American Mineralogist, Volume 97, pages 524–531, 2012

Incorporation of Si into TiO_2 phases at high pressure

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ABSTRACT

Silicon incorporation in TiO_2 phases at increasing pressures until 20 GPa at 1300 °C has been studied by XRD and TEM. Rutile is the stable Si-doped TiO_2 phase until at least 7 GPa, transforming into α-PbO_2 structured TiO_2 between 7 and 10 GPa. The further transformation to the TiO_2 polymorph with the baddeleyite structure, akaogiite, has not been observed on the quenched samples. XRD and TEM-EDX data suggest that the Si-doped TiO_2 akaogiite polymorph is non-quenchable and reverts to α-PbO_2 structured TiO_2 when releasing the pressure. This transformation gives rise to α-PbO_2 structured TiO_2 grains decorated with π fringes stacking faults. Silicon solubility in TiO_2 phases increases with increasing the synthesis pressure until 16 GPa, implying the substitutional solid solution to be the mechanism of solubility. The influence of the dopants on the stability of the rutile and the α-PbO_2 structured TiO_2 has also been analyzed.

Keywords: Rutile, TiO_2-II, akaogiite, silica, high pressure, geobarometer, TEM, solid solutions, π fringes stacking faults