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Molecular dynamics simulation of polymorphic and polyamorphic transitions in tetrahedral network glasses: BeF_2 and GeO_2

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Abstract

It is well know that tetrahedral network glasses have anomalous properties such as a density maximum and bulk modulus minimum. The magnitudes of such anomalous properties are different among tetrahedral network glasses. The origin of this anomaly has not been explained yet. We had already analyzed the local structural changes in SiO_2 in terms of transformation of 'structon'. The fragments of Si_2O_7 were categorized into four types named alpha-, beta-, gamma-, and delta-'structons'. In this study we use molecular dynamics simulations to investigate the structural changes in crystalline and vitreous BeF_2 and GeO_2. First the simulated BeF_2 cristobalite and quartz clearly reproduce their alpha–beta transitions and the density in the vitreous BeF_2 shows a maximum around 2300 K. On the contrary, GeO_2 shows weak alpha–beta like transitions in cristobalite and quartz, and a density maximum is not observed in the vitreous phase. Next we perform the 'structon' analyses on BeF_2 and GeO_2. For the BeF_2 system the conversion between alpha- and beta-'structons' are almost complete, as previously observed in our study on the SiO_2 system. On the other hand, such transformation is incomplete in the GeO_2 system. We discuss similarities and dissimilarities between SiO_2, BeF_2, and GeO_2.

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