Germanium coordination and bond distances in compressed amorphous GeO2 up to 100 GPa by valence-to-core X-ray emission spectroscopy

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Abstract

The application of valence-to-core X-ray emission spectroscopy (vtc-XES) to DAC experiments is a developing field of research. This probe allows insight into the pressure evolution of electron binding energies and electronic transition probabilities.
In the case of germanium oxides, this information can be extracted from the oxygen 2s -> germanium 1s crossover transition emission line, whose energy and intensity are directly proportional to the germanium coordination and the Ge-O bond distances, respectively. This makes vtc-XES a powerful tool for germanium oxides at high pressure, complementary to X-ray diffraction (XRD) and extended X-ray fine structure absorption spectroscopy (EXAFS) measurements. The information from measured and modeled vtc-XES spectra is extracted in a simple straight-forward way, without additional parameters or assumptions concerning density.
We compressed amorphous GeO2 up to 100 GPa in diamond anvil cells (DAC) and measured germanium valence-to-core X-ray emission spectra. The 6-fold coordination is reached at 20 GPa. At about 50 GPa, a further coordination increase is observed, and the average coordination reaches about seven at 100 GPa, in agreement with the recent XRD study of Kono et al. 2016.

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