**Compressibility and Evidence of Amorphisation of 6 nm $TiO_2$ Nano-anatase**

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$TiO_2$ in the macrocrystalline and nanocrystalline forms is an important material with a variety of industrial applications. Recent high pressure experimental studies have demonstrated that the behavior of nano-anatase may be quite different to that of the macrocrystalline form [1],[2],[3]. Although, to date there has been no XRD structural characterization of nano-anatase at high pressures for grain sizes less than ~30nm.

$TiO_2$ nano-anatase with an average grain size of ~ 6 nm has been studied at room temperature and high pressure up to ~30 GPa using synchrotron X-ray diffraction. The nano-anatase phase remains stable up to ~18 GPa, after which the degree of disorder increases progressively and the material becomes completely amorphous at pressures beyond ~24 GPa. The effect of external pressure on ultrafine nano-anatase ($d$<10nm) has been investigated in conjunction with molecular dynamics (MD) simulations, in an attempt to elucidate the mechanism of pressure-induced amorphisation.

Ultrafine nanocrystals are constituted of a core/surface shell structure that may have distinct elastic properties. Above $P$~6 GPa where there is a monotonic decrease of the volume, a Birch-Murnaghan fit to the data yielded a bulk modulus $K = 237 \pm 3$ GPa (with $K' = 4$, fixed). Thus the 6 nm nano-anatase shows an enhanced bulk modulus in comparison with the macrocrystalline counterpart and is equal to that reported for 30 nm nano-anatase[3]. The MD simulations suggest that the disorder is initiated in the shell and propagates to the core of the nano-structure.

[1] Wang Z., Saxena S.K., *Solid State Commun*., 2001, **118**, 75-78. [2] Hearne G.R., Zhao J., Dawe A.M., Pischedda V., Maaza M., Niewoudt M.K., Kibasomba P., Nemraoui O., Comins J.D., Witcomb M.J., *Phys. Rev*., 2004, **B70**, 134102. [3] Swamy V., Dubrovinsky L.S., Dubrovinskaia N.A., Simionovici A.S., Drakopoulos M., Dmitriev V., Weber H.P, *Solid State Commun*., 2003, **125**, 111.

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