On the mechanical quality factors of cryogenic test masses from fused silica and crystalline quartz

A Schroeter$^1$, R Nawrodt$^1$, R Schnabel$^3$, S Reid$^4$, I Martin$^4$, S Rowan$^4$, C Schwarz$^1$, T Koettig$^1$, R Neubert$^1$, M Thür$^1$, W Vodel$^1$, A Tünnermann$^2$, K Danzmann$^3$, P Seidel$^1$

$^1$ Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, D-07743 Jena, Germany
$^2$ Institut für Angewandte Physik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena, Germany
$^3$ Max-Planck-Institut für Gravitationsphysik (Albert-Einstein-Institut) and Leibniz Universität Hannover, Callinstr. 38, D-30167 Hannover, Germany
$^4$ SUPA, University of Glasgow, Glasgow, G128QQ, UK

E-mail: anja.zimmer@uni-jena.de

Abstract. Current interferometric gravitational wave detectors (IGWDs) are operated at room temperature with test masses made from fused silica. Fused silica shows very low absorption at the laser wavelength of 1064 nm. It is also well suited to realize low thermal noise floors in the detector signal band since it offers low mechanical loss, i.e. high quality factors (Q factors) at room temperature. However, for a further reduction of thermal noise, cooling the test masses to cryogenic temperatures may prove an interesting technique. Here we compare the results of Q factor measurements at cryogenic temperatures of acoustic eigenmodes of test masses from fused silica and its crystalline counterpart. Our results show that the mechanical loss of fused silica increases with lower temperature and reaches a maximum at 30 K for frequencies of slightly above 10 kHz. The losses of crystalline quartz generally show lower values and even fall below the room temperature values of fused silica below 10 K. Our results show that in comparison to fused silica, crystalline quartz has a considerably narrower and lower dissipation peak on cooling and thus has more promise as a test mass material for IGWDs operated at cryogenic temperatures. The origin of the different Q factor versus temperature behavior of the two materials is discussed.

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1. Introduction

The current interferometric gravitational wave detectors (IGWDs) \[1, 2, 3\] designed to search for gravitational radiation produced by astrophysical sources are among the most sensitive measurement devices ever built. These instruments operate by sensing changes in the relative positions of test-mass mirrors suspended as pendulums. Noise spectral densities for differential strain measurements lower than \(10^{-22} \text{m}/\sqrt{\text{Hz}}\) at frequencies between 70 Hz and about 400 Hz have been achieved \[4\]. Future generations of gravitational wave detectors (GWDs) aim for even lower noise spectral densities. To achieve this goal noise sources that produce displacements of the interferometer’s test mass surfaces in the direction of the optical axis must be further reduced because their influence mimics that of gravitational waves. Noise sources that exist due to a non-zero temperature are called thermal noise sources. One source for thermal noise originates from thermally driven mechanical vibrations of the test masses themselves.

Until relatively recently the thermal noise from test mass and suspensions was modelled by treating the resonant modes of the systems as damped harmonic oscillators. Applying the fluctuation-dissipation theorem \[5, 6\], the power spectral density of thermal displacement noise for each mode may be found, and the total thermal noise calculated by considering the laser beam reflected from the front face of a test mass as sensing the incoherent sum of the thermal displacements in the tails of the test mass resonant modes (see for example \[7\]).

However a method for calculating thermal noise was developed by Levin \[8\] which showed that the modal approach is accurate only when the off-resonance thermal noise from each mode is uncorrelated. In a system having spatially inhomogeneous mechanical dissipation, correlations exist between the noise from the modes, and the resulting thermal noise can be greater or smaller than a modal treatment would suggest \[8, 9\]. Using Levin’s approach the power spectral density \(S_x(f)\) of thermally excited displacement of the front face of a test mass mirror may be written as

\[
S_x(f) = \frac{2k_B T W_{\text{diss}}}{\pi^2 f^2 F_0^2},
\]

where \(f\) is frequency, \(T\) is the temperature, \(k_B\) is the Boltzmann constant and \(W_{\text{diss}}\) is the power dissipated when a notional oscillatory force of peak magnitude \(F_0\) acting on the face of a test mass mirror has an associated pressure of spatial profile identical to that of the laser beam used to sense the mirror displacement. No general formula can be given if the loss is inhomogeneous, however if the loss is homogeneous, and in the case where a test mass can be approximated as semi-infinite in dimension (compared with the diameter of a sensing laser beam) then it can be shown that the power spectral density of thermal noise of a test mass substrate having mechanical loss \(\phi_{\text{substrate}}(f)\) is given by

\[
S_x(f) = \frac{2k_B T}{\pi f} \frac{1 - \sigma^2}{\sqrt{2\pi}} \phi_{\text{substrate}}(f)
\]
where $E$ and $\sigma$ are the Youngs modulus and Poissons ratio of the material and $r_0$ is the radius of the laser beam at a point where the intensity has fallen to $1/e$ of its maximum.

A direct measurement of the relevant mechanical losses at the frequencies of the detection band of IGWDs is often impracticable as the losses are typically extremely low in this region. A more feasible approach is to determine the mechanical losses at the resonances of the test masses. At a resonant frequency, the reciprocal of the mechanical loss factor is given by the quality factor, or Q factor, of the oscillation. According to the fluctuation-dissipation theorem, the thermal noise can be reduced by decreasing the temperature of the test masses, thus cooling the test masses in IGWDs is of interest as a technique for reducing thermal noise. See for example [11]. The mechanical loss of the test masses generally depends on temperature as well as on frequency, thus for a given material the temperature dependence of mechanical loss is an important parameter to study.

For single relaxation processes with merely one relaxation time $\tau$, the tangent of the mechanical loss $\phi$ can be expressed in the following way [12, 13],

$$
\tan (\phi) = \Delta \frac{2\pi \cdot f \cdot \tau}{1 + (2\pi \cdot f \cdot \tau)^2},
$$

where $\Delta$ is the so-called relaxation strength. For most processes the relaxation time $\tau$ strongly varies with temperature and also the relaxation strength has a temperature dependent component for some processes [13].

Current interferometric gravitational wave detectors are operated at room temperature with test masses made from fused silica. Fused silica shows very low absorption at the laser wavelength of 1064 nm [14]. It is also well suited to realize low thermal noise floors in the detector signal band since it offers low mechanical loss, i.e. high quality factors (Q factors) of up to $2 \times 10^8$ at room temperature [15]. However, for a further reduction of thermal noise cooling of the test masses to cryogenic temperatures may be of interest. Unfortunately, it has been found that Q factors of fused silica samples significantly decrease with decreasing temperatures. Early measurements used the so-called ‘resonant piezoelectric method’ and found a damping peak of fused silica at about $35\,\text{K}$ [16] measured at a resonant frequency of $50\,\text{kHz}$. Other early works were performed at rather high frequencies far above the gravitational wave detection band ($>500\,\text{MHz}$) [17]. More recent investigations used Brillouin spectroscopy and concentrated on small samples ($<1\,\text{cm}^3$). Q factors of the order $10^3$ were achieved [18, 19]. Crystalline quartz also offers very low absorption at the IGWD wavelength of 1064 nm [20]. Q factor measurements on crystalline quartz samples were performed in [21, 22, 23]. A much richer variation of Q factor values with temperature was found. The highest Q factor value observed in those works was slightly below $10^7$ measured on a $2\times2\times2.5\,\text{cm}^3$ natural quartz crystal at a $5\,\text{MHz}$ resonance [23].

In this work we reanalyze the behavior of fused silica and crystalline quartz Q factors using the method of “cryogenic resonant acoustic spectroscopy of bulk materials” [24] using methods based on those described in [25, 26]. In this method excitation and
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readout is realized without mechanical contact providing high measurement accuracies. We used artificially produced samples with a high grade of purity allowing for the resolution of narrow damping structures in the temperature spectrum. Our data shows a greatly increased temperature resolution compared with previous measurements. We also used rather large samples having an increased relevance for test mass applications in gravitational wave detectors and, for crystalline quartz, observed Q factors of up to $7 \times 10^7$ at a 11.5 kHz resonance.

2. Measurement of Q factors

The measurements of the Q factors were performed in a custom made cryostat. Details concerning the measurement system can be found in the work of Nawrodt et al. [27, 28] and Zimmer et al. [24]. In the following, the measuring process is roughly outlined. The mechanical loss at a resonant frequency was determined by cryogenic resonant acoustic (CRA) spectroscopy which is an amplitude ring-down method. For this purpose the substrate was excited to resonant vibrations by means of a comb capacitor which avoids additional losses due to contact to the substrate. After removing the driving electric field the subsequent ring-down of the vibrational amplitude was recorded by a Michelson-like interferometer. From the ring-down time the Q factor was determined. To minimize additional losses due to clamping, the substrate was kept in a loop of wire made of tungsten resulting in a pendulum. For reduction of gas damping the probe chamber was evacuated to a vacuum of better than $10^{-3}$ Pa.

With this set-up, measurements at temperatures between 5 K and 325 K can be realized. For cylindrical samples of isotropic materials the Q factor measured is insensitive to the rotation of the substrate in the suspension. It is plausible that the mode shape is self-aligned with respect to the contact points of the suspension. In anisotropic materials the mode shape is aligned to the coordinate system of the inner structure of the material [29]. Thus, by rotating the substrate in the wire loop the Q factor varies [30]. The position with the highest Q factor at room temperature was adopted for all of the measurement cycles in our investigations.

3. Results and Discussion

In Fig. 1 the reciprocals of the measured Q factors are plotted versus temperature. The data have been taken on two substrates made of fused silica [31] and crystalline quartz [32], both identical in shape (a cylinder 76.2 mm in diameter and 12 mm thick). The excited mode shapes, visualized in Fig. 2 were chosen to be similar for both substrates. The mode shapes are not identical because the fused silica is isotropic, but the crystalline quartz is anisotropic and has different physical properties in the different directions.

For fused silica a large, broad damping peak occurs. No strong dependency of the peak shape or height on the mode shape is visible. The mechanical losses increase about 4 orders of magnitude from room temperature to 30 K finally resulting in a value of $10^{-3}$
Figure 1. Reciprocal of the measured Q factors versus temperature for a fused silica and crystalline quartz substrate both 76.2 mm in diameter and 12 mm thick. The dashed line represents a theoretical model for a dominant loss mechanism at intermediate temperatures around 80 K which was fitted to the measured data of fused silica at 17193 Hz. Details of the fit parameters are given in the text.

Figure 2. Calculated mode shapes and frequencies of the fused silica substrate a) 11548 Hz and b) 17101 Hz at 300 K and the crystalline quartz substrate c) 10792 Hz and d) 16964 Hz at 300 K. The cylinder axis is aligned with the c-axis of crystal. Please note, that the asymmetric mode shape reflects the anisotropy of the quartz crystal. For the numerical simulations the FEA based software ANSYS [33] was used. The essential material parameters have been taken from SCHOTT Lithotec [31] for fused silica and from Smakula et al. [34] (density) and Bechmann [35] (elastic coefficients) for crystalline quartz.

Fused silica is a material with high structural variation. The structural unit, a silicon atom surrounded by 4 oxygen atoms in the form of a tetrahedron, equals that of crystalline quartz. But the variation in bond lengths and bond angles generates its amorphous character. This variation also seems to be the cause for the observed large, broad, damping peak [17, 36, 37, 38]. In general one can assume that a vast number
of different bonding configurations with different bonding energies exist. Considering
the simplest case, the energy landscape of two configurations can be described by
two valleys of an asymmetric double-well potential. The wall height between them is
given by the stiffness of the directed bonding forces and can be overcome by thermal
energy. Three possibilities of the microscopic origin of the mechanical losses have been proposed:
(1) transverse movement of oxygen atoms between two potential minima resulting in
flipping of the bond \[39\]
(2) motion of oxygen atoms in the direction of the bond between two potential minima
\[40\]
(3) rotation of the SiO$_4$ tetrahedrons by small angles \[41\].

Due to the amorphous character of fused silica a wide variation in the height of the energy
barrier occurs and therewith a distribution in activation energies. An activation energy
$E_a$ is needed to overcome the barrier between the two configurations. In combination
with the relaxation constant $\tau_0$ it determines the temperature dependent relaxation time
according to an Arrhenius-like relation,

$$\tau = \tau_0 \cdot e^{\frac{E_a}{k_B T}}$$

where $k_B$ is the Boltzmann constant and $T$ the temperature. A distribution in relaxation
times requires integrating over all contributions at a fixed temperature \[42\]. The
contribution of a single anelastic process is given by Eq.\[3\]. For small losses ($\phi, \Delta \ll 1$)
the tangent is nearly linear,

$$\phi \approx \Delta \frac{2\pi \cdot f \cdot \tau}{1 + (2\pi \cdot f \cdot \tau)^2}$$

The mechanical loss due to a superposition of loss processes with varying relaxation
time can then be written as

$$\phi \approx \Delta \int_\infty^{-\infty} \Psi (\ln \tau) \frac{2\pi \cdot f \cdot \tau}{1 + (2\pi \cdot f \cdot \tau)^2} d \ln \tau,$$

with the following normalized distribution function

$$\int_\infty^{-\infty} \Psi (\ln \tau) d \ln \tau = 1.$$  

The distribution is linearly related to $\ln \tau$, as $\ln \tau$ is linearly related to the activation
energy \[42\]. Assuming a Gaussian distribution of the barrier heights and therewith also
of the activation energies, the relaxation times are lognormal distributed,

$$\Psi (\ln (\tau/\tau_m)) = \frac{1}{\beta \sqrt{\pi}} \exp \left[ -\frac{(\ln (\tau/\tau_m))/\beta)^2}{2} \right],$$

where $\tau_m$ is the most likely value of $\tau$ and $\beta$ is the half-width of the Gaussian distribution
at the point where $\Psi$ falls to 1/e of its maximum value. Since solely a variation in
activation energies and not in the relaxation constant is assumed, $\beta$ is chosen to be
temperature dependent, $\beta = \beta_c/T$ \[42\], where $\beta_c$ is a constant. The measured data
recorded for the resonant frequency of 17193 Hz at 300 K in Fig.1 have been fit using
Eq. \[6\] and \[8\] with the following parameters: $\tau_0 = 1 \times 10^{-13}$s, $\beta_c = 700$ 1/K and
$\tau_m = \tau_0 \times \exp (35.3 \text{meV}/k_B T)$. The parameters used for $\tau_0$ and $\tau_m$ are those reported
in the work of Hunklinger [17], and also successfully describe our measurement data between 50 K and 100 K, see the dashed line in Fig. 1. Differences to the measured values at other temperatures are possibly due to the following mechanisms. For temperatures above 225 K, phonon-phonon interactions are plausible. Phonon-phonon interactions are expected to play a similarly important role in both, fused silica and crystalline quartz, which is indeed found in (Fig. 1). The deviations between 100 K and 225 K and below 50 K are assumed to be due to other loss mechanisms. At 50 K as well as at about 100 K, a small kink in the curve is visible indicating additional damping peaks. Below 50 K a damping peak has been observed by Hunklinger [17] at far higher resonant frequencies (507 and 930 MHz). Due to the much higher frequencies the damping peaks were clearly separated from each other and observed as distinct peaks. Note that a loss peak caused by relaxation processes moves with decreasing frequency to lower temperatures. Peaks having different parameters entering the relation for the relaxation time are not equally shifted. Thus, the peak observed by Hunklinger is likely to appear in our measurements below 50 K partially covered by the damping peak due to structural variations since the resonant frequencies are lower. According to the work of Hunklinger [17] it is caused by relaxation processes of the two-level-systems by resonant absorption or emission of thermal phonons. The origin of the damping peak at about 150 K is not known to our knowledge. An analysis of this problem would require a clearer separation of this damping peak from our fitted damping peak at about 80 K. This could be achieved by measurements at lower frequencies which are, however, experimentally rather challenging.

For crystalline quartz the temperature spectrum of the measured Q factors looks rather different. Below room temperature the damping slightly decreases with decreasing temperature. However, several damping peaks are visible with heights depending on the resonant frequency. In particular the temperature region from 30 K to 50 K is dominated by a rather narrow distinct damping peak. Below 15 K the losses strongly decrease. We found Q values of up to $7 \times 10^7$.

The origin of the losses in crystalline quartz can be found in interactions of the excited acoustic waves with thermal phonons of the crystal and with alkali ions which were introduced during the growth [23]. Relaxations of the perturbed states to new equilibria lead to removal of oscillation energy. However, the defect induced damping peaks can be reduced or removed by sweeping (electrodiffusion) or by irradiating the crystal [43]. For a review on loss mechanisms in crystalline quartz see the work of Zimmer et al. [24]. In contrast to fused silica, crystalline quartz shows a much narrower damping peak because almost no variations in bond lengths and bond angles occur. Quite generally most relaxation processes in crystalline materials depend on parameters with low variations and result in narrow damping peaks. Crystalline quartz is however piezoelectric thus the possibility of excess damping associated with this piezoelectric behaviour is an area which require further investigation. The crystalline structure also causes an anisotropy of the material which explains why the damping depends on the direction of the motion, i.e. on the mode shape.
The advantages of crystalline quartz over its amorphous counterpart as discussed here are evident in other crystalline materials. Crystalline silicon shows very high Q factors at cryogenic temperatures [26] in addition to having other highly desirable thermo-mechanical properties [44] and may be used as a test mass material if future IGWDs operate at a laser wavelengths of 1550 nm, or employ non-transmissive topologies [45, 46, 47, 48, 49, 50, 51]. Another crystalline high Q material is sapphire [25, 52], which is already used in the Japanese cryogenic IGWD prototype [53].

4. Conclusions

We confirmed an increasing mechanical loss of fused silica from room temperature down to a maximum at 30K measured at resonant frequencies of slightly above 10 kHz. The emergence of broad loss peaks is a general behaviour of amorphous solids and cannot be circumvented by higher purities. Therefore, fused silica is not suitable as a material for the test masses of cryogenic gravitational wave detectors. Crystalline quartz, however has more promise. Q factors of up to $7 \times 10^7$ were measured on our quartz test mass, suggesting crystalline quartz may merit further study for IGWDs operated at the laser wavelength of 1064 nm. We note that for frequencies in the gravitational wave detection band around 200 Hz the measured crystalline quartz curves in Fig. [1] need to be shifted to the left by 10 to 20 K. This is a result of the frequency dependence of the loss factor according to Eq. [3]. Assuming frequency independent relaxation strengths and times for four independent damping peaks, as found below 150 K in the crystalline quartz investigated here, 50K might turn out to be a preferred temperature for a low thermal noise performance in the gravitational wave detection band. We note that some of the measured losses which arise due to defect relaxations can possibly be reduced by higher purity, sweeping or irradiating the crystal.

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