Experiment Report

Proposal Code HC-2315

Proposal Title Investigation on the local structure in amorphous Ta2O5 thin films by pair distribution function analysis

Beamline ID31

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The local structure of amorphous films of tantalum oxide (Ta_2O_5) was (and still is) the subject of several investigations on account of its relevance in the field of interferometric gravitational wave detectors. Despite a large number of studies, the structural properties at the local scale of this material still deserve several further investigations. Such information is essential to any attempt aimed to understand the properties of this important technological material and no property modelling efforts can be expected to yield reliable information until the local structure in the amorphous phase is better understood.

The aim of the proposal was to study the local structure of amorphous Ta_2O_5 and amorphous Ti-substituted Ta_2O_5 samples by means of a total scattering experiment with high energy X-rays. This material is applied to build highly reflective mirrors used in interferometric gravitational wave detectors. In order to study the influence of both the annealing and the Ti doping on the coating structure four samples were prepared: pure Ta_2O_5 (annealed and not), Ti-doped Ta_2O_5 (annealed and not annealed). Some of these samples were previously analysed using the same PDF technique at the ID15A beamline, but in that experiment we were able to acquire data for PDF analysis only from two samples. In fact, at first 6 shifts were allocated to analyze the four samples, but afterwards beam time was rescheduled down to only 3 shifts.

PDF data were collected by using a transmission geometry (Fig. 1) from amorphous Ta_2O_5 thin films deposited on amorphous SiO_2 substrates; in order to separate the data from amorphous Ta_2O_5 only, also PDF data from the pure SiO_2 substrate were collected. During the data reduction treatment of the total scattering data, the PDF function of Ta_2O_5 was thus obtained by subtracting the SiO_2 substrate data.

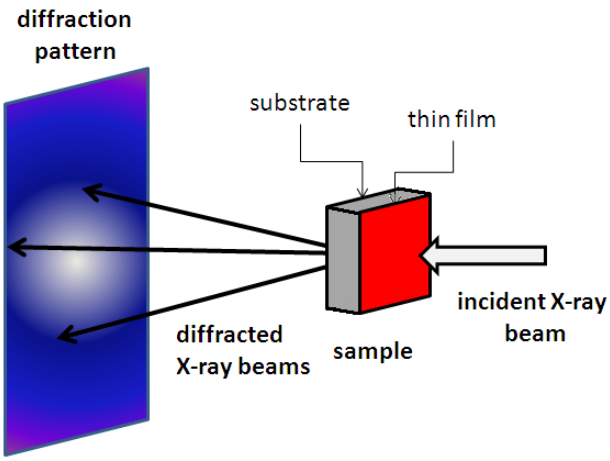

Figure 1: Experimental set-up used for data collection.

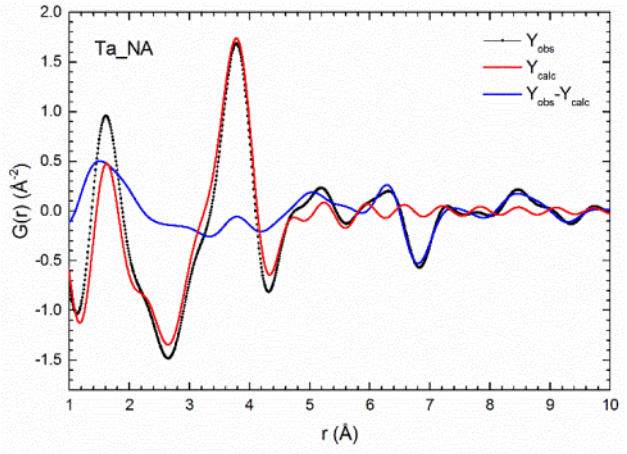

Figure 2: Refinement fit for PDF data of *a*-Ta_2O_5 thin film.

Than the PDF function of Ta_2O_5 was fitted by using several structural models, since that Ta_2O_5 crystallizes with many different polymorphic modifications. As a result we observed a good correspondence (at the local scale, i.e. for r < 5 Angstrom) between the PDF function of amorphous Ta_2O_5 and the monoclinic *C*2 structural model of the *Z*-Ta_2O_5 phase. We further improved the structural model by taking into account the topological properties of O atoms in amorphous Ta_2O_5 as probed by ^{17}O NMR analyses [1], obtaining a reasonably good fitting of our PDF data for all the investigated samples (Fig. 2).

These data provided a relevant step forward in the comprehension of the local structure of amorphous Ta_2O_5 that can find application in the technological development of the future interferometric gravitational wave detectors. At present, a paper has been submitted reporting our findings.

[1] N. Kim, J F. Stebbins, Chem. Mater. **23**, 3460 (2011)