MD calculation of elastic properties and post-rutile transitions of SiO2, GeO2 and MnF2

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Many high-pressure experiments of SiO2 and its analogue materials has been executed to elucidate a post-rutile phase. These studies shows that fluorides directly transforms to the fluorite-type structure having higher cation coordination, but that oxides transform to the CaCl2-type structure without coordination change. Molecular dynamics (MD) calculations with model interatomic potentials also predicted similar phase relations correctly. In this study, from a viewpoint of elastic properties, we discuss the reason that oxide and fluoride rutiles have different high-pressure forms. We predict that stability parameters of SiO2 and GeO2 have opposite temperature dependence to it of MnF2.

The post-rutile transition of stishovite, which is a high-pressure polymorph of SiO2, is quite important to Eath's mantle science. Many high-pressure experiments of SiO2 and its analogue materials has been executed to elucidate a post-rutile phase. These studies shows that fluorides directly transforms to the fluorite-type structure having higher cation coordination, but that oxides transform to the CaCl2-type structure without coordination change. Molecular dynamics (MD) calculations with model interatomic potentials also predicted similar phase relations correctly. In this study, from a viewpoint of elastic properties, we discuss the reason that oxide and fluoride rutiles have different high-pressure forms. We predict that stability parameters of SiO2 and GeO2 have opposite temperature dependence to it of MnF2.