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Effects of Hydrostatic Pressure on the Elastic Anisotropy of SnO_2 Polymorphs: A First-principles Approach

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Cassiterite (SnO_2) is the most important ore mineral used for extraction of metal tin. Using DFT calculations we investigate the pressure-dependent variations of elastic anisotropy in the following SnO_2 phases: *rutile-type* (tetragonal; $P4_2/mnm$), *$CaCl_2$-type* (orthorhombic; *Pnnm*)-, *α-PbO_2-type* (orthorhombic; *Pbcn*)-, and *fluorite-type* (cubic; *Fm-3m*). We estimate the shear anisotropy (A_1 and A_3) on {100} and {001} crystallographic planes of the tetragonal phase, and (A_1, A_2 and A_3) on {100}, {010} and {001} crystallographic planes of the orthorhombic phases. The rutile-type phase shows strongest shear anisotropy on the {001} planes ($A_2 > 4.8$), and the degree of anisotropy increases nonlinearly with pressure. Conversely, the anisotropy is almost absent on the {100} planes (i.e. $A_1 \sim 1$) irrespective of the pressure. The $CaCl_2$-type phase exhibits similar shear anisotropy behavior preferentially on {001} ($A_3 > 5$), while A_1 and A_2 remain close to 1. The α-PbO_2-type phase shows strikingly different elastic anisotropy characterized by a reversal in anisotropy ($A_3 > 1$ to < 1) with increasing pressure at a threshold value of 38 GPa. Furthermore, we show that the electronic density of states and atomic configuration is crucial for this pressure-dependent reversal in shear anisotropy. The DOS of α-PbO_2-type structure at 40 GPa exhibits multi-peaked structure of the valence band which is indicative of underlying layered structure, which corresponds to the anisotropy reversal. Our study also analyzes the directional Young's moduli for the tetragonal and orthorhombic phases as a function of pressure. The rutile-type SnO_2 phase is the stiffest material due to its high Young's modulus, while fluorite-type SnO_2has the lowest stiffness. The directional Young's moduli of both rutile -type and $CaCl_2$ -type, is very pressure sensitive along the diagonals in {001} plane. Furthermore, in the case of α-PbO_2, the Young's modulus is pressure sensitive on {100} and {010}, rather than {001}.

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