Compression Behavior of Zr-doped Nanoanatase

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The compression behavior of Zr-doped nano anatase $T_{i_{0.90}}Zr_{0.10}O_2$ synthesized by the sol-gel method was studied using a diamond anvil cell (DAC) up to ~ 13 GPa. The compressibility parallel to the *a* axis decreases strongly at ~ 4 GPa and other structural parameters also change with pressure. The parameters of the third order Birch-Murnaghan equation of state were fitted to: $V_0 = 139.6(0) \text{ Å}^3$, $K_0 = 213(9)$ GPa and K' = 17.9(2). *Ab initio* electronic structure simulations indicate that the Zr atoms cluster in the crystal. The effects of chemical substitution as well as of microstructure, especially the crystallite size, on the mechanical properties are discussed.

Key words: High-pressure, Nanocrystals, Titania, Zirconia, Anatase, Dopant