

## MD calculation of elastic properties and post-rutile transitions of SiO<sub>2</sub>, GeO<sub>2</sub> and MnF<sub>2</sub>

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Many high-pressure experiments of SiO<sub>2</sub> 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 CaCl<sub>2</sub>-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 SiO<sub>2</sub> and GeO<sub>2</sub> have opposite temperature dependence to it of MnF<sub>2</sub>.

The post-rutile transition of stishovite, which is a high-pressure polymorph of SiO<sub>2</sub>, is quite important to Eath's mantle science. Many high-pressure experiments of SiO<sub>2</sub> 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 CaCl<sub>2</sub>-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 SiO<sub>2</sub> and GeO<sub>2</sub> have opposite temperature dependence to it of MnF<sub>2</sub>.