COMPOSITION INDUCED CHANGES IN OPTICAL RESPONSE OF $Ti_{(1-X)}Si_XO_2$ FROM FIRST PRICIPLES CALCULATIONS

ONDRAČKA Pavel, HOLEC David, FRANTA Daniel, KEDROŇOVÁ Eva, ELISABETH Stéphane, ELIÁŠ Marek, GOULLET Antoine, ZAJÍČKOVÁ Lenka

Masaryk University, Brno, Czech Republic, EU
Institute of Physics of the AS CR, v.v.i. - CEITEC, Prague, Czech Republic, EU;
University of Leoben, Leoben, Austria, EU;
University of Nantes, Jean Rouxel Materials Institute, Nantes, France, EU

Abstract

Mixed TixSiyOz materials offer interesting optical properties due to the high difference between refractive indices (TiO2: ~2.5, SiO2:~1.5) and band gaps (TiO2: ~3.2 eV, SiO2: ~8.5 eV). By changing composition a fine-tuning of the optical properties is possible. This opens new possibilities in design of optical devices.

In the present work, the variation of Ti(1-x)SixO2 optical constants caused by changed Si concentration are examined by employing Density Functional Theory. Special Quasirandom Structures method is used to generate structural models of Ti(1-x)SixO2 disordered solid solutions based on TiO2 and SiO2 phases. These initial supercells are structurally optimized (i.e. optimized with respect to the cell shape, size, and atomic positions) using the Vienna Ab initio Simulation Package. Ab initio Molecular Dynamics approach ("simulated annealing") is used to generate structural models of amorphous phase. Optical

constants of the resulting structures are calculated by the linearized augmented plane wave method as implemented in the Wien2k code together with the recently developed modified Becke-Johnson exchange-correlation potential allowing precise prediction of electronic structure and band gap. The calculated dielectric function is compared to the experimental

data obtained by fitting the optical measurements (ellipsometry, spectrophotometry) carried out on TiO2 and TixSiyOz films prepared by plasma enhanced chemical vapor deposition and atomic layer deposition.

Keywords: Titanium dioxide, silicon dioxide, optical properties, mixed oxide, density functional theory

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