Characterizing Structure in Simulated Silicon Under Shock Compression

Alex Li[1], Rob Rudd[2], Eric Hahn[1], Marc Meyers[1]

[1]University of California, San Diego [2] Lawrence Livermore National Labs

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Motivation

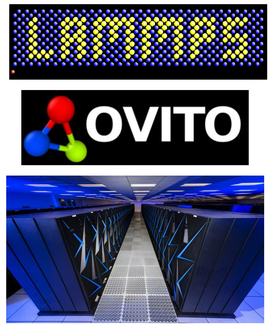
- Silicon is an important material used in many industries and is well studied. Here it is used as a baseline for exploring shock simulations in covalently bonded solids.
- Amorphous structures in shocked silicon have been identified, but some disordered phases have not been as clearly characterized.
- The effects of shock on the structure of silicon can give insight into other covalently bonded solids such as diamond.

Simulation Parameters

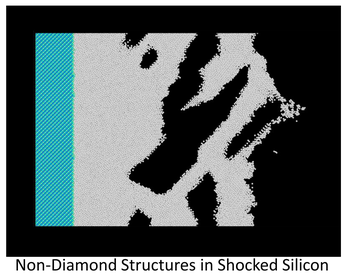
- A piston is formed from silicon atoms frozen such that they cannot deform, essentially an infinite-mass piston
- It is driven at a specified speed into the bulk silicon
- Piston speed was varied to observe onset of amorphization and non-diamond structure formation
  - Speeds varied from 0.8 to 1.5 km/s
  - Results shown here are from 1.25 km/s
- The modified Tersoff potential for Silicon was used (Kumagai et al.)

Simulation Tools

- Simulations were performed using LAMMPS
- Visualization was done using OVITO
- Computing resources were provided by Lawrence Livermore National Labs

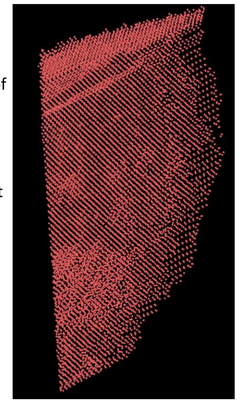


Simulation Results and Exploring Silicon Structure



Non-Diamond Structures in Shocked Silicon

A cutaway of one lamellae of non-diamond Silicon. While some amorphous regions exist at the most disordered places, the majority exhibits some long-range order



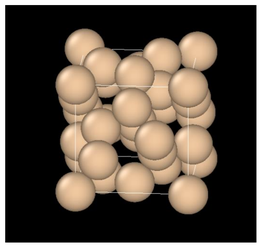
Amorphization has been identified previously in shocked silicon, both experimentally and in simulations. These small pockets of amorphization occur at the highest concentrations of defects within the shocked region, generally at the intersections between different stacking faults formed by the shock.

However, the bulk of the deformed silicon is not amorphous, and is also no longer in its initial diamond cubic phase.

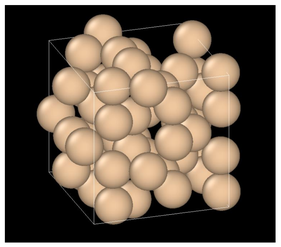
Identifying the phase of this disordered phase was the primary goal of this research, as well as other measures of energy storage and density within the disordered phase.

Some potential structures of silicon were probed using methods such as radial distribution functions and angular distribution functions

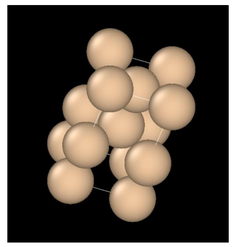
BC8 Silicon



ST12 Silicon



BCT5 Silicon

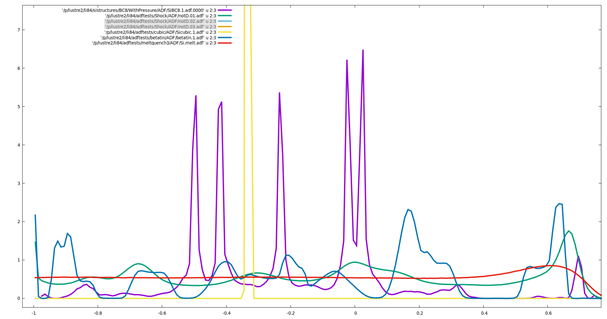


Identifying Structure within the Shocked Region

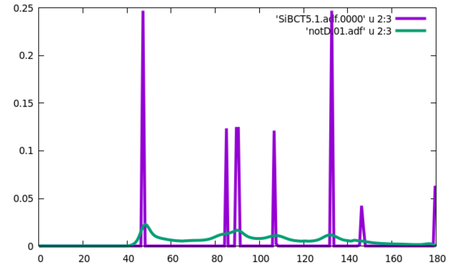
Some known structures of silicon such as beta tin, BC8, ST12, Hexagonal, BCT5, Imma, etc. were modeled using xyz format and replicated into larger systems. Analyses were performed on these larger systems to determine measurements such as their radial distribution functions and angular distribution functions.

The most discernable data came from the angular distribution functions (ADF), which compare the angles between any three atoms within the system within a certain cutoff distance. The ADF for the shocked silicon was compared with the ADF for each of the modeled crystal structures to find the best match. The BCT5 system was found to have the closest match with the shocked silicon region.

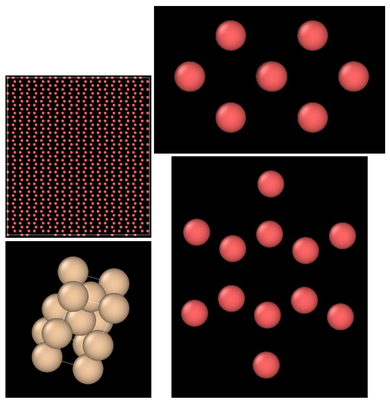
Part of the shocked silicon region was then manually cut apart to isolate a section that could be matched to the structure of BCT5.



ADF for several different Silicon structures



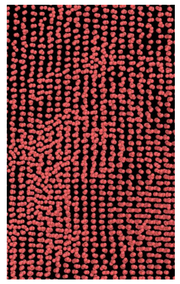
The positive match with the BCT5 structure against the shocked silicon

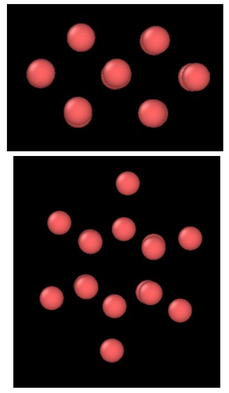


Left: Pristine modeled BCT5 at 1K with no imperfections.

Right: A cut out section of the shocked silicon region, then rotated to orient it along the same axes as the pristine BCT5 model.

The match is very good, with some misalignment in the shocked silicon due to thermal fluctuation and stress.





Summary and Acknowledgments

- Silicon is a well studied material that provides a basis for examining shock in covalently bonded solids
- Structures were identified within the shocked disordered region by matching with known structures using distribution functions.
- These results may be applicable to similarly structured materials such as diamond-like carbon, a material of much interest for future simulations.

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