World Academy of Science, Engineering and Technology
International Journal of Physical and Mathematical Sciences
Vol:11, No:05, 2017

Shock-Induced Densification in Glass Materials: A Non-Equilibrium Molecular Dynamics Study

Authors : Richard Renou, Laurent Soulard

Abstract : Lasers are widely used in glass material processing, from waveguide fabrication to channel drilling. The gradual damage of glass optics under UV lasers is also an important issue to be addressed. Glass materials (including metallic glasses) can undergo a permanent densification under laser-induced shock loading. Despite increased interest on interactions between laser and glass materials, little is known about the structural mechanisms involved under shock loading. For example, the densification process in silica glasses occurs between 8 GPa and 30 GPa. Above 30 GPa, the glass material returns to the original density after relaxation. Investigating these unusual mechanisms in silica glass will provide an overall better understanding in glass behaviour. Non-Equilibrium Molecular Dynamics simulations (NEMD) were carried out in order to gain insight on the silica glass microscopic structure under shock loading. The shock was generated by the use of a piston impacting the glass material at high velocity (from 100m/s up to 2km/s). Periodic boundary conditions were used in the directions perpendicular to the shock propagation to model an infinite system. One-dimensional shock propagations were therefore studied. Simulations were performed with the STAMP code developed by the CEA. A very specific structure is observed in a silica glass. Oxygen atoms around Silicon atoms are organized in tetrahedrons. Those tetrahedrons are linked and tend to form rings inside the structure. A significant amount of empty cavities is also observed in glass materials. In order to understand how a shock loading is impacting the overall structure, the tetrahedrons, the rings and the cavities were thoroughly analysed. An elastic behaviour was observed when the shock pressure is below 8 GPa. This is consistent with the Hugoniot Elastic Limit (HEL) of 8.8 GPa estimated experimentally for silica glasses. Behind the shock front, the ring structure and the cavity distribution are impacted. The ring volume is smaller, and most cavities disappear with increasing shock pressure. However, the tetrahedral structure is not affected. The elasticity of the glass structure is therefore related to a ring shrinking and a cavity closing. Above the HEL, the shock pressure is high enough to impact the tetrahedral structure. An increasing number of hexahedrons and octahedrons are formed with the pressure. The large rings break to form smaller ones. The cavities are however not impacted as most cavities are already closed under an elastic shock. After the material relaxation, a significant amount of hexahedrons and octahedrons is still observed, and most of the cavities remain closed. The overall ring distribution after relaxation is similar to the equilibrium distribution. The densification process is therefore related to two structural mechanisms: a change in the coordination of silicon atoms and a cavity closing. To sum up, non-equilibrium molecular dynamics were carried out to investigate silica behaviour under shock loading. Analysing the structure lead to interesting conclusions upon the elastic and the densification mechanisms in glass materials. This work will be completed with a detailed study of the mechanism occurring above 30 GPa, where no sign of densification is observed after the material relaxation.

Keywords : densification, molecular dynamics simulations, shock loading, silica glass
Conference Title : ICSCCM 2017 : International Conference on Shock Compression of Condensed Matter
Conference Location : Berlin, Germany
Conference Dates : May 21-22, 2017