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Next Generation Coating Research:
Whitepaper for Coating Vendors

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Detection of gravitational waves is based upon experimenter's ability to determine the position of the front face of an interferometer test mass mirrors. Mirror vibrations due to thermally-driven resonant modes will change the position of the mirror face, but these modes are at well known, narrow resonances that are, for the most part, outside of the detection band. However, mechanical dissipation in the mirrors can result in non-resonant fluctuations that will generate "thermal noise" in-band. In electrical systems, thermal noise is also known as Johnson Noise, the thermally-driven voltage noise that results from resistance (dissipation) in a circuit. Using the Fluctuation-Dissipation Theorem of Callen and Green [1], one can calculate the level of thermal noise from the mechanical loss in the mirror. We seek to lower the thermal noise in gravitational wave detectors by minimizing the mechanical loss in the mirrors.

Thermal noise from the optical coatings of mirrors is a limiting noise source in other precision measurements, including laser frequency stabilization and macroscopic measurements of quantum phenomena. The importance of coating thermal noise was first appreciated in the gravitational wave detection community, though, and that application remains the most important [2]. Planning is underway for future interferometric gravitational wave detectors [3], where coating thermal noise may be an even more important limitation on sensitivity than in the detectors now being built. However, there is sufficient time (at least 10 years, and likely more) before the next generation gravitational wave detector will need to be formally designed. So a deliberative approach to understanding and reducing coating thermal noise is both possible and desirable.

Coatings used in interferometric gravitational wave detectors have typically been multi-layer stacks of amorphous oxide dielectrics created using ion beam deposition. This choice was driven by optical considerations, primarily the need for extremely low (<1 ppm) absorption [4]. It is possible that other materials and/or deposition techniques could be suitable, either now or in the future. To understand the causes of mechanical loss in amorphous thin film oxides, research coating runs are planned by a collaboration of researchers working with the LIGO, Virgo, and GEO 600 gravitational wave detectors. The details of these runs will be determined in collaboration with the vendors, to fully exploit what is possible with current coating technology and what is understood about the causes of mechanical loss. These runs will focus on silica, tantala, and titania-doped tantala, the materials used in current detectors, and will try to find variables in the coating process that influence mechanical loss.

The theory of mechanical loss is most developed in silica of all amorphous oxides. Mechanical loss in bulk silica is described using a double well potential in the bond angle between silicon and oxygen atoms, where transitions between the two wells account for loss of elastic energy [5]. This model has been found to accurately describe the mechanical loss in silica with a room temperature frequency dependence of $f^{0.77}$ verified from Hz – MHz [5, 6]. It has also been observed that the surface layer of silica has a different, and higher, value of mechanical loss [6], which may be related to the different elastic moduli and strength properties of the surface of silica. There is insufficient data to determine if the double well potential model adequately explains mechanical loss in silica surfaces. It has been suggested that this higher mechanical loss in the surface may be due to highly stressed Si-O bonds in two member rings that are more prevalent at the surface. It has also been suggested that surface micro-cracks may play a role in excess surface loss, either directly through rubbing friction or as a pathway for greater water (or other impurities) absorption. It has also been found that mechanical loss in both bulk and thin film silica can be improved with annealing [7, 8]. Annealing is shown to minimize stress in the material, thus allowing the molecular bonds to settle into their lowest energy configuration. Correlations of bond angle measurements with mechanical loss models are not fully determined.

It is postulated that this double well potential mechanism may apply in some form to other amorphous oxides. This can be studied by measuring mechanical loss versus temperature to near liquid helium temperatures, where a peak in mechanical loss due to the double well potential is observed (in silica) near 20 K [9]. Tantalum pentoxide, which is used in currently operating gravitational wave detectors, has been studied in this way and found to have a similar loss peak [10], as has titania-doped tantala [11]. Hafnia does not have a low temperature loss peak [12]. The theory of the double well potential in bond angles has not been applied to tantala or hafnia, so the interpretation of these results is not complete.

Doping has been found to affect mechanical loss in the high index materials tantala and titania. Titania as a dopant into tantala significantly reduces mechanical loss [13]. This material is planned for use in the second generation detectors being built now. Silica as a dopant into titania has also been found to affect mechanical loss, while silica doped into tantala has been found to have negligible effect. Cobalt doped into tantala has been reported to greatly reduce mechanical loss. The effect of doping on bond angle distribution has not been studied, nor is it known whether this is the mechanism by which doping is affecting mechanical loss.

It has been speculated that mechanical loss in coatings might correlate with other properties. A preliminary look at mechanical loss data and stress did not provide evidence of a correlation, but this was not done in a systematic way. Other mechanical properties that have been suggested for correlation studies include the real part of Young’s modulus (as the imaginary part is directly related to the mechanical loss), density, hardness, thermal expansion, and thermal conductivity. Optical properties such as absorption, index, or change in index with temperature may also correlate with mechanical loss. Index especially may correlate with mechanical loss through density. Very little research has been done in this area, and it may be a fruitful area for exploration.

Molecular level modeling of thin film oxides is beginning, aimed at comparing structure and specifically bond angle distribution with measured mechanical loss. The priority is to start with silica, including surface and bulk, where there is a literature that compares models with macroscopic properties. Mechanical loss has never been studied this way, but only from lack of motivation, not from any inherent difficulty. If a successful model can be developed that explains mechanical loss in silica as functions of frequency, temperature, and surface versus bulk, the research will proceed to study tantala, the role of dopants, and hafnia.

The research coating runs will focus on parameters that could be important for mechanical loss that are common to all materials. These would include the annealing curve, deposition ion properties, impurities in the coating, and layer thickness. Annealing dependence could come through peak temperature and dwell time as well as ramp up and down rates. Some of these dependencies have been studied in silica [8] and found to influence the mechanical los. The properties of the bombardment ion of most interest include atomic species, energy, and current. Argon is the typical ion used in most coatings that have been studied. It has been found that replacing argon with xenon increased the mechanical loss of tantala, and it has been suggested that going to a lower mass ion like neon might cause the opposite, desirable, effect. Secondary ion beam bombardment with oxygen has also been found to change mechanical loss in tantala, possibly through stoichiometry. Impurities in the coating, including water, metals (iron, chromium, etc.), the bombardment ion, or nitrogen or other air gases, might play a role in determining mechanical loss as well. Intentionally increasing the level of a contaminant to see if mechanical loss changes would be one way to study impurity effects. Finally, the thickness of the layers may be an important parameter in understanding mechanical loss. It was noted above that silica has higher mechanical loss in a thin film than in bulk. In addition to comparing with bulk properties, it is of interest to study any differences between micron-scale layers (typically what is used on optics in detectors) and much thinner, nanometer scale (which can still be used in an optical coating tuned to micron scale wavelengths).

Coating variables specific for the different materials will also be explored. Doping of silica with another low index material like alumina has been suggested. Further studies of titania doped into tantala, including much higher concentrations of titania than the ~50% that have been done so far, would be of interest. A trinary alloy of silica-titania-tantala could be designed with specific optical and mechanical properties that could be beneficial. Trying to change the coefficient of thermal expansion to allow for higher annealing might also be beneficial.

Fully characterizing the resulting coatings from these research coating runs will be an important component of this research. Of primary interest is the mechanical quality factor, which is used to determine mechanical loss. This will be measured on a variety of geometries within the LIGO collaboration, including at cryogenic temperatures. A direct measurement of thermal noise can also be made on occasion at a dedicated LIGO interferometer [14]. Young’s modulus is another important mechanical property. A nanoindenter can be useful for measuring Young’s modulus, but LIGO has relied, in the past, primarily on vendors for this measurement. There is a potential LIGO collaborator who can make Resonant Ultrasound Spectroscopy measurements [15] to determine coating moduli. Absorption, scatter, and index are important optical properties. Absorption and scatter can be measured within the LIGO collaboration [13], while index has been provided by vendors. Changes in index with temperature can also be important to thermal noise [16]. There is a dedicated apparatus to measure this within the LIGO collaboration, but additional ellipsometric measurements could provide valuable data. Thermal conductivity and expansion also enter into thermal noise and are measured with a specific experiment within LIGO [17].

Characterizing the constituents and the structure of the coatings could also prove important to understanding their mechanical loss. In the past, LIGO collaborators have studied impurities in coatings using X-ray techniques like X-ray fluorescence and X-ray Absorption Near Edge Structure analysis. This has provided information on titania dopant concentration and impurity species and levels [18]. Electron beam techniques have also been used, both Electron Energy Loss Spectroscopy for species analysis and electron microscope work to determine layer thicknesses [13]. A new LIGO collaborator is planning on doing radial distribution function analysis to determine short range order, including nearest atomic distances, coordination numbers, and bond angles. This could prove a very useful technique to correlate with both modeling efforts and experimental measurements. Additional techniques that promise information on coating structure and constituents could be valuable, and LIGO would be interested in hearing ideas from vendors on their capabilities and thoughts.

At this stage, LIGO is interested in ideas from coating vendors of how best to pursue this line of research. Ideas for coating runs that would allow multiple theories of possible causes of mechanical loss to be explored are of particular interest. We would also welcome ideas for coating analysis of structure and/or contamination that have been successfully used to study mechanical properties of coatings in the past.

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