MOLECULAR DYNAMICS MODELING OF LASER-PULSE COMPRESSION OF SILICON

E. N. Hahn[1], S. Zhao[1], D. Tramontina[2], E. M. Bringa[2,3], B. A. Remington[4], T. C. Germann[5], M. A. Meyers[1]

[1] University of California, San Diego, [2] Instituto de Ciencias Básicas, Universidad Nacional de Cuyo, Mendoza, Argentina,
[3] CONICET, Mendoza, Argentina, [4] Lawrence Livermore National Laboratory, [5] Los Alamos National Laboratory

Motivation

- The kinetics of high strain-rate compression are fundamental to our understanding of many physical phenomenon.
- Phenomenon critical to defense and energy needs that will benefit from an improved understanding vary from high-speed collisions to inertial confinement fusion implosions.
- Quantitative experimental data at high strain rates is lacking and atomistic molecular dynamics simulations provide a means to accurately model and visualize dislocation kinetics.
- Dislocation slip systems and dislocation velocities determine the kinetic limits of physical deformation phenomenon.
- Silicon is well-suited for molecular dynamics simulations and physical experimentation due to the development of representative interatomic potentials and the availability of high-purity, well-oriented single crystal physical samples.

Model Description

- Code: Large-Scale Atomistic/Molecular Massively Parallel Simulator (lammps.sandia.gov)
- Material: Diamond Cubic Silicon (Potential: Stillinger-Weber)
- Processing: LANL Conejo High Performance Computing, 8 – 1024 Intel Xeon 2.67 GHz Cores
- Simulation Size: 50nm x 50nm x 200 nm, 10^5 – 10^7 Atoms
- Strain Rate: 10^9 – 10^{12} m^{-1}

Conclusions and Future Research

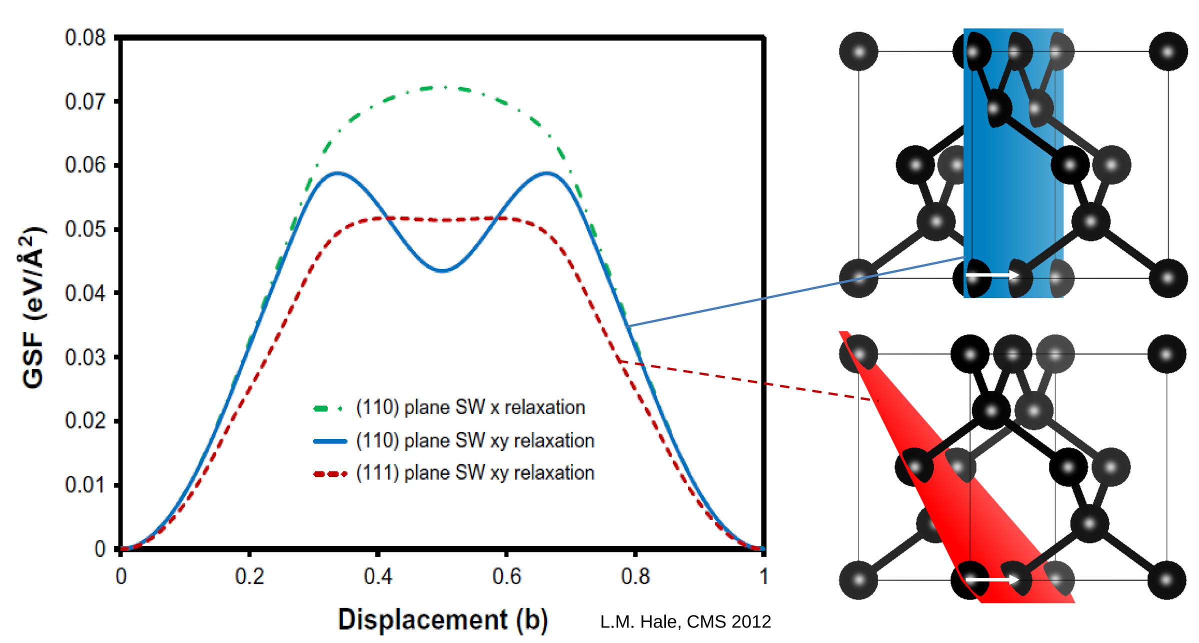
- Large scale simulations up to 14 million atoms were successfully run – future runs will increase this to 100 million atoms
- The measured Hugoniot elastic limit of 18 GPa is within the projection of experimental data and serves to inform experimental conditions necessary to observe plasticity at extreme strain rates
- Both heterogeneous surface nucleation and homogenous bulk nucleation of partial dislocations are observed
- Evolution of partial dislocations bounding a stacking fault to full dislocations is observed and will be explained in terms of dislocation energetics in future work

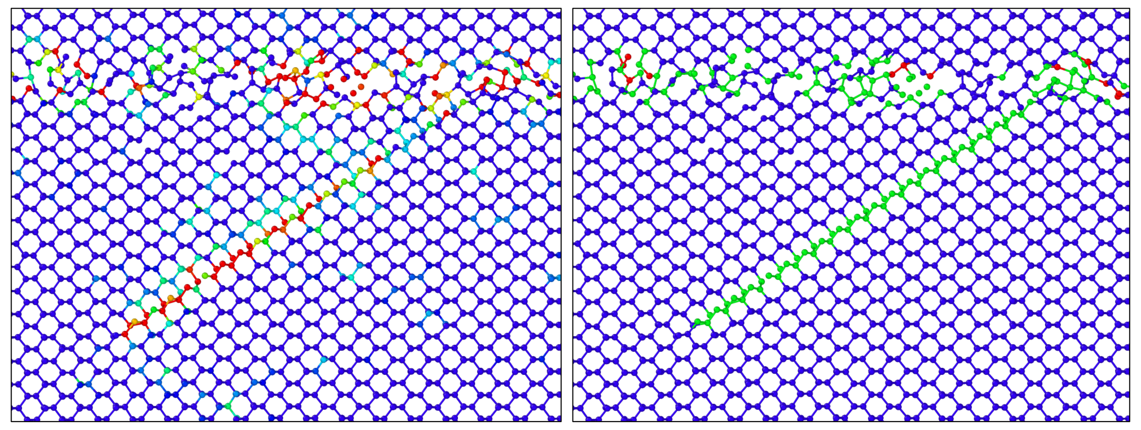
Acknowledgements

Support from NNSA SSAA and Los Alamos National Laboratory Fellowship and Conejo High Performance Computing cluster.

Dislocation Slip-System Evaluation

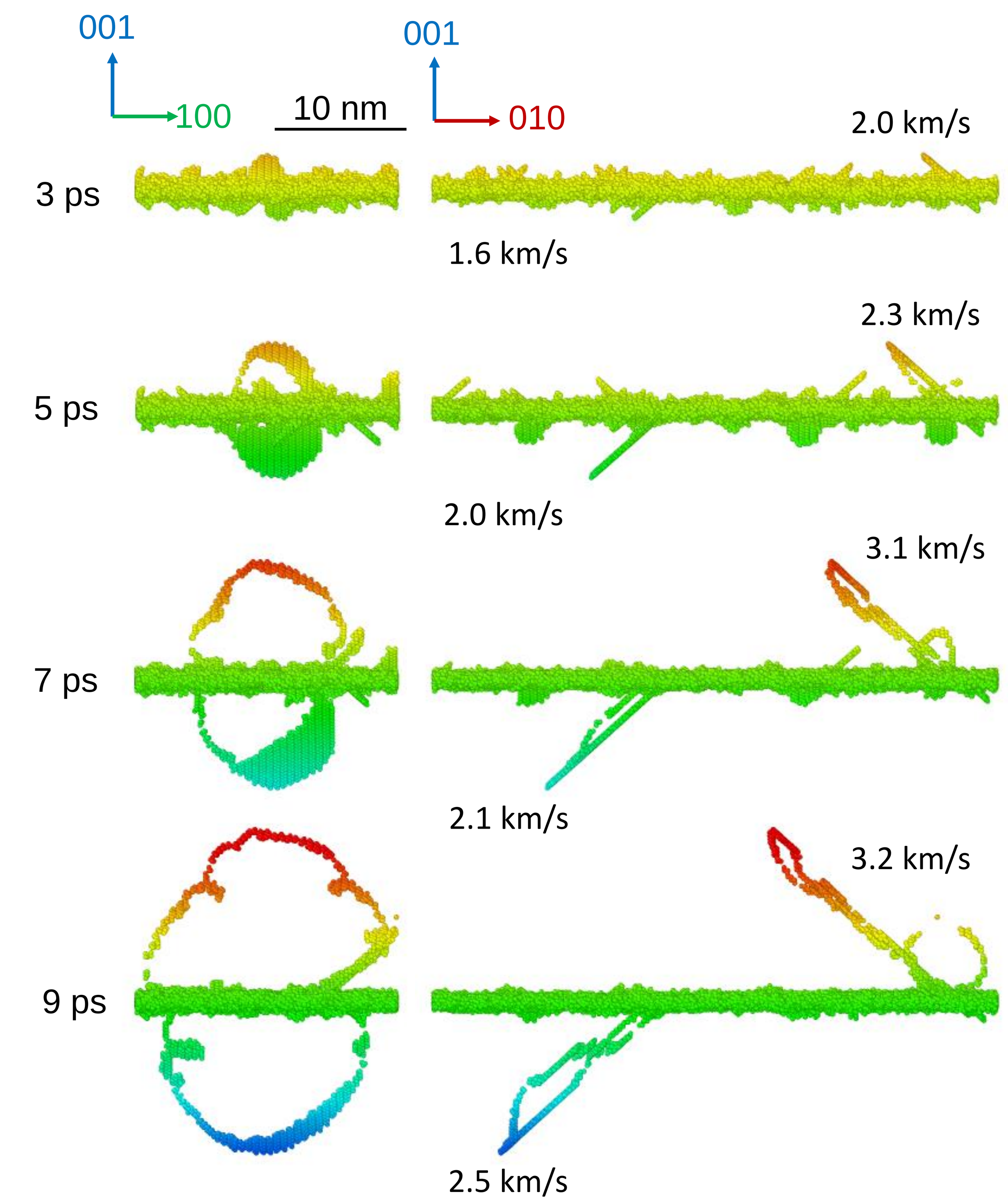
Comparative stacking fault energies showing the potential of both (110) and (111) slip systems with burgers vector b = ½ <110>.



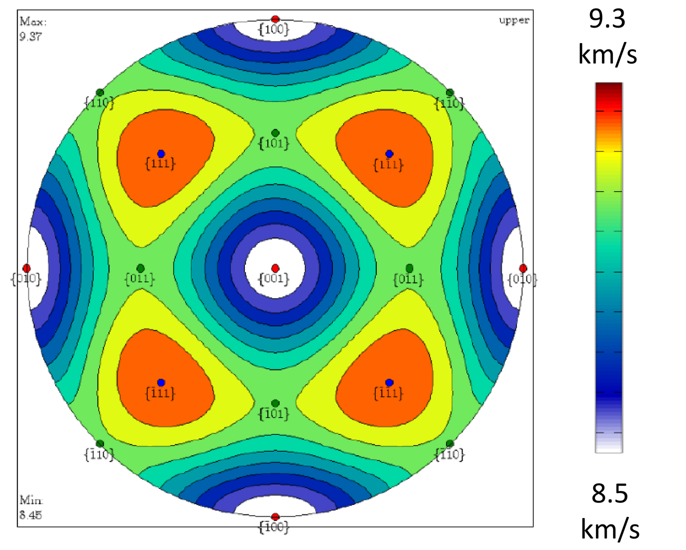


{110} Stacking Fault colored by shear stress (left) and local coordination (right). The {110} stacking fault travels by shifting a metastable body-centered-tetragonal-5 coordination by ¼ <111>.

Dislocation Kinetics



- Simulated compression shock of a <001> single crystal silicon sample
  - Strain-rate of $2.3x10^9$ m^{-1}
  - Flyer plate velocity of 3.0 km/s.
  - Particle velocity is 1.47 km/s
  - Shock front pressure is 34.7 GPa
- Shown are four progressive time steps and the evolution of dislocations and their respective velocities in both the piston (above plane) and sample (below plane)
- The 9 ps time step is most representative of characteristic dislocation velocities as the trailing partial catches the leading partial and removes drag associated with the stacking fault
- The average dislocation velocity is 2.85 km/s relating to 33.5% the <001> speed of sound in silicon
- 2D sound velocity plot shown to the right indicating sound speed varying with crystallographic direction



Defect Structure as a Function of the Deviatoric Shear Component of Shock Pressure