THERMAL CONDUCTIVITY AND STRUCTURAL CHANGES IN ULTRA-HIGH PRESSURE TREATED SILICA GLASS – A MOLECULAR DYNAMICS STUDY

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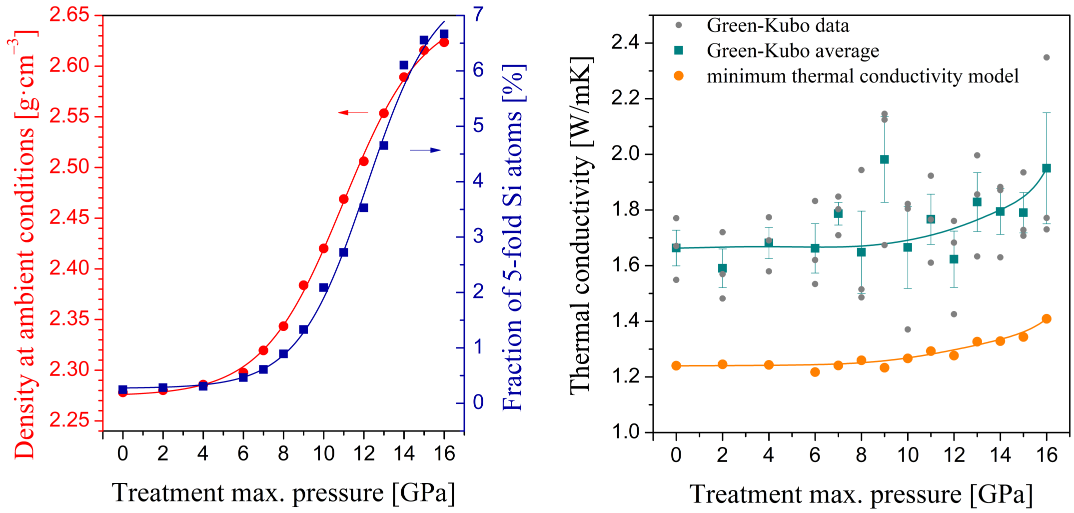

Fig. 1. The calculated density and 5-fold silicon fraction dependence on the maximal treatment pressure as well as the thermal conductivity change.

Silica is a common material with a wide range of commercial applications – including the production of glass, concrete and semiconductors. Amorphous silica is considered an archetypal tetrahedral glass, and is a component of most glasses due to its abundance and exceptional glass-making properties [1]. The objective of this study [2] was to calculate the thermal conductivity of amorphous silicon oxide SiO_2 structures after they were treated under ultra-high pressure using molecular dynamics. Previous studies have concluded that silica glass undergoes permanent densification through the increase of silicon-oxygen coordination number when subjected to ultra-high pressure of the order of GPa [3,4], although to our knowledge no study of the influence of this process on thermal conductivity yet exists.

The amorphous silica structures were obtained by melt-quenching using the LAMMPS [5] molecular dynamics software and the SHIK-1 empirical potential [6]. Then, they were pressed to maximal pressures from 2 GPa to 16 GPa and subsequently relaxed. The thermal conductivity of these samples was determined using the equilibrium Green-Kubo method [7]. The results show an increase in thermal conductivity. They were compared with the minimum thermal conductivity model, which also predicts a rise in thermal conductivity, though not as sharp as the MD simulation suggests.
The increase in density was also investigated and compared with the literature. The local structure of the samples was investigated for high-pressure treatment induced changes. An increase in silicon-oxygen coordination was observed, caused by the increased fraction of 5-fold coordinated silicon. An interesting finding is the tendency of 5-fold silicon atoms to cluster.

This computational study gives a clue that high-pressure treatment of silica glass should lead to a noticeable and permanent increase in its thermal conductivity. Experimental confirmation of this phenomenon is still expected.

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