Allan variance of frequency fluctuations due to momentum exchange and thermomechanical noises

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We investigate the Allan variance of nanoresonators with random rough surfaces under the simultaneous influence of thermomechanical and momentum exchange noises. Random roughness is observed in various surface engineering processes, and it is characterized by the roughness amplitude w, the lateral correlation length ξ, and the roughness exponent $0<H<1$. The roughness influence becomes significant for measurement time τ_A so that $\omega_o\tau_A\sim 1$, with ω_o the fundamental resonance frequency. The Allan variance increases significantly with increasing roughness (decreasing H and/or increasing ratio w/ξ) if the quality factor due to gas collisions is smaller than the intrinsic quality factor associated with thermomechanical noise. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2787169]

Nanoelectromechanical systems (NEMS) represent an important class of devices that combine the advantages of mechanical systems (e.g., applicability as sensor systems and robustness to electrical shocks) with the speed and large scale integration of silicon based electronics.[1–7] However, the performance of NEMS is limited by noise related dissipation effects. Indeed, as the fluctuation-dissipation theorem states, systems that dissipate energy are necessarily sources of noise, while the converse is also often true. Therefore, a self-contained formalism for describing the resonance and noise related properties of NEMS is important. Moreover, as the resonator size is reduced to nanoscales, the surface to volume ratio increases making nanoresonators susceptible to a variety of surface related noise mechanisms (e.g., by gas molecules impinging the surface, loss due to defects and impurities, scattering of surface acoustic waves by roughness etc.).

Studies of SiC/Si NEMS have shown that devices operational in the uhf/microwave regime have low surface roughness, while devices with rougher surfaces cannot be operated higher than the VHF regime.[8] Other studies of Si nanowires have shown the quality factor to decrease by an increment of the surface area to volume ratio.[9] Recently, random surface roughness was shown to affect the quality factor, the limit to mass sensitivity of nanoresonators, and their dynamic range.[10–12] In addition, another important quantity that is very often used to compare frequency standards and thus quantify frequency fluctuations is the dimensionless Allan variance $\sigma(\tau_A)$.[6,13,14] The latter is defined in the time domain as the variance over time in the measured frequency of a source, where each measurement is averaged over a time interval τ_A (with zero-dead time between measurement intervals). However, how the influence of the surface morphology manifests on the Allan variance and the associated phase noise still remains unexplored. This will be the topic of study in the present paper.

For more realistic treatment we will consider the presence of thermomechanical noise generated by the internal loss mechanisms in the resonator and momentum exchange noise generated from impinging surrounding gas molecules. This is because both types of noise lead to random displacements of the resonator, which are translated to frequency fluctuations and influence the Allan variance. Thermomechanical noise arises from coupling between a mechanical resonator and its dissipative reservoir. The coupling damps the resonator motion and induces spatial fluctuations in the resonator's position at nonzero temperature.[6,15,16] It could be a dominant source of frequency noise at a given mode of vibration, and it imposes an ultimate limit of detection for a dynamic micromechanical sensor.[15,16] Notably, due to its small heat capacity, a nanoresonator can be also subject to rather large temperature fluctuations (which induce frequency fluctuations because dimensions and material parameters are both temperature dependent) depending on the thermal coupling strength to the environment.[6] In addition, mass loading of the resonator can also take place due to adsorption and desorption of gas molecules, which is, however, a parametric noise leaving the quality factor unaffected.[6]

Furthermore, the Allan variance, which gives the variance over time in the measured frequency, is defined as $\sigma(\tau_A)=[1/2f_c^2(N-1)]\Sigma_{m=2}^{N}[\langle f_m\rangle-\langle f_{m-1}\rangle]^2$, where $\langle f_m\rangle$ is the average frequency measured over the mth time interval τ_A and f_c is the carrier frequency driving the nanoresonator.[14] The squared Allan variance is related to the phase noise density $S_\varphi(\omega)$ by[14]

$$\sigma(\tau_A)^2 = 2(2/\omega_c\tau_A)^2\int_0^{+\infty} S_\varphi(\omega)\sin^4(\omega\tau_A/2)d\omega, \qquad (1)$$

where ω_c $(=2\pi f_c)$ is the driven carrier frequency acting perpendicular to the cantilever beam and ω is the modulation frequency from the first harmonic ω_o.[14]

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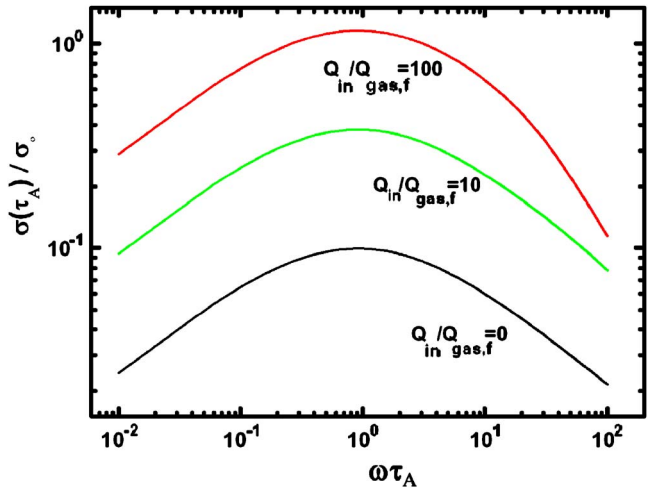

FIG. 1. (Color online) $\sigma(\tau_A)$ as a function of $\omega_o\tau_A$ for $w=3$ nm, $\xi=100$ nm, $H=0.5$, $Q_{\text{in}}=1000$, $\sigma_o=(16A_c/\omega_c^2)$, and $Q_{\text{in}}/Q_{\text{gas,f}}$ as indicated.

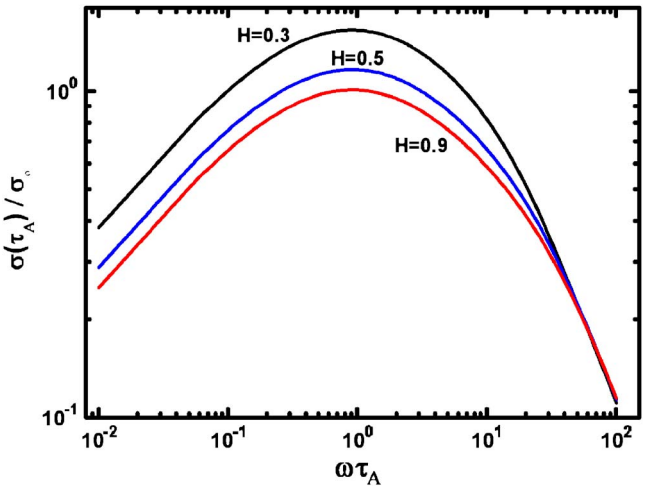

FIG. 2. (Color online) $\sigma(\tau_A)$ as a function of $\omega_o\tau_A$ for $w=3$ nm, $\xi=100$ nm, H as indicated, $Q_{\text{in}}=1000$, $\sigma_o=(16A_c/\omega_c^2)$, and $Q_{\text{in}}/Q_{\text{gas,f}}=100$.

In the presence of both the thermomechanical and momentum exchange noises, the quality factor of the resonator is given by $1/Q=1/Q_{\text{in}}+1/Q_{\text{gas,r}}$. Q_{in} is the intrinsic quality factor associated with thermomechanical noise, and $Q_{\text{gas,r}}$ is the quality factor associated with momentum exchange noise. The quality factor due to momentum exchange noise is given by $Q_{\text{gas,r}}=M_{\text{eff}}\omega_o\sqrt{K_BT/m}(PA_{\text{rou}})^{-1}$, with m the molecule mass, M_{eff} the effective resonator mass that oscillates, and A_{rou} the rough surface area of the resonator.[10] For an oscillating cantilever beam of quality factor Q, mass m, length L, and amplitude factor c_1 of the first harmonic mode with frequency ω_o, the frequency modulated phase noise spectrum $S_\varphi\omega$ has the Lorentzian form[14] $S_\varphi(\omega)=A_o(\omega_o/\{[(\omega+\omega_0)^2-\omega_0^2]^2+\omega_0^4/Q^2\})$, with $A_c=(K_BT)/\pi|c_1|^2L^2mQ_{\text{in}}$. Substitution in Eq. (1) yields

$$\sigma(\tau_A)^2=(16A_c/\omega_c^2)(1+Q_{\text{in}}/Q_{\text{gas,r}})\times\int_0^{+\infty}(\omega_0\tau_A)\sin^4(x)/[(4\omega_0\tau_A+4x^2)^2+(\omega_0\tau_A)^4/Q^2]dx. \quad (2)$$

Our study will be performed for random self-affine rough surfaces observed in a wide range of surface engineering processes.[17] If we assume for the roughness profile a single valued random function $h(r)$ of the in-plane position $r=(x,y)$ and a Gaussian height distribution, the rough area is given by $A_{\text{rou}}/A_{\text{flat}}=R_{\text{rou}}=\int_0^{+\infty}du(\sqrt{1+\rho^2u})e^{-u}$ (Ref. 18), with $\rho=\sqrt{\langle(\nabla h)^2\rangle}$ the average local surface slope $[\rho=(\int_{0\le q\le Q_c}q^2\langle|h(q)|^2\rangle d^2q)^{1/2}]$,[19] and $A_{\text{flat}}=2w_bL$ the average flat surface area of the cantilever beam of width w_b. $Q_c=\pi/a_o$, with a_o a lower lateral cutoff. As a result, we obtain $Q_{\text{gas,r}}=R_{\text{rou}}Q_{\text{gas,f}}$ with $Q_{\text{gas,f}}=M_{\text{eff}}\omega_o\sqrt{K_BT/m}(PA_{\text{flat}})^{-1}$. $\langle|h(q)|^2\rangle$ is the roughness spectrum, which is required to calculate $\sigma(\tau_A)$. A wide variety of surfaces possesses, the so-called self-affine roughness,[18] with a roughness spectrum that scales as $\langle|h(q)|^2\rangle\propto q^{-2-2H}$ if $q\xi\gg1$, and $\langle|h(q)|^2\rangle\propto$ const. if $q\xi\ll1$.[18,20] This scaling is satisfied by the analytic model[20] $\langle|h(q)|^2\rangle=(2\pi w^2\xi^2)/(1+aq^2\xi^2)^{(1+H)}$, with $a=(1/2H)[1-(1+aQ_c^2\xi^2)^{-H}]$ if $0<H<1$, and $a=1/2\ln(1+aQ_c^2\xi^2)$ if $H=0$. Small values of H (~0) characterize jagged or irregular surfaces, while large values of H (~1) characterize surfaces with smooth hills/valleys.[17,20] For other roughness models see Ref. 21

The calculations of the Allan variance $\sigma(\tau_A)$ were performed for roughness amplitudes observed in real resonators in the range $w\sim2-8$ nm,[8] and $a_o=0.3$ nm. Figure 1 shows calculations of $\sigma(\tau_A)$ for two different values of the ratio $Q_{\text{in}}/Q_{\text{gas,f}}$. It becomes evident that the momentum exchange noise and through it the surface morphology of the resonator has strong influence for $Q_{\text{in}}\gg Q_{\text{gas,f}}$. Under these conditions as Fig. 2 indicates, the influence of the roughness exponent H appears to play significant role for relatively low frequencies $\omega_o\tau_A\leqslant10$. This is also shown in Fig. 3 which shows the Allan variance for two different roughness amplitudes. In any case, the Allan variance increases with increasing roughness (decreasing H and/or increasing roughness ratio w/ξ) if the quality factor due to gas collisions is smaller than the intrinsic quality factor associated with thermomechanical noise.

For frequencies well off the peak resonance, but small compared to the resonance frequency or $\omega_o/Q\ll\omega\ll\omega_o$, the

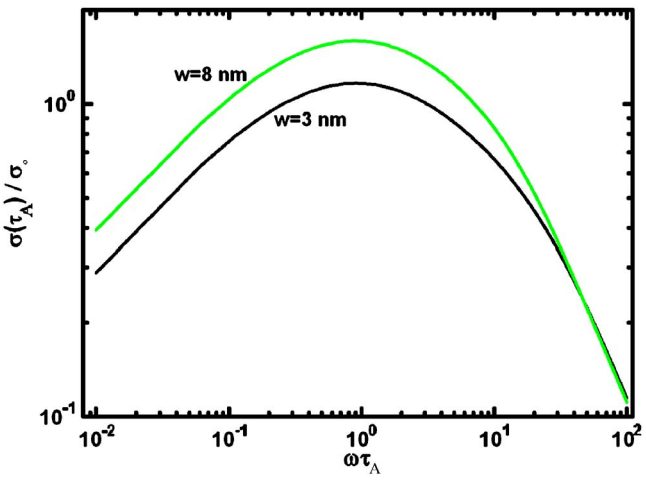

FIG. 3. (Color online) $\sigma(\tau_A)$ as a function of $\omega_o\tau_A$ for w as indicated, $\xi=100$ nm, $H=0.5$, $Q_{\text{in}}=1000$, $\sigma_o=(16A_c/\omega_c^2)$, and $Q_{\text{in}}/Q_{\text{gas,f}}=100$.

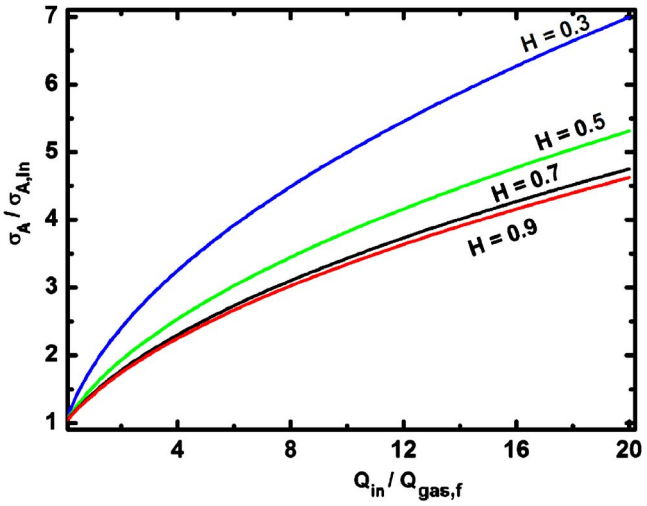

FIG. 4. (Color online) $\sigma(\tau_A)$ as a function of $Q_{\rm in}/Q_{\rm gas,f}$ using the approximate theory of Eq. (3) for $w=3$ nm, $\xi=100$ nm, $H=0.5$, and $Q_{\rm in}=1000$.

phase noise has the form $S_\varphi(\omega)\approx(1/4\pi\varepsilon_c Q)(\omega_o/\omega)^2$ and Eq. (1) gives $\sigma(\tau_A)=1/\sqrt{4\varepsilon_c\omega_c\tau_A Q}$, where $\varepsilon_c=\omega_o^2/\pi A_c$. $\sigma(\tau_A)$ falls inversely with the square root of the measurement time τ_A, the quality factor Q, and the resonator frequency ω_o. Increment of any of these factors leads to lower Allan variance. Notably, this approximate form applies quite well for τ_A sufficiently large so that $\omega_o\tau_A>10$. For the case of thermomechanical and momentum exchange noises, the Allan variance obtains the more intuitive form of

$$\sigma(\tau_A)=\sigma_{\rm in}(\tau_A)[1+(Q_{\rm in}/Q_{\rm gas,f})R_{\rm rou}]^{1/2}, \tag{3}$$

with $\sigma_{A,\rm in}=1/\sqrt{4\varepsilon_c\omega_c\tau_A Q_{\rm in}}$. Figure 4 shows the calculation using Eq. (3) of the Allan variance as a function of the quality factor ratio $Q_{\rm in}/Q_{\rm gas,f}$. Significant influence of surface roughness takes place for $Q_{\rm in}\gg Q_{\rm gas,f}$. In the opposite limit, $Q_{\rm in}\ll Q_{\rm gas,f}$, we obtain from Eq. (3) $\sigma(\tau_A)\cong\sigma_{A,\rm in}[1+(Q_{\rm in}/Q_{\rm gas,f})R_{\rm rou}+\cdots]$.

In conclusion, we investigated the simultaneous influence of thermomechanical and momentum exchange noises on the Allan variance of nanoresonators with random rough surfaces. The influence of the roughness is becoming significant for measurement time τ_A such that $\omega_o\tau_A\sim 1$ with ω_o the fundamental resonance frequency of the resonator. The Allan variance increases with increasing roughness (decreasing roughness exponent H and/or increasing roughness ratio w/ξ) if the quality factor due to gas collisions is smaller than the intrinsic quality factor associated with thermomechanical noise. The present results are expected to be important in noise studies of NEMS where understanding the influence of surface morphology can be of significant importance.

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