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Electronic and structural properties of 181Ta in anatase and rutile: Experimental study and ab initio calculations

Ab initio calculation of Ta doped anatase and rutile

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oral

Summary

The study of the properties of Titanium Dioxide (TiO2) has been a subject of interest for its wide ranging applications in different fields. However, the current renewal of interest in this material is due to the synthesis of TiO2 nanoparticles and its numerous potential applications [1]. As it is well known that the hyperfine-interaction measurements provide local information as a result of the interaction at the probe nucleus and the surrounding electronic charge distribution, in this study we report the result of hyperfine interaction measurement at 181Hf (181Ta) probes present as an impurity in the anatase phase of TiO2. In addition, we have performed first principle calculations in both phases of TiO2, anatase and rutile, and analyzed the electronic environment around the Tantalum probe atom.

We have performed our calculations based on the density functional theory (DFT) with local orbitals in addition to the augmented plane wave (APW+LO) method as embodied in the WIEN2K code [2]. In order to introduce the Ta impurity a 2×2×3 super cell with 72 atoms in case of rutile and a 2×2×1 super cell with 48 atoms in case of anatase were constructed. Thereafter one of the Ti atoms was replaced by a Ta atom in each case. We optimized the internal position parameter of all atoms and kept the lattice parameters constant. It is observed that for relaxation beyond optimum oxygen nearest neighbor (ONN) distance the change in the electric field gradient (EFG) at Ta sites is insignificant. Calculations were performed with the optimized structure in each case and a reasonable agreement is observed with the experimental results as shown in the table below. However, the nonzero value of for anatase has been attributed to a large distribution width of Q and the poor crystallinity of the anatase sample [3]. We find no significant change in EFG calculated with a charged Ta state in either case. Calculations are in progress to elucidate the variation in experimentally measured TDPAC parameters in Zr-doped rutile TiO2 carried out recently by us.

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