Non-equilibrium simulations of 4H silicon carbide.

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Objective

Using non-equilibrium molecular dynamics simulations, we aim to validate experimental results of laser shock-recovery experiments, where post-mortem high-resolution transmission electron microscopy revealed that above a certain shock threshold, directional amorphous bands form following the formation of stacking faults.

Introduction

Silicon carbide is used in armor¹ and as a semiconductor for high temperature applications¹. There are over 200 polymorphs, whose structural variations arise from different stacking sequences of Si-C double layers.¹,² Figure 1 compares the 3C and 4H SiC structures. In past experiments and simulations, 3C SiC (cubic with periodicity of 3 Si-C double layers) has been shown to undergo a phase transformation to 2H (hexagonal with periodicity of 2 Si-C double layers) when subjected to pressures ranging from 70 to 140 GPa.²,⁹,¹¹ 4H SiC is under-explored in comparison to 3C SiC.

Experiments were performed to explore the behavior of 4H SiC subject to extreme shock loading². Figure 4c shows a high-resolution TEM image of an amorphous domain embedded in a crystalline matrix that was shocked at approximately 50 GPa. These experiments motivated simulations of 4H SiC since the formation of directional amorphous bands was unexpected. The goal of these simulations is to verify experimental results while attempting to explore the mechanisms of phase change. Experimental and simulation results show strong agreement.

Method

Simulations of SiC were performed using the LAMMPS package¹. Initially, a modified Tersoff interatomic potential¹ was considered, but the Vashishta interatomic potential² was used since it is better suited for desired pressure regimes. Figure 2 compares selected values of elastic constants produced by both potentials, illustrating how the modified Tersoff potential behaves unrealistically at pressures greater than 35 GPa.

Results

Using a controlled piston, we produce a shock wave along the [0001] axis and observe the formation of defects along the basal plane, perpendicular to the shock front. Figure 4a shows the formation of lattice rotation and stacking faults following the shock wave. Figure 4b shows how these defects nucleate to form a seemingly amorphous phase. Shear-driven defects continue to evolve as the shock wave propagates through the system and new phases form, leading to further directional amorphization. As shown in figure 4c, present results agree with experiments¹² where horizontal stacking faults and amorphization are observed following laser shock compression and recovery. Post-mortem high-resolution transmission electron microscopy revealed that above a certain shock threshold, directional amorphous bands are observed in the vicinity of the shock surface. The directionality of the bands tends to show agreement between the simulations and the experiment.

Conclusions

• Formation of directional amorphous bands in the vicinity of the shock surface is supported by both experiment and simulation.
• Examination of individual atoms indicate that silicon and carbon atoms tend to stay coordinated in the amorphous phase.
• This phenomenon may be analogous to the transformation of 3C SiC to 2H SiC at high shock pressures.
• Early results show that what seems to be an amorphous phase may partially be nanograins of other silicon carbide solid phases. Further study is being performed to identify these phases and verify their existence.

References