Graduate Student Research Seminar

Fall 2022

Molecular dynamics simulation of fused silica under shock impact: parameter characterizations

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Advisor: Dr. Huijuan Zhao

Monday, September 26th

3:00 pm (EST) – 132 Fluor Daniel Building

Abstract

Silica is one of the most abundant substances on earth. Chemically expressed as SiO2, silica exhibits a complicate phase diagram with multiple crystalline structures (polymorphs) at different temperature and pressure conditions. Under a shock impact, a significant amount of energy will be effectively absorbed due to the phase transition of fused silica to stishovite, thereby taking most of the destructive energy away from these structures. Therefore, it is important to have a reliable method to investigate the mechanism behind the phase transition between fused silica and stishovite in order to better adopt this material as energy absorption and protection materials for future combat protection applications. In this work, multi-scale shock technique (MSST) method is characterized to study the shock impact of fused silica. The BKS potential is employed to define the interatomic potential of fused silica. We calibrate two artificial MSST parameters, Q and tscale, with respect to the simulation box size and understand the impact of cutoff radius r_c to the phase transition of fused silica under various shock velocity conditions. We found that the selection of r_c in the BKS potential can influence the nucleation, formation, and growth of stishovite at different shock velocity conditions. Future work will be focusing on the development of MSST method to eliminate the parameter calibration and better predict the material behavior under shock impact.

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