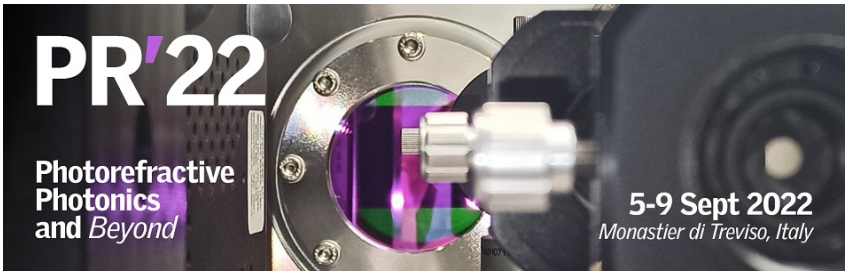

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Optical response of the newly discovered hexagonal phase of Ta2O5 (calculated) from first principles

Thursday, 8 September 2022 16:40 (1h 30m)

Ta2O5 is known as a relatively chemically inert material with high density and high refractive index. It has low absorption and is therefore usually employed in optical coatings for applications from near-UV to near-IR, e.g. for mirror coatings in gravitational-wave detectors.

Experimental studies of thermically produced nanocrystals in amorphous Ta2O5 thin films indicate a new crystalline phase of Ta2O5. These crystals were characterized by Grazing Incidence X-Ray Diffraction (GIXRD). The phase has a hexagonal structure with cell parameters of around 7.2 Å and 3.8 Å. The unit cell includes four Tantalum and ten Oxygen atoms as shown in Fig.1.

This new phase is modeled from first principles in the framework of the Density Functional Theory (DFT) as implemented in VASP [1]. In this work we present, besides the ground state structural properties, the optical response of the newly proposed hexagonal Ta2O5 phase. The optical properties are calculated with different approaches of different precision, ranging from the independent particle approximation to the GW-approach. Additionally, we compare the optical responses of the new hexagonal phase with those of known phases of Ta2O5, e.g. orthorhombic and monoclinic phases.

First results indicate remarkable differences between the investigated phases regarding their linear optical responses. Therefore, it should be possible to differentiate between crystal structures of Ta2O5 by optical measurements, e.g. by comparing their absorption spectra.

In addition, we analyze non-linear optical properties of the hexagonal phase, e.g. THG.

[1] G. Kresse, J. Furthmüller, Computational Materials Science 6, 15 (1996), and G. Kresse, J. Furthmüller, Phys. Rev. B 54, 11169 (1996).

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