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

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Introduction

Ta_2O_5 is known as a relatively chemically inert material with high density and high refractive index. It has low absorption coefficients from near-UV to near-IR and is therefore usually employed in optical coatings, e.g. for mirror coatings in gravitational-wave detectors. One of the main problems gravitational-wave interferometer coatings face is the Brownian thermal noise which is always present at non-zero temperature. In the case of amorphous materials used for these coatings this problem is also coupled with a requirement of very low optical absorption. The main idea therefore is to partially crystallize these coatings to reduce Brownian noise without introducing too much unwanted optical effects like scattering.

Experimental studies of thermically produced nanocrystals in amorphous Ta_2O_5 thin films indicate a new crystalline phase of Ta_2O_5. 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.

Theoretical investigations

This new phase is modeled from first principles in the framework of the Density Functional Theory (DFT) as implemented in VASP [1, 2]. In this work we present, besides the ground state structural properties, the optical response of the newly proposed hexagonal Ta_2O_5 phase. The optical properties are calculated with different approaches of different precision, ranging from the independent particle approximation to the GW-approach (many body perturbation theory). Additionally, we compare the optical responses of the new hexagonal phase with those of known phases of Ta_2O_5, e.g. the orthorhombic and monoclinic phases.

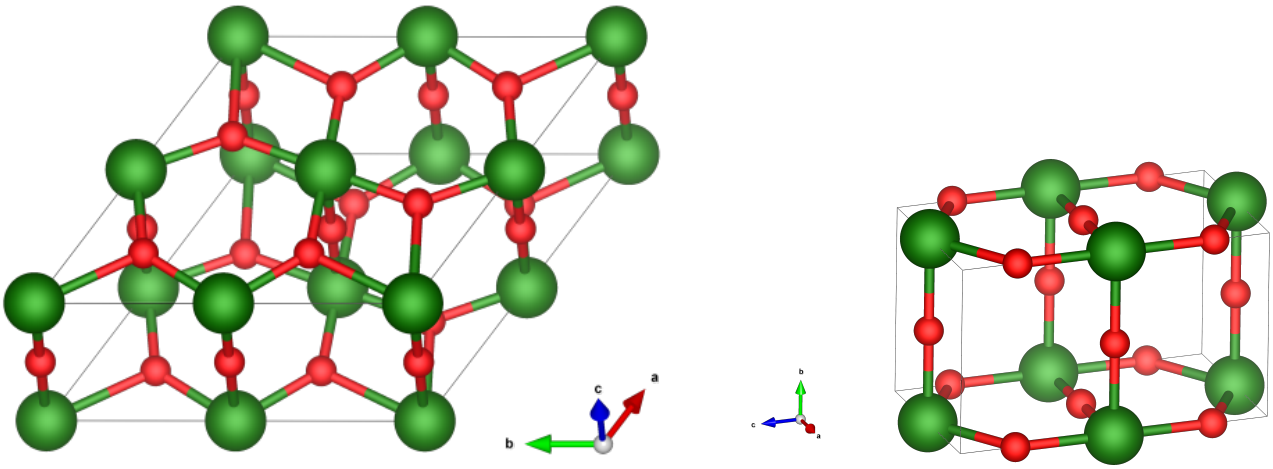

Figure 1: *Left*: Atomic structure of hexagonal δ-Ta_2O_5. The unit cell includes 4 atoms of Tantalum (green) and 10 atoms of Oxygen (red). *Right*: Atomic structure of simplified orthorhombic Ta_2O_5 [3]. The unit cell includes 2 atoms of Tantalum (green) and 5 atoms of Oxygen (red).

First results

Firstly, the experimentally measured cell parameters are in good agreement with the theoretically calculated values with deviations less than 1 %.

In addition, our results indicate remarkable differences between the investigated phases regarding their linear optical responses. E.g. from dielectric function we observe differences between the phases regarding the positions of the main absorption edges. Therefore, it should be possible to differentiate between crystal structures of Ta_2O_5 by optical measurements, e.g. by comparing their absorption spectra.

Conclusions

As the first results are in good agreement with the experiment and in addition predict optical differences between different phases, they could be quite useful to identify crystalline structures of Ta_2O_5 by their optical properties. Additional calculations with a higher precision will be performed for a better quantitative comparison with experimental results.

References

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