Properties of Optical Coatings

ET-0003A-14

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Where possible, properties of optical coating materials at cryogenic temperatures relevant to KAGRA (and also ET) have been included in this document. However, there is limited data for some of the important properties, particularly at cryogenic temperatures, and thus, in some sections only room temperature measurements are given.

1. Mechanical loss of coating materials

1.1 Single layers of individual coating materials

1.1.1 Tantala coatings

Effect of heat-treatment on loss in tantala

Post-deposition heat-treatment is used to relieve the stress and reduce the optical absorption in multi-layer optical coatings. Silica/tantala coatings for GW detectors have typically been heat-treated at temperatures between 500-600 °C. There is evidence of heat-treatment reducing the mechanical loss of single layers of tantala at room temperature (Cesarini, Prato, & Lorenzini, 2010), and detailed studies of the effect of heat-treatment on the temperature dependence of the loss of tantala have been carried out (Martin, et al., 2010).

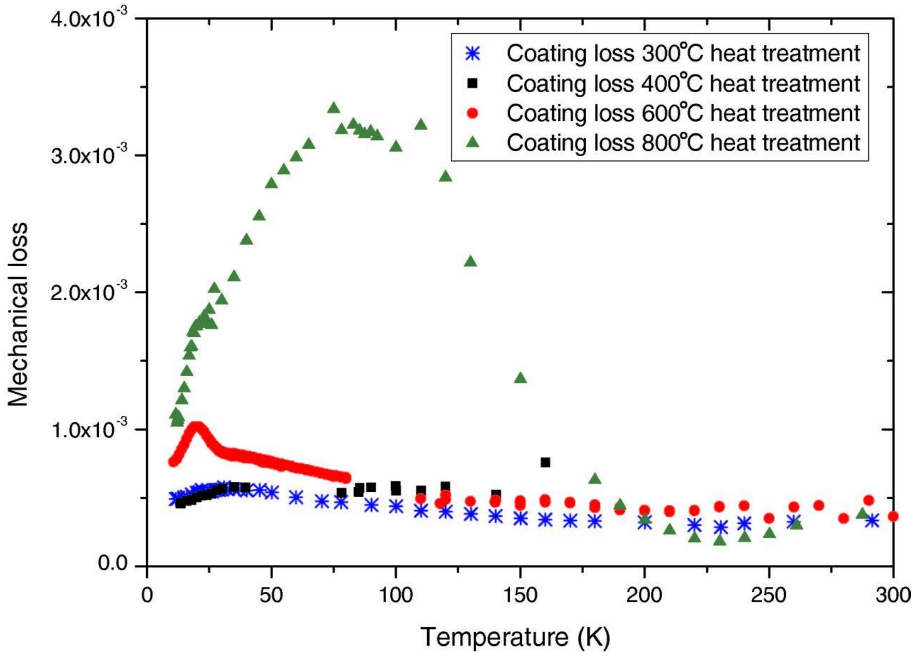

Figure 1 – Calculated mechanical loss factors of various Ta_2O_5 coatings at approximately 1000 Hz.
(tantala_undoped_300.txt, tantala_undoped_400.txt, tantala_undoped_600.txt, tantala_undoped_800.txt)

Effect of titania doping on loss of tantala

Doping the tantala layers of silica/tantala multilayer coatings with titania has been shown to reduce the mechanical loss of the coating at room temperature (Harry, et al., 2006, Harry, et al., 2007). A similar reduction in loss has been demonstrated in single layers of tantala doped with titania at room temperature (Flaminio, Franc, Michel, Morgado, Pinard, & Sassolas, 2010) and throughout the majority of the temperature range 10-300 K (Martin, et al., 2009). The latter measurements show evidence that doping may reduce the activation energy of the dissipation peak at 20 K. The current best loss for titania-doped tantala at room temperature is – 2.44×10^{-4} (Flaminio, Franc, Michel, Morgado, Pinard, & Sassolas, 2010).

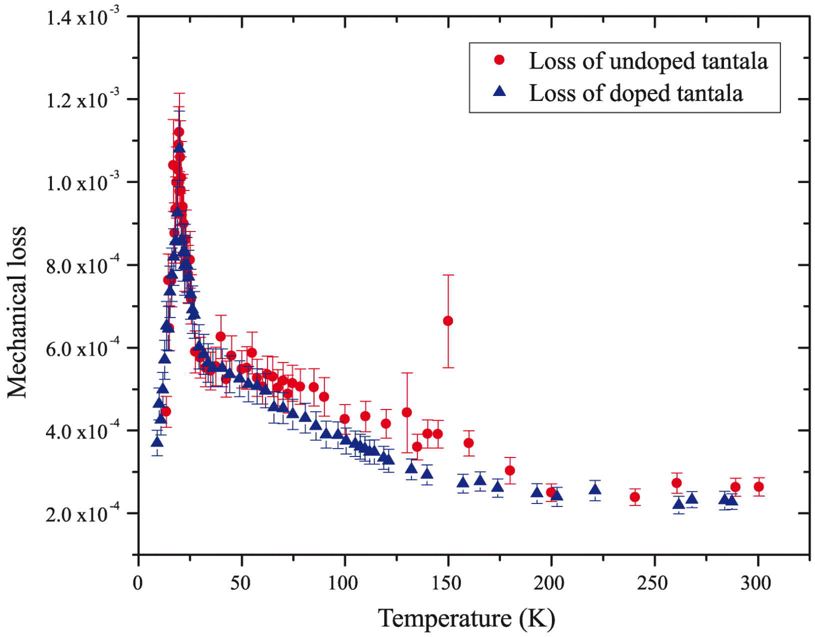

Figure 2 - Comparison of the loss of an undoped Ta_2O_5 and a Ta_2O_5 coating doped with TiO_2 at approximately 1000 Hz.
(doping_comparison_undoped_1kHz.txt, doping_comparison_14_5%_1kHz.txt)

Effect of alternative dopants

Some studies of the effect of alternative dopants on the mechanical loss have been carried out (Flaminio, Franc, Michel, Morgado, Pinard, & Sassolas, 2010). Of the dopants tested (Ti, Co, W, W+Ti), Ti was the only dopant found to reduce both the mechanical loss and the optical absorption.

Coating	Refractive index	Optical absorption (ppm)	Mechanical loss
Ta_2O_5	2.035	1.22	3×10^{-4}
Ta_2O_5:Co	2.11	5000	11×10^{-4}
Ta_2O_5:W	2.07	2.45	7.5×10^{-4}
Ta_2O_5:W+Ti	2.06	1.65	3.3×10^{-4}
Ta_2O_5:Ti	2.07	0.5	2.4×10^{-4}

Table 1 - Comparison of refractive indices, optical absorption and mechanical loss of alternative dopants.

1.1.2 Silica coatings

Temperature dependence of the loss of silica coatings

A dissipation peak has been observed in a single layer of ion beam sputtered (IBS) silica at approximately 20 K (Martin, et al., 2014). The loss at temperatures close to this peak is of a similar magnitude to the loss of tantala. Thus for multilayer silica/tantala coatings it is expected that both of the coating materials will make a significant contribution to the total coating loss at cryogenic temperatures. The loss peak observed in a 1 µm thick IBS silica coating heat-treated at 600 °C is at a significantly lower temperature than the well-known dissipation peak in bulk silica, which may imply a different microscopic dissipation mechanism is responsible for the peak. There is evidence that the magnitude of the loss around the peak is also significantly lower in IBS silica than in bulk silica (Martin, et al., 2014, Cagnoli, 2013), with recent measurements showing losses as low as ~2.5×10^{-4} at the loss peak.

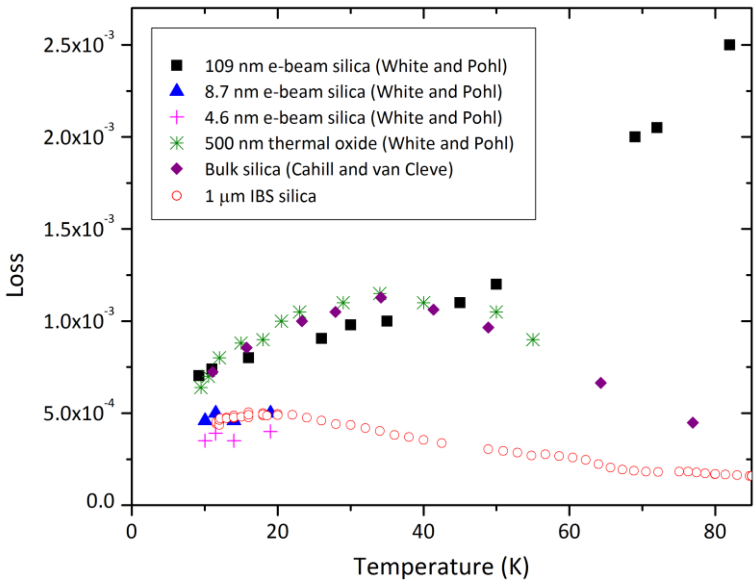

Figure 3 - Comparison of the mechanical dissipation of ion-beam sputtered silica with bulk silica, e-beam evaporated silica and thermal oxide grown on silicon.
(IBS_Silica_7kHz.txt)

1.1.3 Silica-doped hafnia coatings

Alternative IBS amorphous coatings are currently under investigation, with silica-doped hafnia being one interesting alternative high-index material to tantala. Initial results indicate that the loss of this coating can be reduced by heat-treatment to be up to a factor of two lower than for tantala heat-treated at 600 °C (Craig, et al., in prep.).

1.1.4 Other coating materials e.g. crystalline coatings

The coatings discussed so far are all amorphous materials deposited by IBS. The use of epitaxially grown crystalline coatings is also currently under investigation following promising optical absorption and mechanical loss results in coatings based on AlGaAs. A 3-fold reduction in thermal noise has been observed through the use of an AlGaAs mirror coating on the end mirrors of a Fabry-Perot cavity (Cole, et al., 2010, Cole, Gröblacher, Gugler, Gigan, & Aspelmeyer, 2008). These coatings were produced by growing them epitaxially on GaAs substrates and then transferring, and bonding, them to the final mirror substrate. Recent measurements on a multilayer GaAs/AlGaAs mirror coating also showed a factor of three improvement in the displacement thermal noise (Cole, Zhang, Martin, Ye, & Aspelmeyer, 2013).

Material	Crystal structure	Lattice const. (A)	Modulus (GPa)	Density (kg/m^3)	CTE ($\times 10^{-6}$ K^{-1})	Refractive index
GaAs	zinc blende	5.6455	85.3	5320	5.73	3.4804
AlAs	zinc blende	5.6533	83.5	3760	5.20	2.9383
Al_2O_3	hexagonal	4.785	345	3980	5.50	1.76

Table 2 - Properties of crystal structure grown using molecular beam epitaxy and metal organic chemical vapour deposition (Cole, Ways to bring down thermal noise, 2011)

Multilayer stacks of gallium phosphide (GaP) and aluminium gallium phosphide (AlGaP) are of interest to the GW community as they have their crystal structure lattice matched to silicon, meaning the coating can be grown directly onto a silicon test mass mirror substrate, without the need to transfer from an initial substrate. Recent measurements (Cumming, et al., in prep.) of the mechanical dissipation of a multilayer crystalline GaP/AlGaP coating grown directly onto a silicon substrate, show that the coating loss ranged from 1.6 – 3.7 $\times 10^{-5}$ at 12 K which is a significantly lower mechanical losses than IBS silica/tantala coatings at similar temperatures.

1.2 Multilayer coatings

1.2.1 Advanced LIGO coating

The mechanical loss of an Advanced LIGO silica/titania-doped tantala coating stack applied to a silicon cantilever has been studied between 10 and 300 K (Granata, et al., 2013). As expected from the loss measurements of single layers of silica and tantala, a low-temperature loss peak was observed. However, the temperature of the loss peak was somewhat higher than would be predicted by single-layer measurements. This may be related to slightly differing heat-treatments and doping concentrations between the various coatings and is an area of on-going research.

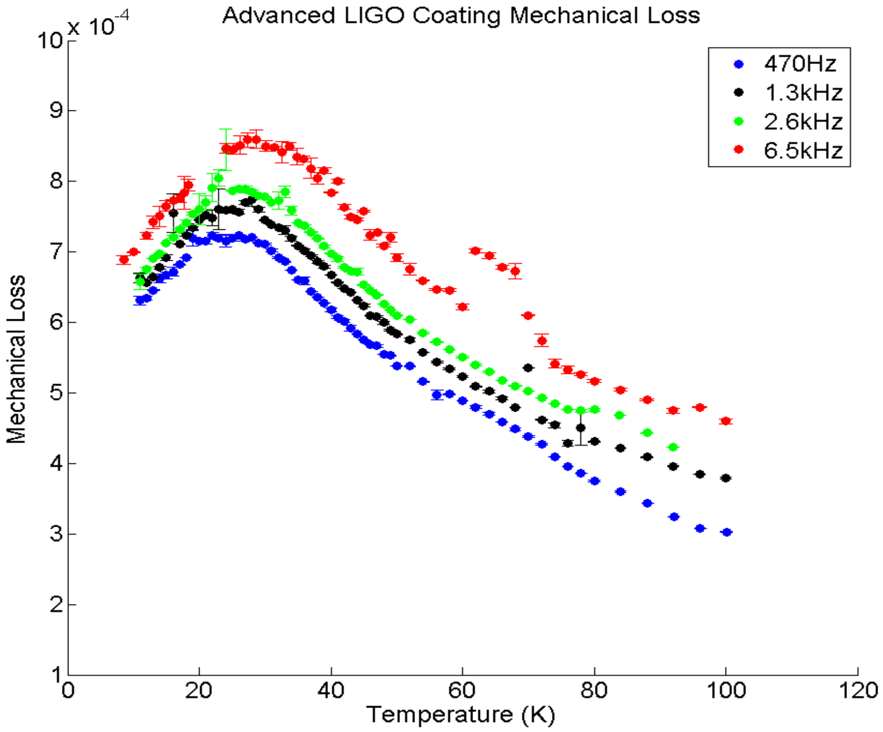

Figure 4 – Mechanical loss of an Advanced LIGO silica/titania-doped tantala coating on a silicon cantilever.

1.2.2 Multilayer silica/tantala coating measurements at ICRR

Previous loss measurements on multilayer silica/tantala coatings on sapphire disks did not show evidence of a low temperature loss peak (Yamamoto, et al., 2006). These measurements have been repeated (using un-doped tantala layers) in more detail as part of the Elites project (Hirose, et al., in prep.). The repeated measurements show no evidence of a sharp peak in the coating loss for an as-deposited coating, while a coating heat-treated at 500 °C did show a loss peak at ~28 K. It is interesting to note that both the position and magnitude of the loss peak are broadly consistent for both this coating (un-doped tantala layers, quarter wavelength design) and the Advanced LIGO coating (titania-doped tantala layers, optimised thickness design).

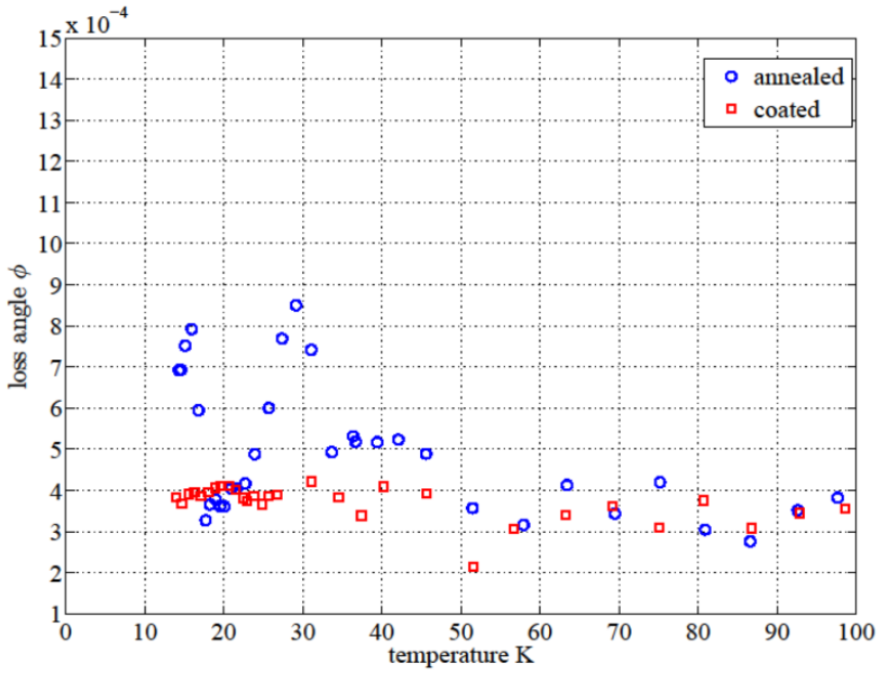

Figure 5 – Mechanical loss of an as-deposited (coated) and a 500 °C heat treated (annealed) multilayer silica/tantala coatings on sapphire disks.

2. Young’s modulus of coating materials

The material properties of silica are well documented. Nanoindentation measurements of the Young’s moduli of various tantala and titania-doped tantala thin films have been made at room temperature (Abernathy, et al., 2014). Indents were made to assess the effects of both titania doping concentration and post-deposition heat-treatment on the measured values. Young's modulus measurements on pure tantala and 25% and 55% titania-doped tantala show a wide range of values (132 to 177 GPa), dependent on both titania concentration and heat-treatment.

%Ti	Heat Treatment (°C)	Substrate	Young’s Modulus (GPa)
0	300	SiO_2	152 ± 9
0	400	SiO_2	137 ± 8
0	600	SiO_2	133 ± 8
0	800	SiO_2	162 ± 11
0	300	Si	160 ± 15
0	400	Si	146 ± 5
0	600	Si	137 ± 6
25	AD	SiO_2	143 ± 9
25	300	SiO_2	137 ± 8
25	400	SiO_2	145 ± 9
25	600	SiO_2	132 ± 8
55	AD	SiO_2	145 ± 10
55	300	SiO_2	158 ± 10
55	400	SiO_2	142 ± 8
55	600	SiO_2	177 ± 11

Table 3 - Young's moduli measured for various titania-doped tantala films. The Young's moduli are stated with the combined uncertainty from the measured indents on each sample, systematic uncertainty arising from the softer substrate and uncertainty in the Poisson ratio of the coating materials (Abernathy, et al., 2014).

Coating Young's moduli as measured on silica substrates are shown below plotted as a function of heat treatment. In the pure tantala coatings the Young's modulus appears to decrease with increasing heat-treatment until the coating begins to crystallize (600 – 800 °C). A similar trend can be seen for the 25% titania-doped samples, with the exception of the 400 °C sample.

The opposite trend is observed on the 55% titania-doped samples, again, with the exception of the 400 °C sample. This is most likely due to the high abundance of titania, which is known to have a low crystallization temperature and a high Young's modulus.

It is known that both 400 °C treated samples were produced together, and perhaps may not have been fully heat treated. Further evidence of this comes from the fact that the two samples give approximately the same moduli as the as deposited coatings.

Overall, the average Young’s moduli of all the coatings was found to be 147 ± 3 GPa which ties in with the commonly used value of 140 GPa (Martin, et al., 1993), but care should be taken as the Young's modulus of tantala, it is dependent upon both the doping and heat-treatment of the coating.

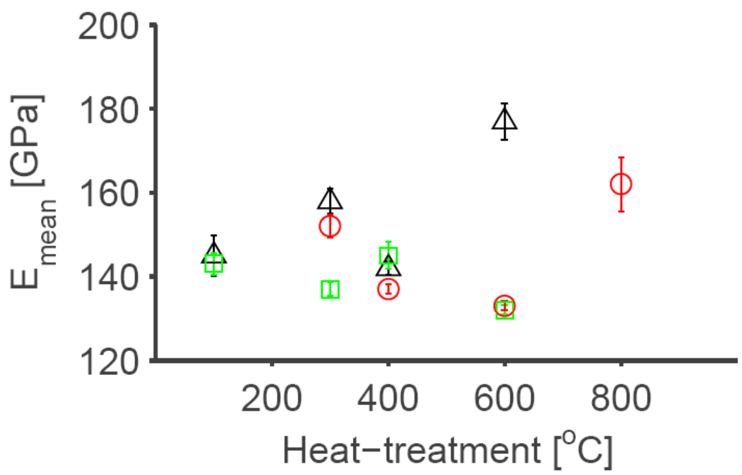

Figure 6 - Mean Young's moduli of tantala samples measured on silica substrates, plotted for different heat-treatments. Red circles are pure tantala, green squares are 25% titania-doped tantala, and black triangles are 55% titania-doped tantala.

3. Other properties of coating materials

Density

Density measurements of a 400 °C heat-treated Ta_2O_5 Coating were made at the University of Glasgow (Bassiri, 2011) by measuring the mass of a coated silicon cantilever, using a microbalance, and then etching the cantilever in 40% unbuffered hydrochloric acid for an hour to completely remove the coating and then weighing it again. After taking in to consideration that there was a thin SiO_2 layer also present, they determined the measured density of the Ta_2O_5 coating to be

$$\rho_{Tantala} = (7.68 \pm 0.46)\ g/cm^3.$$

LMA used Rutherford Backscattering Spectrosopy (RBS) to determine the structure and composition of materials by measuring the backscattering of a beam of high energy ions impinging on tantala coatings (Morgado, 2009).The densities of both pure and titania doped tantala coatings sputtered in two different chambers are detailed below. Further, they saw that annealing the samples under vacuum showed no change in density.

Coating	Density (g/cm^3)
Ta_2O_5 [1]	7.1
Ta_2O_5 [2]	6.8
55% TiO_2 – Ta_2O_5	5.5
75% TiO_2 – Ta_2O_5	6.4

Table 4 - Summary of RBS density measurements by LMA on both pure and doped tantala samples.

Titania (TiO_2) was added as a dopant to Ta_2O_5 in an attempt to improve the mechanical loss without significantly degrading the optical absorption, because it has a high Young's modulus, its atomic size allows for dense packing in the Ta and O matrix and the melting point of the TiO_2/Ta_2O_5 alloy is relatively high which is indicative of a stable amorphous structure.

A series of silica substrates were coated with the TiO_2-doped Ta_2O_5/SiO_2 coating using ion beam deposition (Harry, et al., 2007). After coating, each sample was annealed at 600 °C and further x-ray examination showed that no large crystals had formed in the coating after annealing. Each coating comprised of 30 $\lambda/4$, at 1.064 µm, layers alternating between the two materials, TiO_2-doped Ta_2O_5, the high index layer, and SiO_2, the low index material. The average coating thickness for the coatings was measured to be 4.5 ± 0.1 µm. The single layer of TiO_2-doped Ta_2O_5 was 4.7 µm thick.

The concentration of TiO_2 in Ta_2O_5 for the different coatings was measured in two different ways. Firstly, an estimate was made by comparing the index of refraction of the TiO_2-doped Ta_2O_5 with pure Ta_2O_5 and pure TiO_2. Here, a linear relationship was assumed between TiO_2 concentration and index so the TiO_2 concentration was obtained by interpolation, as indicated in the table below. A more detailed measurement was made on some samples using electron energy loss spectroscopy and appeared to agree reasonably well with the other technique.

[1] Coated in a small IBS DIBS chamber
[2] Coated in a large IBS GC chamber

Optical absorption was measured using photothermal common-path interferometry. The **index of refraction at 1064 nm** was also measured with the results shown below [Harry 2007].

Coating	[TiO_2] Index	[TiO_2] EELS	Index *n*	Absorption (ppm)
0	0 %	-	2.065 ± 0.005	0.9 ± 0.2
1	6 ± 0.6 %	8.5 ± 1.2 %	2.075 ± 0.005	1.1 ± 0.1
2	13 ± 1 %	20.8 ± 4.4 %	2.092 ± 0.005	1.0 ± 0.1
3	24 ± 2 %	22.5 ± 2.9 %	2.119 ± 0.005	1.1 ± 0.1
4	54.5 ± 5 %	54 ± 5 %	2.180 ± 0.005	2.5 ± 0.5
5[3]	14.5 ± 1 %	-	2.070 ± 0.005	0.9 ± 0.1
6[4]	6 ± 0.6 %	-	2.075 ± 0.005	4.5 ± 0.5

Table 5 - Concentration of TiO_2 in Ta_2O_5 as measured by change in index of refraction and by electron energy loss spectroscopy (EELS) compared with the optical absorption of TiO_2-doped Ta_2O_5/SiO_2 coatings and indices of refraction of individual TiO_2-doped Ta_2O_5 layers within those coatings. Note that the index of refraction comparisons is only valid between coatings from the same coating chamber.

The addition of TiO_2 appears to slightly increase the optical absorption. Using low concentrations of TiO_2 dopant will be useful. Further, it is known that changes in the heat treatment and annealing cycles are known to affect optical absorption, along with levels of contamination.

Other thermal and mechanical properties

Many of the properties of IBS tantala and silica films which are required for calculating coating thermal noise have not been well characterised. The following table (Fejer, et al., 2004) lists commonly-used values for some of these properties at room temperature.

	α (K^{-1})	C (Jkg^{-1}K^{-1})	κ (Wm^{1}K^{-1})	ν
Tantala [5]	3.6×10^{-6}	306	33	0.23
Silica [6]	5.1×10^{-7}	746	1.38	0.17

Figure 7 – List of commonly used values of coefficient of linear thermal expansion, specific heat capacity, thermal conductivity and Poisson's ratio.

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[3] Coated in a large coating chamber
[4] Single layer of TiO_2-doped Ta_2O_5
[5] (Tien, Jaing, Lee, & Chuang, 2010, Samsonov (Ed.) & Kubaschewski, 1982, Fejer, et al., 2004)
[6] (Musikant, 1985, Waynant & Ediger, 2000)

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