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Novel pressure induced transition sequence in engineering high entropy rutile TiO_2

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Rutile structure is a highly stable phase among all polymorphs of TiO_2 at ambient conditions. A number of experimental and theoretical studies indicate that TiO_2 has a series of high-pressure phases such as baddeleyite. Rutile TiO_2 is a good analogue system for the key mineral SiO_2, especially under high pressure conditions, since it would undergo pressure induced phase transitions at significantly lower pressure range compared to silica. Shock wave modification on the phase transition sequence on rutile TiO_2 was reported recently. Here we would like to demonstrate other approach for simulations of the real complicated multiple element situations in mantle environments. High entropy oxides (HEO) are single-phase oxides composed of muti-elements developed from high entropy alloys. The compositional flexibility of HEO provides infinite possibilities for the application of high entropy oxides in various fields. By taking advantage of the potential cocktail effect of HEO, we designed and synthesized rutile-type HEO ($Ti_{0.2}Fe_{0.2}Ta_{0.2}Sn_{0.2}Ge_{0.2}O_2$) and its referenced samples ($Ti_{0.33}Fe_{0.33}Ta_{0.33}O_2$ and $Ti_{0.25}Fe_{0.25}Ta_{0.25}Sn_{0.25}O_2$) by solid-phase method. The structures and properties of these HEOs were analyzed by X-ray diffraction (XRD), SEM, high resolution TEM, X-ray absorption spectra, Raman and UV-VIS, and heat capacity measurements, to reveal their disorder, local lattice strain, and entropy features. In order to detect the local structure distortion of rutile-type HEO and potential phase transition under pressure, *in situ* high-pressure Raman spectra were measured in a diamond anvil cell (DAC) at room temperature. The *in situ* high pressure synchrotron XRD experiments were carried out up to 60 GP, to reveal the pressure induced phase transitions in these 3 types rutile-type HEOs. Although the structural transition under high pressure of conventional rutile TiO_2 has been extensively studied, the influence of high configuration entropy on the structural stability of rutile-type HEO under high pressure conditions offer us new opportunity to discover the unconventional phase transition sequence upon compression. This will shed light on the structural transitions in the complicated compositional real world case.

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