K134-P012 **Room: Poster Session Hall** **Time: May 16**

Phase transition in TiO2 at high pressure and the bulk modulus of TiO2 polymorphs

Daisuke Hamane[1]; Taku Okada[2]; Takehiko Yagi[2]

[1] ISSP Tokyo Univ.; [2] Inst. Solid State Phys, Univ. Tokyo

Titanium dioxide (TiO_2) has many polymorphs with a series of the structural phase transformation at elevated pressure with anatase, brookite and rutile being the most abundant in nature. Under high pressure, TiO_2 transforms to the alpha-PbO_2 phase, the baddeleyite phase, the OI phase, and the cotunnite phase with increasing pressure. The bulk modulus for the cotunnite phase was reported to be 431 GPa that is close to the bulk modulus for diamond, 444 GPa (e.g. Dubrovinsky et al., 2001). It is, however, noted that the bulk modulus for the cotunnite phase was obtained under the non-hydrostatic condition using unknown pressure scale. Recently, a fluorite-like cubic phase was also proposed as a stable phase at the pressures above 40 GPa rather than the cotunnite phase (Mattesini et al., 2004). However, the fluorite cubic phase was not found even at 60 GPa in the previous studies (e.g. Dubrovinsky et al., 2001), and thus the phase relation in TiO2 above 40 GPa is still controversial.

In this study, we report the phase transitions in TiO_2 at high pressure up to 70 GPa and the bulk modulus for the high pressure polymorphs of TiO_2 under the quasi-hydrostatic conditions using a diamond anvil cell combined with a laser heated technique.

The transition sequence was rutile, alpha-PbO_2 phase, baddeleyite phase, OI phase, and cotunnite phase with increasing pressure. The fluorite-like cubic polymorph was not found at least up to about 70 GPa in this study. The Birch-Murnaghan equation of state under the quasi-hydrostatic conditions using the platinum pressure scale by Holmes et al. (1989) yields V_0 = 18.40 (11) cm^3/mol and K_0 = 206(4) GPa for the alpha-PbO_2 phase, V_0 = 17.36 (4) cm^3/mol and K_0 = 175(5) GPa for the baddeleyite phase, V_0 = 16.83 (10) cm^3/mol and K_0 = 222(14) GPa for the OI phase, and V_0 = 15.09 (7) cm^3/mol and K_0 = 309(12) GPa for the cotunnite phase. Although the cotunnite phase is least compressible among the TiO_2 polymorphs, the isothermal bulk modulus is much smaller than that of the diamond.