Abstract Submitted
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Amorphization and nanocrystallization of silicon under laser shock compression: bridging experiment with atomic simulation.[1]
SHITENG ZHAO, BIMAL KAD, ERIC HAHN, Univ of California - San Diego, BRUCE REMINGTON, CHRISTOPHER WEHRENBERG, Lawrence Livermore National Laboratory, EDUARDO BRINGA, Universidad Nacional de Cuyo, CHANNING HUNTINGTON, HYE-SOOK PARK, Lawrence Livermore National Laboratory, KARREN MORE, Oak Ridge National Laboratory, MARC MEYERS, Univ of California - San Diego — Terawatt, nanosecond-duration, laser-driven, shock compression and recovery experiments on [001] silicon unveiled remarkable structural changes above a pressure threshold. Two distinct amorphous regions were identified: (a) a bulk amorphous layer close to the surface and (b) amorphous bands initially aligned with {111}slip planes. Further increase of the laser energy leads to the re-crystallization of amorphous silicon into nanocrystals with high concentration of nano-twins. Shock-induced defects play a very important role in the onset of amorphization. Calculations of the free energy changes with pressure and shear, using the Patel-Cohen methodology, are in agreement with the experimental results. Molecular dynamics simulation corroborates the amorphization, showing that it is initiated by the nucleation and propagation of partial dislocations. The nucleation of amorphization is analyzed by classical nucleation theory.

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