Probing the atomic structure of amorphous Ta_2O_5 mirror coatings for advanced gravitational wave detectors using transmission electron microscopy

Riccardo Bassiri[1], Konstantin B. Borisenko[2], David J. H. Cockayne[2], James Hough[1], Ian MacLaren[1], Sheila Rowan[1]

[1] Department of Physics and Astronomy, University of Glasgow, Glasgow G12 8QQ, United Kingdom

[2] Deapartment of Materials, University of Oxford, Oxford OX1 3PH, United Kingdom

E-mail: r.bassiri@physics.gla.ac.uk

Abstract. Advanced generations of ground-based gravitational wave detectors will use ultra-low-loss amorphous dielectric multilayer mirror coatings in order to minimise thermal noise, a limiting factor in detector sensitivity. Transmission electron microscopy is a promising way to probe the atomic structure of these coatings in an effort to better understand the causes of the observed mechanical loss (internal friction) and hence thermal noise.

1. Introduction

Gravitational radiation emitted from astrophysical sources is currently being searched for by long-baseline interferometric gravitational wave detectors. They are designed to monitor displacements in test masses, which are coated to produce highly reflective mirrors. The detectors themselves are the most sensitive displacement instruments ever to be developed and are able to detect strains from gravitational waves as small as 1 part in 10^{22} [1].

The test mass mirrors are made from ultra pure fused silica or SiO_2 with multilayer amorphous dielectric mirror coatings required for high reflectivity. The coatings currently used in the GEO600 detector in Germany and the LIGO detectors in the US are made up of multiple $\lambda/4$ thickness layers of Ta_2O_5 and SiO_2 [2].

Noise from various sources is a major challenge when attempting to reach such sensitivities. At the highest sensitivity range (from a few 10s Hz to several 100 Hz) thermal noise is a significant noise source. The S5 run from LIGO shows sensitivity of about 1 part in 10^{22}, with planned upgrades to the Advanced LIGO achieving another factor of 10 to 15 improvement in sensitivity [1, 3].

A dominant source of thermal noise is from the mechanical loss of the mirror coatings. The fundamental processes which cause mechanical loss in these coatings are not well understood. The aim of this research is therefore to understand the processes behind the mechanical losses on an atomic scale. Here we use transmission electron microscopy and associated analysis techniques to study for the first time the local structures and bonding in ion-beam-sputtered Ta_2O_5 which has been heat treated to a variety of temperatures. This is an important preliminary step

towards identifying a quantitative relation between atomic structure and macroscopic coating mechanical loss.

2. Experimental methods

The transmission electron microscope (TEM) gives the ability to probe and characterise the atomic structure of the amorphous mirror coatings using reduced density functions (RDFs). Figure 1 (left) shows an image of a typical multilayer mirror coating, the darker sections are the Ta_2O_5 layers. For the purposes of this research, the samples used for analysis have only a single layer of Ta_2O_5 deposited on a silica substrate. Figure 1 also shows a typical amorphous diffraction pattern one would get when looking at only the Ta_2O_5 layer. It is these diffraction patterns that act as the raw data for the RDFs.

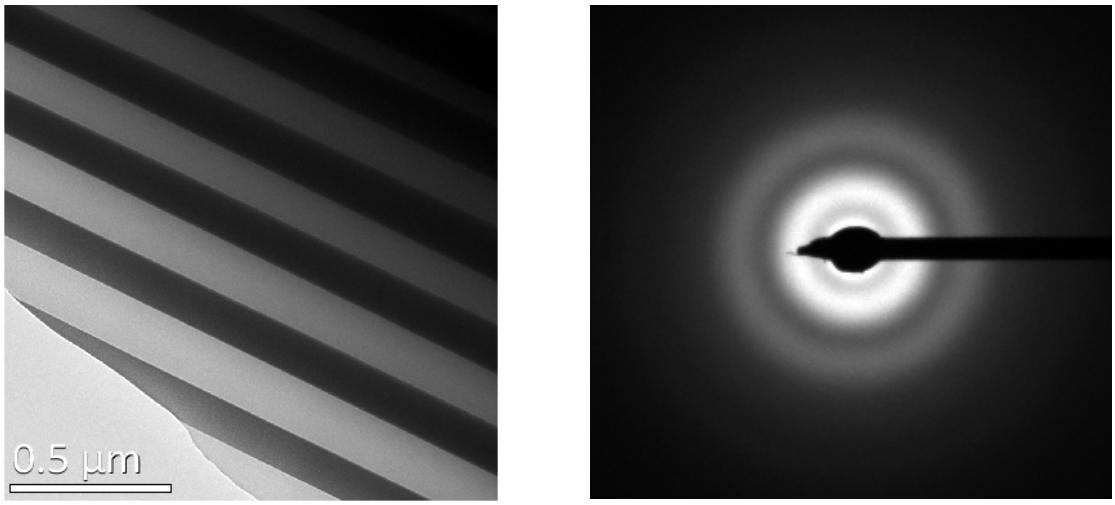

Figure 1. Bright field image of a multilayer coating of dark Ta_2O_5 and light SiO_2 layers (left), CBED amorphous diffraction pattern

The RDF is a statistical representation of where atoms sit with regards to a central atom [4] and can be effectively described as the Fourier transform of the intensity profile one would get from an amorphous diffraction pattern,

$$G(r) = 4\int_0^\infty \varphi(q)\sin(qr)dq, \tag{1}$$

where $q = 4\pi sin\theta/\lambda$, r is the distance from a central atom and $\varphi(q)$ is the reduced intensity function derived from the intensity profile [4].

The peaks of this distribution give information about the nearest atomic neighbours such as the peak intensity, which describes the probability of finding a particular atom at a certain distance. Also, the peak widths are mainly governed by the width of the distribution of interatomic distances with contribution from thermal vibrations, which may be useful for understanding the mechanical loss.

To gain the maximum amount of data from the RDFs, reverse Monte Carlo modelling can be used to model the amorphous structure. Modelling can also be used to find the interatomic bond angles and co-ordination numbers.

The model is produced by firstly randomly packing a defined number of atoms in an defined area and given the atomic boundary conditions of a typical crystalline phase of the material. It is then compared to the experimental RDF via reverse Monte Carlo simulations where the

atoms in the model are re-arranged randomly until they sit in a configuration that agrees with the RDF data, and hence the amorphous phase. Energy optimisation of the model was then carried out using DFT modelling to make sure the atoms are sitting in physically reasonable positions.

Any information we can gain on the atomic structure of these coatings will be interesting in terms of how it relates to the mechanical loss.

3. Results

The RDF and modeling procedure was carried out on three Ta_2O_5 argon-ion beam sputtered coatings that were heat treated at 300, 400 and 600°C. These coated samples were single layers of Ta_2O_5 on a SiO_2 substrate. The process of heat treatment is to leave the sample in an oven under normal atmospheric conditions at a defined temperature for 24hrs.

The mechanical losses of these samples were measured at cryogenic temperatures because new generations of detectors may work at cryogenic temperatures to further reduce noise sources. The samples show that higher heat treatment temperatures correspond to an increasing loss peak at cryogenic temperatures.

The aim of this experiment was to see if there was any difference in the amorphous structures measured using RDFs.

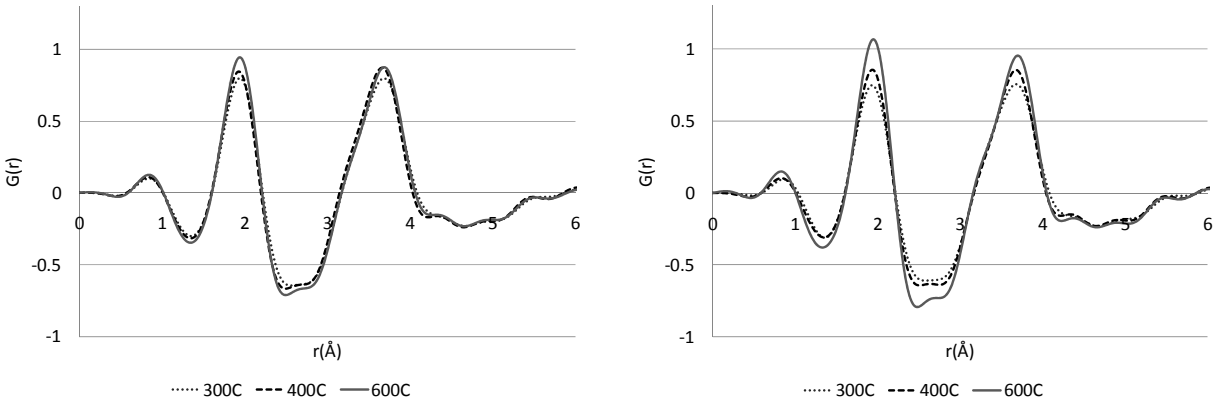

Figure 2. Average RDFs of coatings heat treated at 300, 400 and 600^{o}C (left), Local structure variation showing a greater difference in RDFs at 300, 400 and 600°C (right).

Figure 2 (left) shows three reduced density functions from a tantala layer of mirror coatings heat treated at 300, 400 and 600°C. The averaged RDFs, where RDFs from various areas in the same sample are averaged, show a negligible change as the heat treatment temperature rises. However preliminary investigations into local structural changes, as opposed to averaged areas, suggest that there may be a change in the Ta - O coordination as the heat treatment temperature rises as can be seen in the right of figure 2. Further investigation is required to understand the nature of this change and to relate it to the mechanical loss measurements.

Figure 3 shows the amorphous model generated from the reverse Monte Carlo process and energy optimisation based on the 400°C RDF data. Preliminary results from this model show an average Ta to Ta bond length of 3.28Å and Ta to O bond length of 2.10Å.

What is planned next is to relate this model using the reverse Monte Carlo procedure to the local RDF variation from the 300 and 600°C samples and compare the data, looking for any differences that can be related back to changes in the mechanical loss.

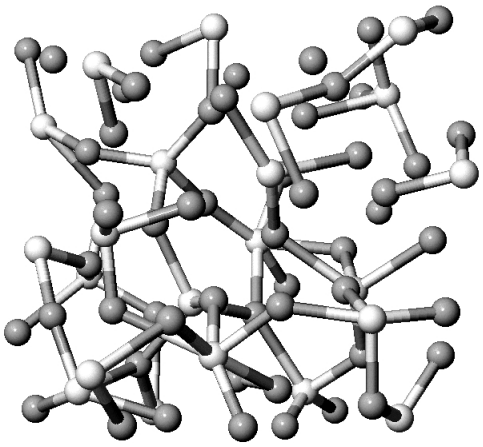

Figure 3. Atomic model of amorphous Ta_2O_5 with dark coloured oxygen and light coloured tantalum atoms, based on the 400°C RDF.

4. Conclusions

We have made major advances in our ability to characterise the atomic structure of amorphous mirror coatings and are working to use this to understand measured mechanical losses. The results from the averaged RDFs of three Ta_2O_5 coatings heat treated at 300, 400 and 600°C show a negligible change in amorphous structure. However, there may be some local changes from area to area in the samples showing an increase in the Ta to O coordination as the heat treatment temperature increases. Reverse Monte Carlo modelling combined with energy optimization of the amorphous structure provides a promising way to probe the maximum amount of information possible from these samples. The main emphases on future research will be to understand how these results relate to the mechanical loss of these coatings.

5. Acknowledgements

We would like to thank our colleagues at IGR, LIGO and the University of Oxford for useful discussions. We would also like to thank EPSRC, SFTC, SFC and the University of Glasgow in the UK and the NSF in the US for financial support.

References

[1] R. Frey, LIGO: Status and Recent Results, LIGO-P070079-01-Z, (2007).
[2] P. Saulson, Fundamentals of Interferometric Gravitational Wave Detectors, World Scientific, (1994).
[3] P. Fritschel, Second generation instruments for the laser interferometer gravitational wave observatory, ArXiv ,(2003).
[4] D.J.H. Cockayne,The Study of Nanovolumes of Amorphous Materials Using Electron Scattering, Annu.Rev.Mater.Res,37:159-87,(2007).