Structural study of amorphous GeO₂ under high pressure by

means of X-ray absorption spectroscopy

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Amorphous germanium dioxide (GeO₂) is a structural equivalent of silicon dioxide (SiO₂) that undergoes structural changes under high pressure. It is already known from previous studies, that in the range of 0-6 GPa the bond length and the coordination number of the first Ge-O coordination shell remain almost unchanged, while at higher pressures (6-12 GPa) a gradual shift from the tetrahedral to the octahedral arrangement takes place [1,2]. In this contribution, besides the analysis of the first coordination shell, the evolution of other structural parameters (Ge-Ge distance and coordination number, O-Ge-O and Ge-O-Ge bond angle distribution) is investigated using EXAFS data analysis (peak-fitting approach). Spectra collected in the range from 0.0 to 5.1 GPa are analyzed. A clear decreasing trend with pressure can be seen for the Ge-Ge distance, which may indicate pressure-induced changes in the packing of the tetrahedral primary structural units. Further insight into this will be gained by Reverse Monte Carlo analysis using the RMC-GNXAS code [3,4].

References

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