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Packing systematics of the silica polymorphs: The role played by O-O nonbonded interactions in the compression of quartz

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Abstract

The anion skeleton of quartz is a distorted body-centered cubic (BCC) arrangement. A hypothetical ideal BCC crystal structure for quartz has been derived and used to locate and describe the unoccupied tetrahedral sites, quantify the distortion of the quartz anion arrangement from ideal BCC, and characterize the role of tetrahedral distortion and O-O interactions in the compression of quartz. Quartz has eight crystallographically nonequivalent tetrahedra, one occupied by silicon and seven unoccupied. These tetrahedra completely fill space, something that cannot be done using only regular tetrahedra. In ideal BCC quartz, the nonequivalent tetrahedra are identical in size and shape with a unique geometry and are referred to as Sommerville tetrahedra. In reality, the unoccupied tetrahedra of quartz are very distorted from both regular and Sommerville tetrahedra. Changes in the unoccupied tetrahedra are responsible for most of the compression in quartz with pressure, as the volume of the Si tetrahedron decreases by <1% over 10.2 GPa, but the volume of the bulk structure decreases by almost 16%. The ideal BCC quartz has been used to quantify the distortion from ideal BCC of the O arrangement in quartz at several pressures up to 10.2 GPa. Distortion decreases by over 60% across this domain. Other parameters have been derived to quantify the distortion of the unoccupied and occupied tetrahedra in quartz from Sommerville tetrahedra, the characteristic tetrahedra of BCC. By all measures, the anion packing in quartz approaches ideal BCC as pressure increases. The compression mechanisms of quartz are compared to those of cristobalite and coesite. Si-O-Si angle-bending controls compression in each of these minerals. The bulk moduli of these minerals are shown to correlate with average nearest inter-tetrahedral anion distances, consistent with the hypothesis that anion-anion interactions stiffen the Si-O-Si angle as inter-tetrahedral anion distances decrease. The tetrahedral distortion in quartz with pressure is attributed to anion-anion interaction, and is not considered a compression mechanism.

Keywords: Quartz, high pressure, body-centered cubic, packing