Thermal, Optical and Mechanical Properties of Nanocrystalline Silicon Optomechanical Cavities

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ABSTRACT

Nanocrystalline silicon is a material that shows highly interesting properties for both electronic and photonic applications. Recently, it has also been employed as the core material for building optomechanical systems, showing some novel features. In this work we provide insight in the optical, mechanical and thermal properties of nanocrystalline silicon as a material platform of optomechanical crystal cavities. The results of this work, extracted by means of a combination of complementary experimental techniques, can be useful to evaluate the potential benefits as well as disadvantages of this material highly relevant for the development of nano-opto-electro-mechanical systems (NOEMS). We show that the specific microscopic nature of the nanocrystalline material has a dominant effect in the optical and mechanical losses and in the thermal properties. More specifically, we find strong correlations between the measured parameters and the volume fraction of grain boundaries, which has been tuned by adjusting the annealing temperature of the layers.
1. Introduction

Nano-opto-electromechanical systems (NOEMS) are a relatively new class of hybrid systems that offer unique opportunities to dynamically control light flow at relatively high speeds and low input powers. When in form of nanoscale optomechanical cavities, they promise a route to realisation of flexible, efficient and reliable interfaces to transfer classical and/or quantum information between microwave and optical domains in a single chip. In the non-linear regime these devices are highly attractive for room temperature applications, such as mass/force sensing, non-volatile memories, chaos-based applications and coupled oscillator networks for neuromorphic computing applications, among others. Many different material platforms have demonstrated significant potential to fulfil those goals. Indeed, a strong interaction between light and mechanical deformation has been demonstrated in nanoscale optomechanical cavities with high enough quality factors, fabricated in technologically relevant material platforms such as silicon nitride (Si$_3$N$_4$), gallium arsenide (GaAs), aluminium nitride (AlN), diamond and, crystalline silicon (c-Si). In particular, the well-established Silicon-On-Insulator (SOI) technology is the key behind most of the best experimental results obtained in optomechanical crystal cavities (OMCs) so far, including ground state cooling and observation of single photon/phonon quantum correlations. Nanocrystalline silicon (nc-Si) is polycrystalline Si in which the grain size is well below 1 μm. It is used in MEMS due to the relatively easy tuning of the mechanical, optical, electrical and thermal properties by tailoring the grain-size and stress. In a recent work, it was demonstrated that nc-Si could also constitute an excellent and cost-competitive alternative to c-Si to build new functional nanoscale optomechanical devices operating at ambient conditions relying on non-linear effects. Non-linear dynamical functions such as phonon lasing and chaos have been reported with a much broader frequency bandwidth.
than that of equivalent devices fabricated on SOI wafers \textsuperscript{17}. In the present work we investigate in detail the properties of nc-Si films by studying a set of nominally identical OMCs fabricated on wafers annealed at different temperatures and, consequently, having different grain size distribution and tensile stress.

2. Description of the layers and structural characterization

The nominal structure of the nc-Si SOI-like wafers was designed to have a 220 nm thick nc-Si film on a 1000 nm thick oxide layer. The fabrication process included growth of a thick SiO\textsubscript{2} layer by wet oxidation at 1050 °C and a layer of amorphous Si at 574 °C by low pressure chemical vapour deposition (LPCVD). A set of four wafers annealed at different temperatures were used in the experiments. The annealing temperatures were 650°C (OMS1), 750°C (OMS2), 850°C (OMS3) and 950°C (OMS4) and annealing time 60 min. The thickness and refractive index of the resulting layers at a wavelength of 633 nm were measured to be 212 nm and 3.87 respectively using spectroscopic reflectometry. Amorphous Si deposited by LPCVD is under compressive stress that can be converted to tensile by annealing. The measured tensile stress of the samples after annealing were 290 MPa (OMS1), 250 MPa (OMS2), 170 MPa (OMS3) and 90 MPa (OMS4). The residual stress was estimated from the change in the curvature of the wafers before and after the deposition and annealing of the nc-Si films. The annealing step transforms the amorphous film to nanocrystalline with the grain size ranging from a few nm to few hundreds of nm. In order to elucidate the structural details we performed a transmission electron microscope (TEM) study of the different films.

Figure 1(b) shows a bright-field TEM micrograph of OMS4, which is representative of the whole set and displays grains with seemingly random orientation. Selective area electron diffraction (SAED) confirmed that the all samples annealed at different temperatures are polycrystalline (see
the inset of Figure 1(b)) with no preferential crystalline orientation. To measure the sizes of
grains, we have employed a standard dark-field analysis methods (DF-TEM, see details in the
Supporting Information file). In the TEM, an aperture is placed in the diffraction plane,
effectively blocking electrons diffracted outside the range covered by the aperture. This creates
images in which only grains with specific crystalline orientations appear bright, on a dark
background. The aperture is then displaced to acquire images so that all grain orientations are
covered. The size of the grains is measured on all images by identifying the brightness threshold
along two perpendicular directions fixed for each samples. Statistics have been done on over 150
grains –300 measurements– for each sample. From the data we have extracted an average grain
size and size distribution for each of the samples. The average size increases with the annealing
temperature from 163 nm to 215 nm and the size distribution broadens towards larger grain size,
as illustrated in Figure 1(a). Consequently, the volume fraction of the grain boundaries within the
layers decreases with the annealing temperature.

We have performed Raman spectroscopy on the nc-Si layers and on a reference c-Si sample
using a 532 nm pump laser. The power of the laser was kept below 1 mW to avoid self-heating
effects. The typical optical-phonon mode of crystalline Si appears in all the cases centred at 520
\( \text{cm}^{-1} \). The nc-Si films show asymmetric broadening at smaller energies, which can be associated
to the presence of a minor amorphous phase, nanocrystallites of different sizes and grain
boundaries \(^{18}\), the most important scattering mechanisms being probably the latter two since the
amorphous phase contribution is expected to be peaked at significantly lower energies (\(~480 \text{ cm}^{-1}\) \(^{19}\)). This is also supported by the SAED images which show that the films are polycrystalline
with no halos arising from amorphous phase. The expected impact of the broadening of the
nanocrystallite size distribution on the Raman signal would be to increase the peak linewidth but,
on the contrary, the linewidth decreases by increasing $T_a$ (inset of Figure 1). The peak broadening can be associated to grain boundaries and the observed tendency to the size distribution shift towards larger domains with $T_a$ as discussed above.

**Figure 1.** a) From top to bottom, histograms of the grain size of samples with increasing annealing temperature $T_a$. A log-normal distribution curve (blue line) is used to fit the histograms. Analysis includes more than 500 grains for each sample and the average grain size ($x_c$) is shown by the vertical dashed black lines. b) Bright field TEM planar image of the OMS4 sample, showing the randomly oriented grains. Inset: Selective area electron diffraction image. c) Raman spectra of a monocrystalline silicon sample (blue) and the nc-Si layers annealed at 650°C and 950°C (green and black, respectively). Inset: Linewidth of the Raman peak as a function of the annealing temperature. The dashed horizontal line corresponds to the value measured from the c-Si reference sample.

The sound velocities in the nc-Si films were measured using a method based on picosecond acoustics.\textsuperscript{20} Interestingly, the sound velocity in all the annealed samples was around 8510 m/s, which is slightly higher than that in (100) Si but lower than in (111) and (110) Si. This may be a
consequence of the polycrystalline nature, averaging the velocities in different crystallographic
directions.

The optomechanical crystals were fabricated on the nc-Si wafers in the same way as reported
elsewhere\textsuperscript{21}. The OMC geometry is based on a unit-cell consisting of a parallelogram with a
cylindrical hole in the centre and two symmetric stubs on the sides (see the SEM image in Figure
2). The cavity region consists of 12 central cells in which the pitch ($a$), the radius of the holes ($r$)
and the length of the stubs ($d$) decrease quadratically way towards the centre of the beam. At
both sides of the central defect region a 10 period mirror is included. The nominal geometrical
values of the cells of the mirror are $a = 500$ nm, $r = 150$ nm, and $d = 250$ nm. The ratio of the
geometrical parameters of the central cell with respect to those of the mirror cells is 0.85. The
length of the OMC beam is about 15 μm and the beam is anchored from the two ends, forming a
stripe clamped at both ends, suitable for optical actuation.

Concerning the geometries designed to be characterized using a time-domain thermo-reflectance
technique, a central gold pad of thickness 80 nm is positioned between two membranes made of
the nc-Si material and it serves both as a heater and sensor (a SEM image of one the resulting
geometries is included as an inset of Figure 5, where the thermo-reflectance measurements are
discussed). The geometries are fabricated using e-beam lithography on a 300 nm thick layer of
PMMA positive resist. Alignment marks were included during the silicon structures fabrication
step to ensure the right placement of the gold squares. After developing the PMMA resist, 4 nm
of chromium and 80 nm of gold were thermally evaporated. Finally, a lift-off process was carried
out using n-methyl pyrrolidinone (NMP) as resist solvent. After that, the BOX silica was
removed by a 10 minutes of HF vapour process to ensure a complete releasing of the
membranes.
3. Experimental setup for optomechanical measurements

The optical and mechanical characterization of the modes supported by the OMCs was performed using the set-up illustrated in Figure 2. The light of two tuneable lasers (L1 and L2), whose polarization states are independently controlled, is multiplexed into a tapered fibre. The thinnest part of the tapered fibre is placed parallel to the OMC, in contact with an edge of the etched frame. The gap between the fibre and the OMC is about 0.2 μm. The long tail of the evanescent field of the fibre mode locally excites the resonant optical modes of the OMC. If not explicitly stated otherwise, the experiments showed in this manuscript are performed by using L1 in a transmission configuration, with L2 switched off. Optical signal decoupled from the OMC can be measured either in transmission or in reflection using InGaAs fast photoreceivers (bandwidth of 12 GHz) PD1 or PD2, respectively. Once in optical resonance, the mechanical motion activated by the thermal Langevin force causes the decoupled signal to be modulated around the static value, which was spectrally decomposed by a spectrum analyser (SA) with a bandwidth of 13.5 GHz. All the measurements were performed in an anti-vibration cage at atmospheric conditions of air pressure and temperature.
Figure 2. Sketch of the experimental setup to measure the optical and mechanical properties of the optomechanical crystals. A SEM image of one of the studied OMCs has been greatly increased for clarity, the total length of the beam being approximately 15μm. λ-mux wavelength multiplexer; λ-filter Fabry-Perot wavelength filter; SG signal generator; VOA, variable optical attenuator; FPC, fibre polarizer controller; SA, spectrum analyser; PD, photodetector.

4. Optical and thermal characterization

Low excitation power optical spectra using L1 of the set of analysed OMCs revealed that they are very similar in terms of the spectral position of the resonant peaks, which is consistent with the fact that all layers have roughly the same thickness and material refractive index. However, the intrinsic optical decay rate of the fundamental mode ($\kappa_{i,1}$, appearing at $\lambda_{r,1} \approx 1.54$ μm), which is extracted indirectly by measuring the overall decay rate ($\kappa_i$) and the power coupled fraction in resonance, shows a clear decreasing tendency as a function of $T_a$ (see the inset in Figure 3). The best $\kappa_{i,1}$ value remains a factor of 1.5 larger than that of the c-Si OMC with equivalent geometry. Material losses are hence the dominant mechanism in nc-Si based OMCs, since radiative losses are unrelated to $T_a$ or to whether the Si material is polycrystalline or not. We associate the main intrinsic optical loss to scattering and absorption at the grain boundaries, e.g. absorption by interface states, since its dependence with $T_a$ is again consistent with the decreasing volume fraction of grain boundaries.

We have also studied the dependence of $\kappa_{i,1}$ with the number of intracavity photons ($n_o$). In Si-based optical resonators there are two main power dependent nonlinear optical losses to be considered when operating at near-infrared optical energies below the gap, namely two-photon absorption (TPA) and free-carrier absorption (FCA). The former scales with $n_o^2$ while the latter is linear with the free-carrier density (N) and depends on the intragap defect states density. In
order to identify and quantify those loss mechanisms we have implemented an optical pump and probe technique in which the 2nd order mode of the OMC is pumped using L1 at high input power \( P_\text{in} \), i.e., \( n_o \) accommodates to the spatial distribution of that mode, while the fundamental mode is probed with L2 at low enough power that its effect on \( \kappa_{i,1} \) can be neglected. In order to adjust \( n_o \) we have fixed \( P_\text{in} \) and changed the relative detuning between the laser wavelength \( (\lambda_{L1}) \) and the resonance wavelength of the 2nd order mode \( (\lambda_{r,2}) \), i.e.,

\[
n_o = n_{o,\text{max}} \frac{\Delta \lambda_{r,2}}{4(\lambda_{r,1} - \lambda_{r,2})^2 + \Delta \lambda_{r,2}^2}.
\]

When the laser is in perfect resonance with the cavity the expression becomes

\[
n_o = n_{o,\text{max}} = \frac{2P_\text{in} \lambda_{L1} \kappa_{r,2}}{\kappa_{2}^2 \hbar c}, \quad \kappa_{r,2} \text{ and } \kappa_2 \text{ being the optical extrinsic and overall optical decay rates of the 2nd order mode, respectively.}
\]

In this particular experiment, light decoupled from the fundamental cavity mode is collected in reflection using a circulator and a tuneable Fabry-Perot filter \( (\lambda\text{-filter}) \) resonant with L2 to filter out the contribution of light decoupled from the 2nd mode. In order to improve the signal-to-noise ratio, the output of L2 is modulated using a signal generator (SG), whose output is used as a reference on a lock-in amplifier that received the signal coming from PD2 (see Figure 2). It is worth noting that we have experimentally verified by inverting the roles of the optical modes, namely the fundamental mode was pumped at high power and the second mode spectrally probed at low power, that \( \kappa_2 \) and \( \kappa_{r,2} \) are not in practice modified up to \( n_o \approx 10^4 \).

Figure 3 summarizes the obtained results, showing that \( \kappa_{i,1} \) increases with \( n_o \) in all the nc-Si samples as a consequence of FCA losses from free-carriers generated by absorption of light stored in the 2nd mode, as described below. Interestingly, the results corresponding to OMS3 and OMS4 show a single linear behaviour with a similar slope

\[
(\kappa_{i,1}(n_o) = \kappa_{i,1}(0) + \frac{\partial \kappa_{i,1}}{\partial n_o} n_o),
\]

where
\[ \frac{\partial \kappa_{i,1}}{\partial n_o} \bigg|_{n_o} = \sigma_{FCA} \left( \frac{c}{n_g} \right) N_o^{1/2} \text{ where } \frac{\partial \kappa_{i,1}}{\partial n_o} \approx 2 \times 10^7 \text{ s}^{-1} \text{ photon}^{-1} \text{ as extracted from the linear fitting of the data and } \sigma_{FCA} \text{ and } n_g \text{ are the free-carrier absorption cross section and the group velocity index, respectively). This result indicates that free-carriers are generated by single-photon absorption from intragap states with similar concentration } (N_o), \text{ excitation cross section } (\sigma_{FC}) \text{ and free-carrier recombination rate } (\Gamma_{FC}) \text{ in both samples. Thus, it is possible to express } N \text{ as } N \approx \left( \frac{\sigma_{FC} N_o}{\Gamma_{FC}} \right) n_o. \text{ The c-Si sample does not show any significant dependence of } \kappa_{i,1} \text{ on } n_o, \text{ i.e., neither FCA nor TPA affect } \kappa_{i,1} \text{ in a way that can be measured under our experimental conditions, which allows us both to neglect TPA in the nc-Si OMCs and state that the concentration of defect states in the c-Si OMC is much lower than on the nc-Si case. Regarding OMS1, two linear regimes appear, the transition between them being found at rather low } n_o \text{ values around } n_{o,t} = 0.2 \times 10^3, \text{ with a lower } \frac{\partial \kappa_{i,1}}{\partial n_o} \text{ in the higher } n_o \text{ region. The slope of the linear fit in the latter region is similar to the other nc-Si sample, i.e., } \frac{\partial \kappa_{i,1}}{\partial n_o} \approx 2 \times 10^7 \text{ s}^{-1} \text{ photon}^{-1}. \text{ Therefore, its origin is probably associated to the same kind of defect states, which are present in a similar concentration in all nc-Si samples. The regime observed at low } n_o \text{ seems to be associated to a different kind of defect states, owning a larger } \sigma_{FC} \text{ value and whose carrier population is depleted at } n_o \approx n_{o,t}. \text{ Concerning sample OMS2 (not shown), the coupled fraction was too small for an accurate determination of } \kappa_{c,2} \text{ and, consequently, of } n_o \text{ and } \frac{\partial \kappa_{i,1}}{\partial n_o}. \text{ Anyhow, the measured } \kappa_{i,1} \text{ values lie between those of OMS1 and OMS3 as expected.} \]
Figure 3. Evolution of the intrinsic optical decay rate as a function of the intracavity photon number for the different samples under study. Inset: Intrinsic losses when the pump laser (L2) is switched off, i.e. for $n_o=0$, as a function of the annealing temperature of the nc-Si layers. The dashed horizontal line corresponds to the value measured on the c-Si sample.

We have also explored the behaviour of the heat dissipation rates of the OMCs as a function of $T_a$. We have a single laser configuration to excite the fundamental optical mode $\lambda_{r,1}$ and adjusted $P_{in}$ to obtain $n_{o,max} \approx 2700$ in all samples. As expected, there is a red-shift of $\lambda_{r,1}$ associated to thermo-optical (TO) dispersion in response to an effective temperature increase ($\Delta T$) of the cavity region. The TO contribution is indeed the origin of a typical saw-tooth spectral shape obtained when measuring a spectrum from short to long wavelength, with the longest wavelength verifying that $\lambda_{L2}=\lambda_{r,1}$ and $n_{a}=n_{o,max}$ (see the inset in Figure 4). Under these experimental conditions it is possible to compare directly the TO contribution in each of the OMCs by
inspecting the maximum $\lambda_{r,l}$ shift. Moreover, since the TO coefficient ($\partial \lambda_{r,l}/\partial \Delta T$) was determined in a previous work to be $\partial \lambda_{r,l}/\partial \Delta T = 0.09 \text{nm/K}$ regardless of the crystalline arrangement of the nc-Si films,\textsuperscript{17} the spectral shifts can be directly related to $\Delta T$. At this point it is worth to point to the results reported in Figure 3, showing that the free-carrier generation rate does not relate with $T_a$, with the exception of the high slope region observed in the OMS1 at low $n_o$, whose contribution can be neglected given that $n_{o,max} >> n_{o,l}$. Furthermore, in previous works we have demonstrated that FCA and subsequent non-radiative recombination within the conduction band are the main source of heating in our Si-based OMCs \textsuperscript{5,17,23}. Thus, in the equilibrium and by using the previously found relations between $N$ and $n_o$, it is possible to derive the following expression:

$$\frac{n_o^2}{\Delta T} = \left( \frac{\Gamma_{FC}}{\alpha_{FCA} \sigma_{FC} N_o} \right) \Gamma_{th} \tag{1}$$

, where $\alpha_{FCA}$ is defined as the rate of temperature increase per photon and unit free-carrier density and $\Gamma_{th}$ as the rate at which heat is leaking out of the cavity, through the anchor points at the ends of the OMC beam or by convection and/or conduction to the surrounding environment. In Figure 4, we have plotted the left hand side of Equation (1) as a function of $T_a$. Since $N_o \sigma_{FC}/ \Gamma_{FC}$ does not depend on $T_a$ and assuming that $\alpha_{FCA}$ is independent of $T_a$, the different values obtained in the plot scale with $\Gamma_{th}$. Therefore, there is a clear increase of $\Gamma_{th}$ with $T_a$, which is directly connected to an increase of the thermal diffusivity and conductivity of the material. The increase in grain size with $T_a$ is in agreement with the increasing thermal conductance of the OMC beams. Indeed, smaller grains lead to enhanced phonon scattering at the grain boundaries and hence to lower thermal conductivity\textsuperscript{24–26}. Samples with smaller grains, i.e., lower $T_a$ in this.
case, therefore display lower thermal conductivity and conductance. This direct comparison of \( \Gamma_{th} \) between samples cannot be made with the c-Si OMC because Equation 1 does not hold for single crystalline silicon. Although the value of \( n_o^2/\Delta T \) extracted for c-Si is much larger than those of nc-Si, one can state that \( \Gamma_{th} \) is larger in c-Si as a consequence of phonon scattering at the grain boundaries in nc-Si\(^{27}\).

![Figure 4](image)

**Figure 4.** Square of the intracavity photon number per effective temperature increase of the cavity as a function of the annealing temperature. The magnitude represented in the y-axis is proportional to the rate at which heat is leaking out of the cavity, as stated in Equation 1.

To independently confirm this trend, we have performed thermal measurements using the time-domain thermo-reflectance technique. A central metal pad of thickness 80 nm, here made of gold, is positioned between two membranes and serves as a heater and sensor (see inset of Figure
5). Its temperature is directly correlated with its reflectivity, which is probed by a continuous-wave laser (532 nm). A 405 nm pulsed laser periodically heats the pad until the system reaches the steady state. The temperature gradient through the membranes normalizes as the heat flows from the central pad to the heat bath. The heat dissipation rate is measured by recording the cooling speed of the system, which takes the form of a single-parameter exponential decay curve \( \exp(-\gamma t) \), where \( \gamma \) is the heat dissipation rate of the system. It is important to note that this heat dissipation rate is not strictly equivalent to \( \Gamma_{th} \) due to the added contribution of the central suspended section and gold pad. The measurement system is directly inspired by previous works, in which more details are given\textsuperscript{27–30}.

We have measured the thermal dissipation rate of identical suspended membranes fabricated in the samples with different \( T_a \). Measurements were performed on three nominally identical structures on each of the samples. The errors bars are calculated as the standard deviation of the three measurements. The results are shown in Figure 5 and clearly show the increasing heat dissipation rate with annealing temperature, which resembles the trend observed in Figure 4.
Figure 5. Heat dissipation rate as measured with the thermoreflectance technique for nc-Si membranes as a function of the annealing temperature. Inset. SEM micrograph of a structure fabricated for the thermal characterization.

5. Mechanical characterization

When the excitation laser is in resonance with the optical cavity mode, it is possible to transduce the thermally activated mechanical modes in all the samples. In Figure 6 we show the RF signals of mechanical breathing modes appearing at about 2.4 GHz on a normalized frequency scale. We have studied the behaviour of the mechanical Q-factor ($Q_m$) and its dependence on $T_a$. The results are shown in the inset of Figure 6. It is clear that the $Q_m$ increases with $T_a$, i.e., it decreases when plotted versus the tensile stress of the material. For the highest annealing
temperature, $Q_m$ is a factor of 2-3 higher than what found in equivalent c-Si OMCs at room temperature.

Thermoelastic damping (TED), resulting from heat generation due to vibration and dissipation from thermal diffusion, is very often the dominant factor which determines the mechanical energy dissipation in micro/nano-scaled beam resonators. An experimentally validated theory to describe TED was first established by Zener for homogeneous materials. This theory was recently extended to polycrystalline materials, in which an enhancement of TED is predicted due to both a reduction of the overall thermal diffusivity of the material and to inter-crystalline damping as a consequence of additional dilatational strains created at the grain boundaries. It is also a well-known that providing mechanical pre-stress (or strain) is an effective way to reduce mechanical losses, which has been in part associated to mitigation of the TED.

The results depicted in Figure 6 reflect that a balance between the two contributions described above determine the overall mechanical dissipation rates in the mechanical modes under study: (i) mechanical tensile strain and (ii) TED. Our results suggest that TED has a much stronger impact on $Q_m$ than the tensile strain. However, the fact that the highest $T_a$ displays a higher $Q_m$ than c-Si, which releases stress after the substrate removal (the OMC are buckled), indicates that TED in OMS4 is weaker than tensile stress effects.
Figure 6. Normalized RF spectrum of a mechanical breathing mode appearing at about 2.4 GHz. The frequency scale has been normalized to allow the linewidth comparison among different samples. Inset: Evolution of the mechanical Q-factor as a function of the annealing temperature and the tensile stress values. The dashed horizontal line corresponds to the value measured from the c-Si sample.

6. Conclusions

In summary, we have used complementary experimental techniques to investigate the optical, mechanical and thermal properties of optomechanical crystal cavities made of nanocrystalline silicon and their dependence on the annealing temperature. We compared the results with those measured from cavities made of single crystalline silicon with identical geometry. Since the comparison has been performed using equivalent geometries, the significant differences found can be ascribed to intrinsic characteristics of the nanocrystalline material. The structural
properties have been characterised by transmission electron microscopy, picoacoustic methods and Raman spectroscopy. The grain size distribution in the nc-Si films shifts towards larger crystalline domains with increasing the annealing temperature. The associated reduction of the volume fraction of grain boundaries within the layers appears to be the origin of the extracted tendencies of optical, mechanical and thermal decay rates, suggesting that the dominant factors are associated with physical phenomena occurring in the grain boundaries. Regarding optical losses of the photonic cavities, intrinsic damping losses decrease with annealing temperature probably due to scattering at the grain boundaries. The relatively strong free-carrier absorption losses are due to carriers generated from single-photon absorption, which appears to be almost unaffected by the annealing temperature. The thermal decay rate significantly increases with annealing temperature due to enhanced thermal conductivity and diffusivity, which is again associated to phonon scattering at the grain boundaries. Finally, mechanical decay rates seem to be dominated by thermoelastic dissipation, which depends directly on the thermal diffusivity and, therefore, decreases with annealing temperature. These results indicate that nanocrystalline silicon has a significant potential to become a material platform for NEMS and or NOEMS with advanced functionalities.

Associated Content

Supporting Information. Further details on the analysis of the dark field TEM images are provided i.

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Supporting Information: Thermal, Optical and Mechanical Properties of Nanocrystalline Silicon Optomechanical Cavities

Dark-field TEM analysis

Dark-field TEM (DF-TEM) is an imaging technique that is diffraction-sensitive. It can be used to analyse from atomic layers to several hundreds of nanometre thick samples and is particularly suitable to analyse grains in polycrystalline materials. First, we have acquired a bright-field TEM image and its corresponding selective area electron diffraction (SAED) pattern, an example of which is shown in Figure S1(a). Then, we have selected five separate diffraction areas, delimited by the colour circles in Figure S1(a). An aperture is placed in the diffraction plane of the TEM so that only electrons within a small range of scattering angles are reaching the detector. The real-space image obtained in that way shows only the grains with in-plane lattice orientations scattered within the aperture, on a dark background, hence the name of the technique. By overlaying the dark-field images obtained for the different aperture positions, we are able to reconstruct most of the map of grain structures. Due to symmetry considerations, covering the whole ring is redundant; diffraction areas were selected so that the overlap in identifiable grains would be minimal. An example of this reconstruction is shown in Figure S1(b) in which only easily identifiable grains are retained.

The analysis of the sizes of grains was performed on the dark-field images with the software DigitalMicrograph® (Gatan). Two perpendicular lines were drawn for each identified grain. The histograms of the intensity on the grayscale were used to precisely delimit the boundaries of the grains. The software then directly converted the size in pixel to a dimension in nanometres. For
each sample, i.e., each annealing temperatures, this process was repeated at different positions on the sample, until more than 150 grains, i.e., more than 300 dimensions, were recorded. We have verified that grains were not taken into account more than once. The histograms are then plotted and fitted by a lognormal distribution, from which the average grain size is extracted.

Figure S1. Dark-Field TEM grain analysis. a) Electron diffraction pattern of sample OMS1. The rings are a signature of poly-crystallinity. Each circle represents one of the apertures selected for DF-TEM, where the selected diffraction pattern is shown. b) Bright-field TEM image of OMS1 with colorized grains. The colours represent the different grain orientations.