Res. Rev. J Mat. Sci. 2018, Volume 6
DOI: 10.4172/2321-6212-C1-015

Investigation of anisotropic mechanical properties of textured $KSr_2Nb_5O_{15}$ ceramics by ab-initio calculation and nanoindentation

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By applying first-principles calculation based on density functional theory (DFT), elastic properties of $KSr_2Nb_5O_{15}$ (KSN) crystals were derived, involving elastic constants, Young's modulus, Poisson's ratio, bulk modulus and shear modulus, hardness, and universal anisotropy index. Calculated results show that in the KSN lattice, Nb-O forms relative strong covalent effect and Nb-O octahedral distortion causes spontaneous polarization in the KSN crystal. To verify the simulated results experimentally, textured KSN ceramics with highly oriented grains with tetragonal symmetry were fabricated by RTGG (Reactive Template Grain Growth) method. Nanoindentation was carried out on textured samples in parallel and perpendicular to the elongated-shape grains oriented to [001] direction. Measured indentation modulus values are in accordance with the predictions which show an anisotropic ratio of ~10% between the two tested orientations. Predictions of Young's modulus revealed a more pronounced anisotropy with a ratio of ~40% between the [100] direction and at a tilt angle of about 45° from the [001] direction towards the [100].

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