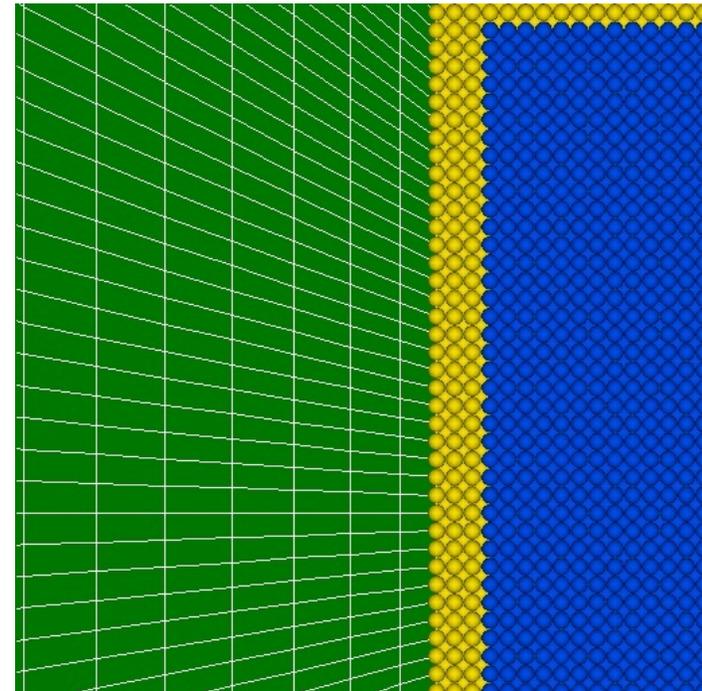


MD and FE run with same time step and integrator.  
Cures numerical instability seen previously. (Kohlhoff, et al)

2D FEM/MD Coupling: Broughton, et al, PRB 1999

## CLS Handshake: FS Ta

- Tri-linear 8-node brick FEM
- Refined to crystal unit cell at FEM/MD interface
- Energy is conserved.
- Hamiltonian dynamics:  
$$H = H^{MD} + H^{FE} + H^{HS}$$
- $H^{HS}$  corrects for bond termination
- HS region spans range of the potential, in current implementation for metals



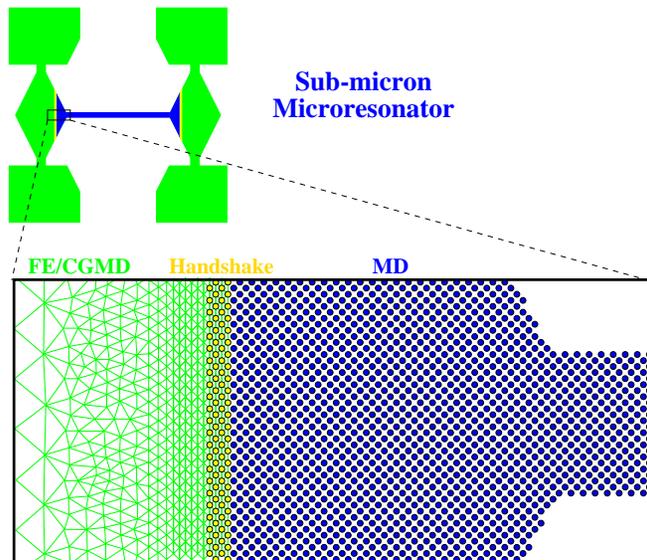
HS region in CLS void simulation

- FEM/MD void growth system:
  - Total simulated system: 12 million atoms
  - Actual MD atoms: 0.5 million
  - FEM nodes: 0.16 million; FEM cells: 0.16 million

# Coarse-Grained Molecular Dynamics (CGMD)

- **Basic Idea:** A replacement for FE, which matches smoothly onto MD as the mesh is refined to atomic spacing.
- **Approach:** Use statistical mechanics to remove MD degrees of freedom on the irregular FE mesh.

$$\mathbf{E}(\vec{u}_k, \dot{\vec{u}}_k) = \int d\vec{r}_\mu d\vec{p}_\mu \mathbf{H}_{\text{MD}} e^{-\mathbf{H}_{\text{MD}}/kT} \Delta(\vec{r}_\mu, \vec{p}_\mu; \vec{u}_k, \dot{\vec{u}}_k) / Z$$



## CGMD Steps:

1. Harmonic expansion of forces in MD at T
2. Average: CGMD equations of motion.
3. Run as if MD but with CGMD eq. of motion on the mesh. Ordinary MD forces are used in the atomistic region.

Note: No mesh refinement is done.

## Formulation of CGMD

- **Micro-Macro Correspondence:**  
Macroscopic fields defined as best fit to microscopic quantities.
  - e.g. Displacement field expressed via shape functions:

$$\vec{u}(\vec{x}) = \sum_j \vec{u}_j \mathbf{N}_j(\vec{x}) \rightarrow \min \chi^2 = \sum_\mu |\vec{u}_\mu - \vec{u}(\vec{x}_{0\mu})|^2$$

- Short wavelength modes are taken to be in thermal equilibrium.
- These modes are “integrated out” via a thermal averaging procedure assuming they evolve adiabatically.
- Equations of motion for remaining long wavelength modes are derived analytically using pert. theory about a harmonic lattice.

The resulting forces are essentially weighted averages of the interatomic forces, with the CG weights determined by stat. mech. This leads to a form of finite elements with non-linear, finite temperature, scale-dependent constitutive equations:

$$\mathbf{M}_{ij} \ddot{\vec{u}}_j = -\mathbf{K}_{ij} \vec{u}_j + \dots \text{ with } \mathbf{M}_{ij} = \sum_\mu \mathbf{N}_{i\mu} \mathbf{m}_\mu \mathbf{N}_{j\mu} \text{ etc.}$$

## Derivation of the CGMD Hamiltonian

- The best fit CG fields are:  $\mathbf{u}_i = (\mathbf{N}_{i\nu}\mathbf{N}_{j\nu})^{-1}\mathbf{N}_{j\mu}\mathbf{u}_\mu \equiv \mathbf{f}_{i\mu}\mathbf{u}_\mu$
- Thus the CGMD Hamiltonian is given by:

$$\mathbf{E}(\vec{u}_k, \dot{\vec{u}}_k) = \mathbf{Z}^{-1} \int d\vec{r}_\mu d\vec{p}_\mu \mathbf{H}_{\text{MD}} \Delta \exp \left[ - \left( \frac{|p_\mu|^2}{2m_\mu} + \frac{1}{2} \vec{r}_\mu \mathbf{D}_{\mu\nu} \vec{r}_\nu + \dots \right) / kT \right]$$

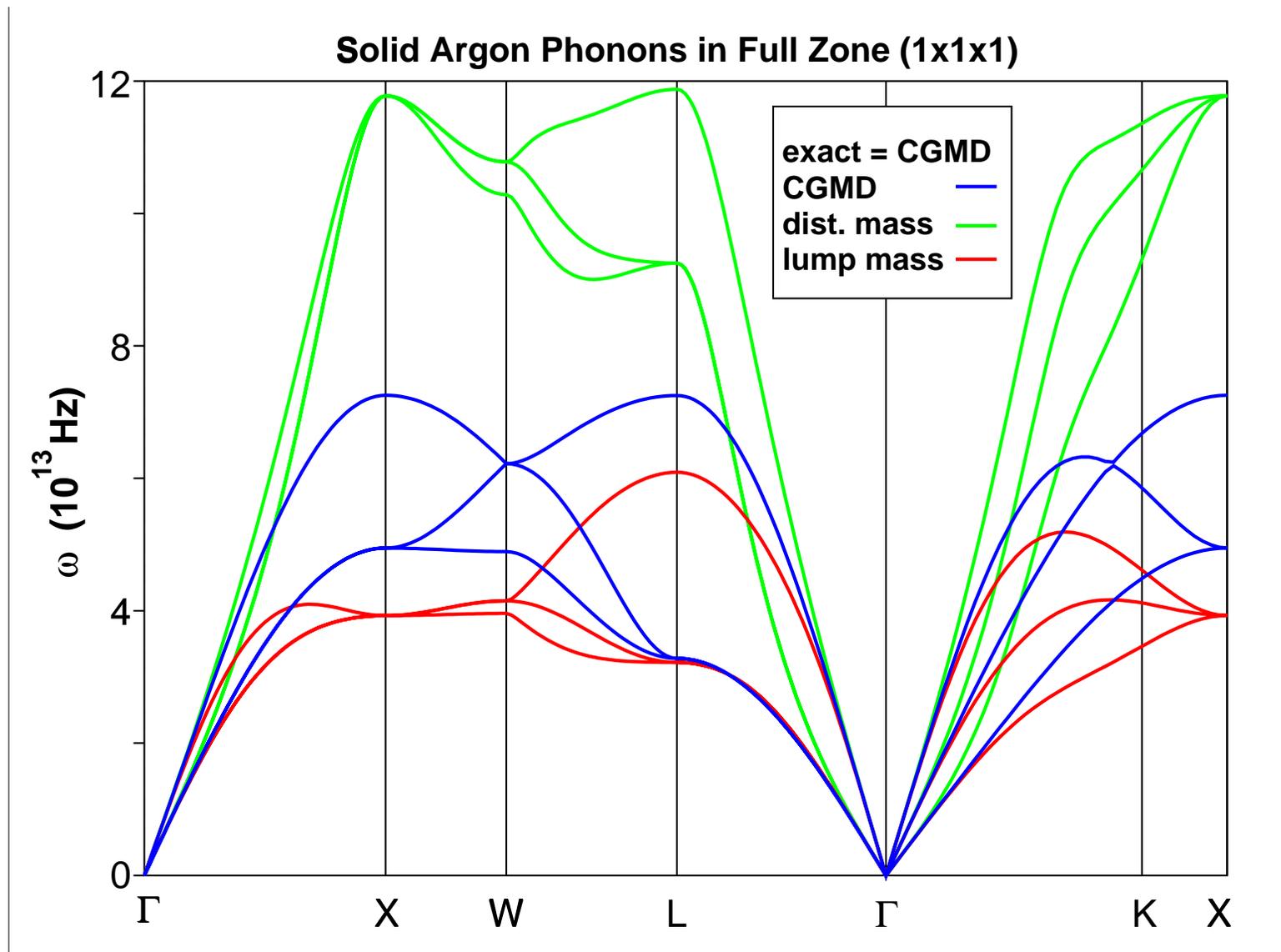
where the constraint factor is given by  $\Delta = \prod_i \delta^{(3)}(\mathbf{u}_i - \mathbf{f}_{i\mu}\mathbf{u}_\mu)$

- This can be reexpressed in terms of Lagrange multipliers:

$$\delta(\mathbf{x}) = \frac{1}{2\pi} \int d\lambda e^{i\lambda\mathbf{x}}$$

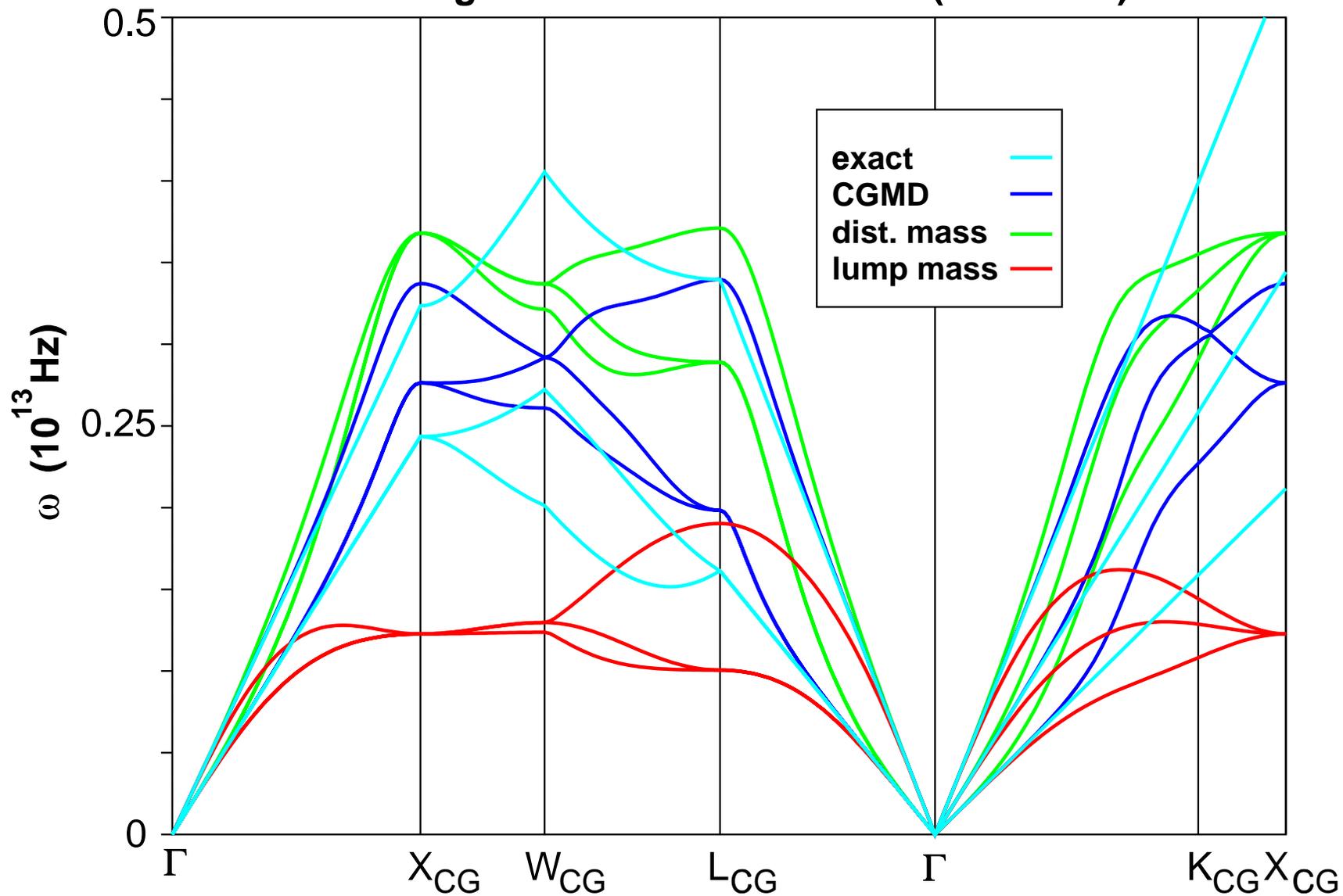
- The anharmonic terms are expanded in a Taylor series, leaving a Gaussian integral. The integral is elementary, so we are left with an analytic expression.
- At zeroth order, the CGMD Green function is a simple average:  
 $G_{ij}^K = N_{i\mu}N_{j\nu}G_{\mu\nu}^H$ .
- The entire perturbation series has been given a diagrammatic representation. Terms up to  $u^4$  are used in  $\mathbf{H}_{\text{CGMD}}$ .

# CGMD Phonons – Atomic Limit

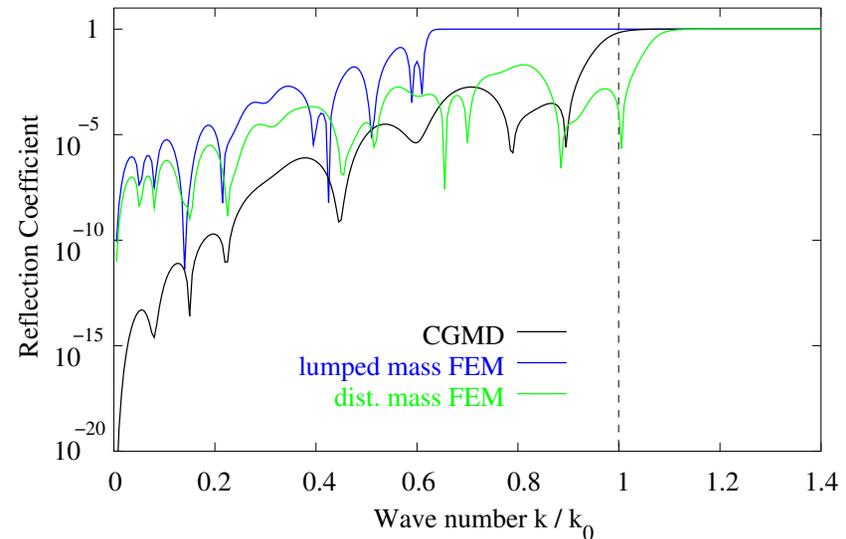
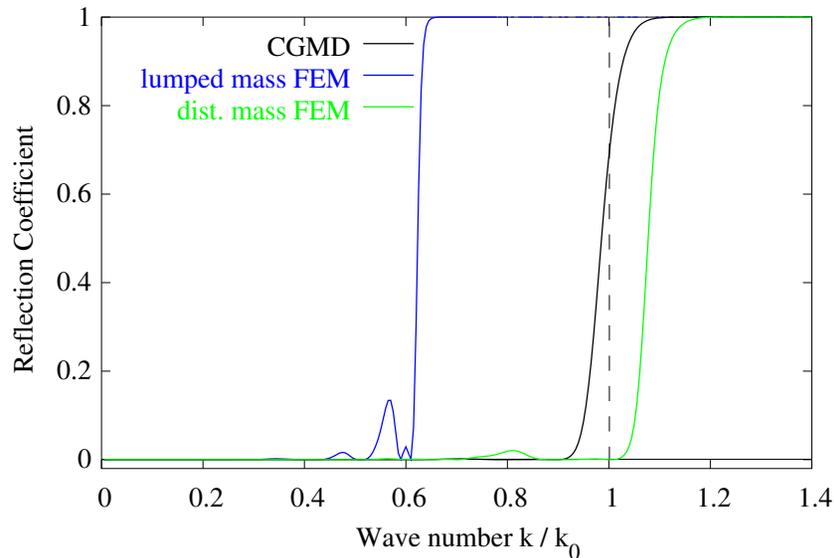


# CGMD Phonons – Continuum Limit

## Solid Argon Phonons in CG Zone (32x32x32)



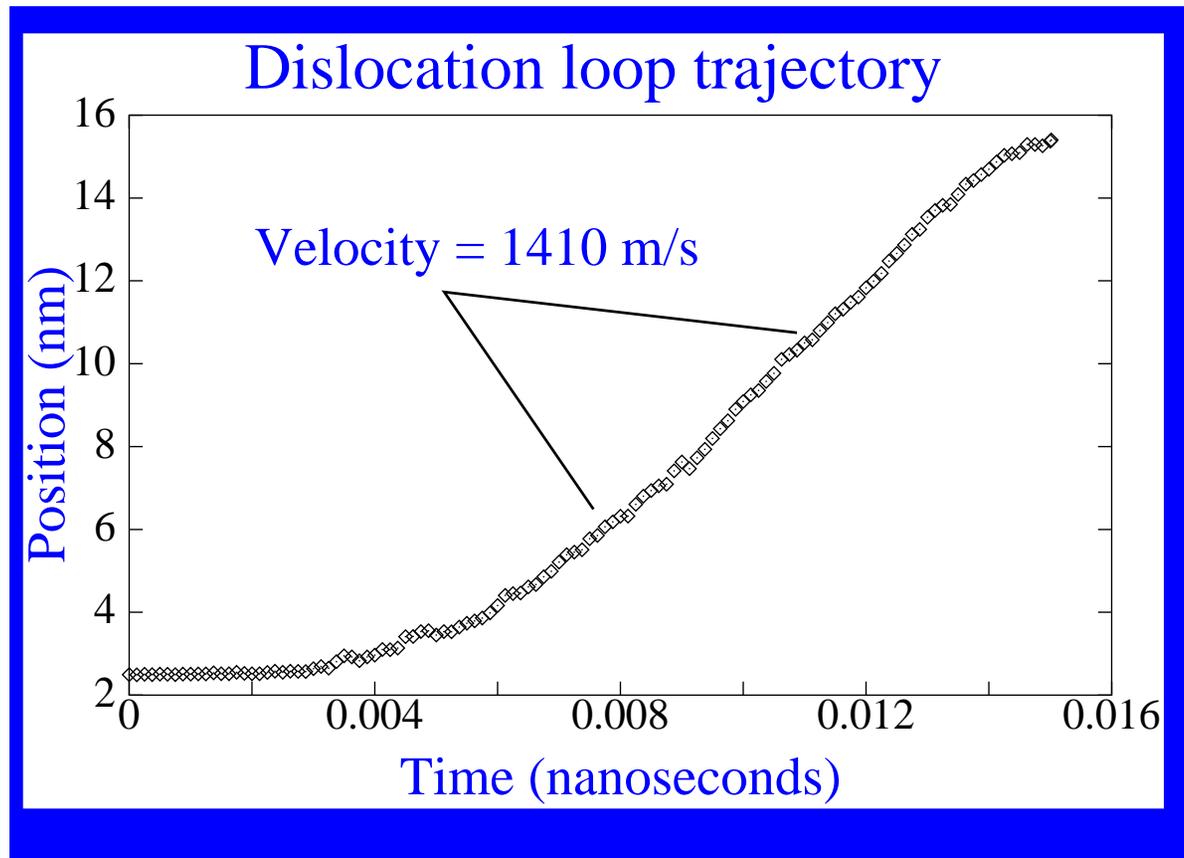
# Elastic Wave Scattering



**Conservative CGMD** already eliminates spurious resonances in the elastic wave scattering.

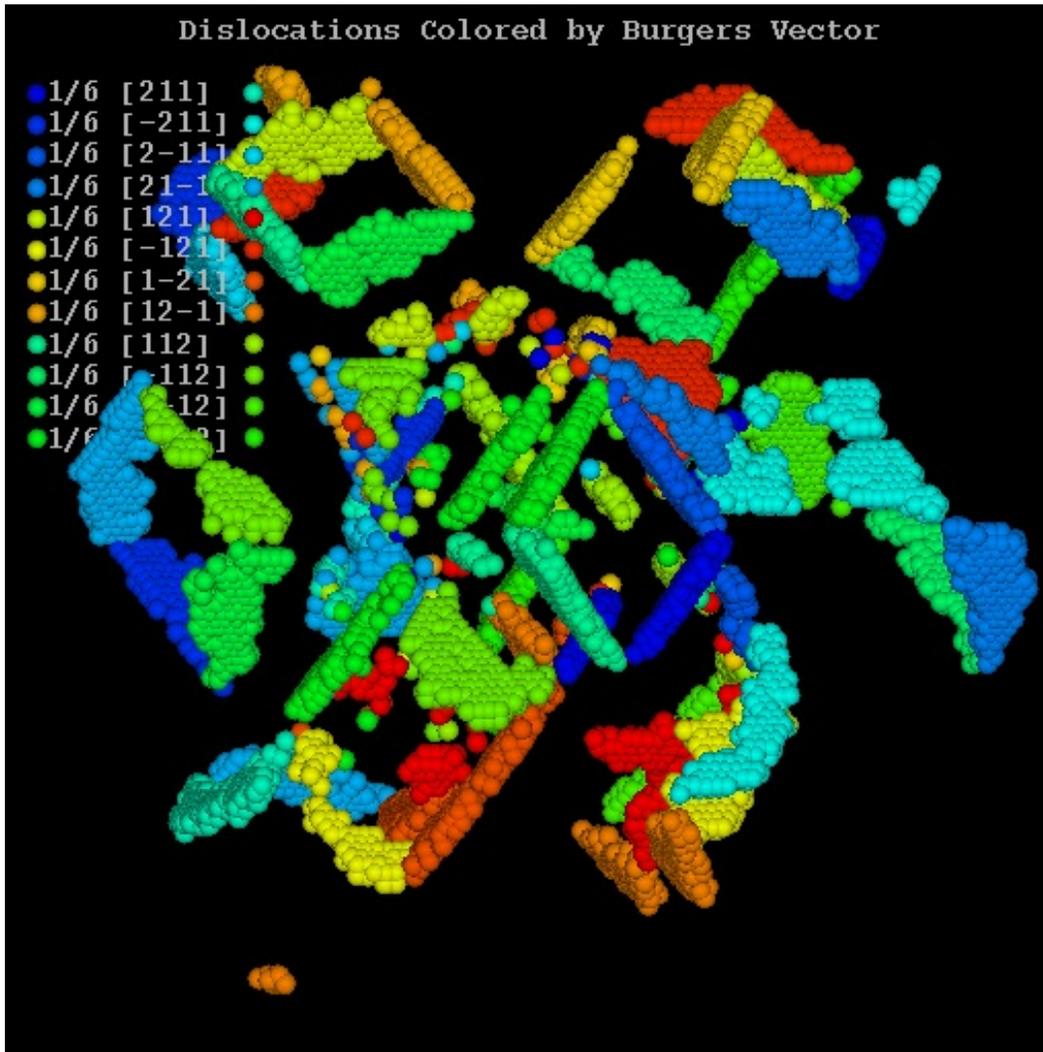
Use of projection operator techniques and Langevin CGMD further reduces scattering of extremely short wavelength modes.

# Outlook for Coarse-graining with Dislocations



The dislocation velocity increases to 1410 m/s, or about 60% of the shear wave velocity. Presumably the limiting velocity is due to phonon drag, but we have not confirmed this directly.

# On-the-fly Dislocation Characterization



The figure shows a complete characterization of the dislocations emitted during void growth at a constant triaxial strain rate.

This characterization was produced automatically based on structural (not energetic) characterization of the dislocations at finite temperature.

# Conclusions from Void Studies

- **Void Nucleation**

- Polycrystalline void nucleation at grain boundary junctions
- Very complex dislocation activity due to GB sources and sinks

- **FCC Void Growth under Triaxial (Hydrostatic) Tension**

- Void growth laws show exponential growth dep. on shape
- Void faceting related to plasticity
- MD results on loop activity used to inform DD simulation

- **FCC Void Growth under Uniaxial Tension**

- Demonstrates interplay of flow and cavitation
- Prolate-Oblate-Equiaxed evolution

- **BCC Void Growth under Triaxial (Hydrostatic) Tension**

- Strong rate sensitivity in MD regime
- Asymmetric plasticity due to high Peierls barrier

- **New Tools**

- On-the-fly dislocation characterization
- High fidelity void surface and volume analysis
- Shape characterization through multipoles
- Goal: 3D MD/DD/FEM code

# Acknowledgments

This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory, under Contract No. W-7405-Eng-48.

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