Study of silica glass using density functional tight-binding approach

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Abstract

In order to explore the structural mechanisms responsible for the plastic behaviour and polyamorphism in silica glass, we perform Molecular Dynamics (MD) simulations within the framework of Density Functionnal Tight-Binding (DFTB) approach (1). The DFTB method provides a description of atomic interactions with an accuracy almost similar to standard ab initio methods used in materials science (e.g. Density Functional Theory), but with a computational loading considerably lower. Recently, the DFTB approach applied to compressed silica (SiO2) glasses has shown that the structural changes from low- to high-density amorphous structures occur through a sequence of percolation transitions (2). These transitions also provide an explanation of some of the mechanical properties of silica glass such as the Bulk modulus. Thus, the presence of percolation networks in silica glass sheds light on amorphous-amorphous phase transitions.
In the present work, we present a more in details analysis of the local structures, their connectivity and features at medium range order. Hence, we have studied how the conformation of various polyhedra does change under compression, as well as how the network connectivity evolves from corner-sharing to edge- and face-sharing. We have also investigated the rings distribution and their conformation under pressure. We also present some results obtained for decompressions starting at pressures above the elastic to plastic limit around 10 GPa. In particular, we have observed various hysteresis for the pressure dependence of the density, the structural properties and percolation transitions.

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