APPLIED PHYSICS LETTERS **90**, 041914 (2007)

Random surface roughness influence on gas damped nanoresonators

G. Palasantzas[a)]
Department of Applied Physics, Materials Science Center, University of Groningen, Nijneborgh 4, 9747 AG Groningen, The Netherlands

(Received 15 November 2006; accepted 21 December 2006; published online 25 January 2007)

The author investigates quantitatively the influence of random surface roughness on the quality factor Q of nanoresonators due to noise by impinging gas molecules. The roughness is characterized by the amplitude w, the correlation length ξ, and the roughness exponent H that describes fine roughness details at short wavelengths. Surface roughening (decreasing H and increasing ratio w/ξ) leads to lower Q, which translates to lower sensitivity to external perturbations, and a higher limit to mass sensitivity. The influence of the exponent H is shown to be important as that of w/ξ, indicating the necessity for precise control of the surface morphology. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2435328]

Today microelectronics technology is pushing into the submicron range, which inspires the extension of electromechanical systems in the nanometer range leading to nanoelectromechanical systems (NEMSs).[1–14] The latter attain extremely high fundamental frequencies (approximately gigahertz),[4,15] mechanical quality factors $Q\sim 10^3-10^5$,[4,16] femtogram active masses ($\sim 10^{-15}$ g),[4] and heat capacities below a yoctocalorie (10^{-18} cal).[17] The quality factor Q, which is associated with damping, measures the ratio of the stored energy E_{stor} to the dissipated energy E_{dis} (within an oscillation cycle) so that $Q=2\pi(E_{\text{stor}}/E_{\text{dis}})$. For larger factor Q the resonance system has higher sensitivity to external perturbations. Q also determines the level of fluctuations that degrades the resonance spectral purity and determines the minimum intrinsic power $\sim K_BTQ/\omega_0$ at which the device can operate with ω_0 the resonance frequency, T the temperature, and K_B the Boltzmann factor.[4]

The quality factor Q of a mechanical oscillator is determined by various multiple loss mechanisms as $Q^{-1}=\Sigma_j Q_j^{-1}$. The index j includes attachment loss due to gas molecules impinging the resonator surface, loss due to bulk defects and impurities, losses due to thermoelastic effects and other phonon-phonon scattering phenomena, and losses due to surface effects.[18] Indeed, surface roughness has shown to decrease Q.[9,19] Studies for SiC/Si NEMS have shown that devices operating in the uhf regime had low surface roughness ($\sim$2.1 nm), while devices with rougher surfaces ($\sim$7.1 nm) were operational only up to the VHF regime.[19] In other studies of Si nanowires, it was shown that the Q factor was decreased from $Q\sim 3000$ to 500 by surface area to volume ratio increment from $\sim$0.02 to 0.07.[9]

So far none of the former studies either in gas atmosphere or in vacuum showed any direct quantitative calculation of the surface roughness influence on the factor Q. This will be the topic in this letter for the case of gas damping due to impingement and momentum exchange of gas molecules on a random rough surface. Modeling of the latter will be considered for the case of self-affine roughness, which is observed in a wide variety of thin film deposition processes and surface engineering procedures.[20]

For a resonator in a gas atmosphere the Knudsen number K_n, which measures the ratio of the mean free path L_{mph} of gas molecules to the beam size, determines operation in the continuum regime if $K_n<0.01$ and operation in the molecular regime for $K_n>10$.[21] For a beam of length $L_b>10w_b$, where w_b is the beamwidth, we have $K_n=L_{\text{mph}}/w_b$, where $L_{\text{mph}}=0.23K_BT/(Pd^2)$ for a dilute gas of pressure P and assuming the molecules as hard spheres with diameter d.[21] For example, with $d=0.37$ nm, $T=300$ K, and $P=1$ atm we have $L_{\text{mph}}=65$ nm meaning that a resonator with width $w_b=10$ μm operates in the continuum regime if $P>1$ atm, while with $w_b=100$ nm it operates in the molecular regime even for $P>10$ atm.[22] Indeed, in the molecular regime the resonator equation of motion has the form (inset of Fig. 1)[5]

$$M_{\text{eff}}\ddot{u}+M_{\text{eff}}\omega_0^2u=-(M_{\text{eff}}\omega_0/Q_{\text{in}})\dot{u}-(PA_{\text{rou}}/v_T)\dot{u}+F(t), \quad (1)$$

where $u(t)$ is the displacement coordinate, $F(t)$ is the external drive force, $v_T=\sqrt{K_BT/m}$ is the thermal molecule velocity, m is the molecule mass, M_{eff} is the effective resonator mass participating in the oscillation, A_{rou} is the resonator rough surface area, and $-(M_{\text{eff}}\omega_0/Q_{\text{in}})\dot{u}$ is the force due to intrinsic damping with quality factor Q_{in}. $-(PA_{\text{rou}}/v_T)\dot{u}$ is the drag

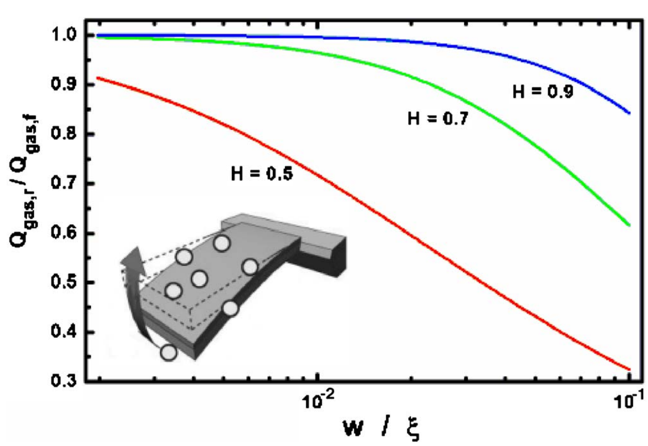

FIG. 1. (Color online) Calculations of the quality factor ratio $Q_{\text{gas},r}/Q_{\text{gas},f}$ due to gas dissipation as a function of the long wavelength roughness ratio w/ξ for $w=10$ nm and various roughness exponents H. The inset shows an example of a resonator oscillating within gas molecules.

[a)]Author to whom correspondence should be addressed; electronic mail: g.palasantzas@rug.nl

force due to impingement and momentum exchange by gas molecules. If we write $-(PA_{\rm rou}/v_T)\dot{u} \equiv -(M_{\rm eff}\omega_0/Q_{\rm gas})\dot{u}$ then we obtain the quality factor due to gas damping by $Q_{\rm gas}=M_{\rm eff}\omega_0\sqrt{K_BT/m}(PA_{\rm rou})^{-1}$.

If we assume for the roughness profile a single valued random fluctuation $h(r)$ of the in-plane position $r=(x,y)$ and a Gaussian height distribution, the rough surface area $A_{\rm rou}$ is given by $A_{\rm rough}=A_{\rm flat}\int_0^{+\infty}du(\sqrt{1+\rho^2u})e^{-u}$ with $\rho=(\int_{0\leq q\leq Q_c}q^2C(q)d^2q)^{1/2}$.[23,24] $\rho=<\sqrt{\langle(\nabla h)^2\rangle}$ is the average local surface slope, $A_{\rm flat}$ is the average flat surface area, $Q_c=\pi/a_0$, where a_0 is the lower roughness cutoff of atomic dimensions, and $C(q)=\langle|h(q)|^2\rangle$ is the roughness spectrum. Upon substitution we obtain

$$Q_{{\rm gas},r}=M_{\rm eff}\omega_0\sqrt{K_BT/m}(PA_{\rm flat})^{-1}\times\left\{\int_0^{+\infty}du(\sqrt{1+\rho^2u})e^{-u}\right\}^{-1}, \quad (2)$$

where $Q_{{\rm gas},f}\approx M_{\rm eff}\omega_0\sqrt{K_BT/m}(PA_{\rm flat})^{-1}$ and $A_{\rm flat}=2w_bL_b$ (the factor 2 accounts for the upper and lower surface areas; see inset of Fig. 1).

Calculations of factor Q from Eq. (2) require knowledge of $\langle|h(q)|^2\rangle$. Indeed, a wide variety of surfaces possesses the so-called self-affine roughness,[20] with a spectrum that scales $\langle|h(q)|^2\rangle\propto q^{-2-2H}$ if $q\xi\gg1$ and $\langle|h(q)|^2\rangle\propto$const if $q\xi\ll1$.[20] This scaling is satisfied by the analytic model[25] $\langle|h(q)|^2\rangle=(2\pi w^2\xi^2)/(1+aq^2\xi^2)^{(1+H)}$, 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 $H\sim0$ characterize very jagged or irregular surfaces, while large values of $H\sim1$ refer to surfaces with smooth hills and valleys.[20,25] For other models see Ref. 26. In addition, we obtain for the local slope ρ the simple analytic form $\rho=(w/\sqrt{2}\xi a)\sqrt{(1-H)^{-1}[(1+aQ_c^2\xi^2)^{1-H}-1]-2a}$.[27] For weak roughness ($\rho\ll1$) we have $A_{\rm rough}/A_{\rm flat}\approx1+(\rho^2/2)$, which is independent of the assumption of a Gaussian height distribution. We obtain for the Q factor the analytic form

$$Q_{{\rm gas},r}\approx Q_{{\rm gas},f}[1-(w^2/4\xi^2a^2)\{(1-H)^{-1}\times[(1+aQ_c^2\xi^2)^{1-H}-1]-2a\}].$$

Figure 1 shows calculation of the quality factor as a function of the ratio w/ξ for various exponents H. With increasing roughness (decreasing H and/or increasing ratio w/ξ), the Q factor decreases significantly and has a sensitive dependence on the exponent H. Indeed, for $H\leq0.5$ the influence of the roughness ratio w/ξ becomes also very pronounced. Furthermore, Fig. 2 depicts the influence of the roughness amplitude w for various correlation lengths ξ, because in many studies only the amplitude w is considered to describe surface roughening.[19]

The significance of $Q_{\rm gas}$ derives by comparison to Q's from other dissipation sources. Indeed, the thermoelastic effect yielded $Q_{\rm th}^s\sim(3-80)\times10^5$ for Si at $T=300$ K, and the phonon-phonon interaction gave large factors $Q_{\rm ph-ph}\gg Q_{\rm th}^s$.[1,28] In addition, from Fig. 6 in Ref. 4, we have $Q_{\rm th}^s\approx Q_{\rm gas}$ at relatively high gas pressures ~10 mTorr for He^3 and He^4. Therefore, gas dissipation and intrinsic thermoelastic effects could give comparable contribution, while surface roughening can significantly decrease $Q_{\rm gas}$ making it the dominant quality factor.

Furthermore, the spectral density of the randomly fluctuating force due to impingement of molecules is given by $S_{P,{\rm rou}}(\omega)=S_{P,{\rm flat}}(\omega)(A_{\rm rou}/A_{\rm flat})$, where $S_{P,{\rm flat}}(\omega)=4mv_T(PA_{\rm flat})$.[5,29] The resonator responds to the random force by displacement fluctuations with spectral density $S_{x,{\rm rou}}(\omega)=(S_{P,{\rm rou}}(\omega)/M_{\rm eff}^2)/\{(\omega^2-\omega_0^2)^2+\omega^2\omega_0^2Q_{{\rm gas},r}^{-2}\}$,[5] and frequency fluctuations with spectral density $S_{\omega,r}(\omega)=(\omega_0/2Q_{{\rm gas},r})[S_{x,{\rm rou}}(\omega)/\langle u_c^2\rangle]$ and thus a frequency shift $\delta\omega_r=\int_{\omega_0-\Delta f\leq\omega\leq\omega_0+\Delta f}S_{\omega,r}(\omega)d\omega\approx(E_{\rm th}/E_C)^{1/2}(\omega_0\Delta f/Q_{{\rm gas},r})^{1/2}$ (for $Q_{{\rm gas},r}\gg1$ and $\omega_0/Q_{{\rm gas},r}\gg2\pi\Delta f$, where Δf is the measurement bandwidth). $E_{\rm th}=K_BT$, and $E_C=M_{\rm eff}\omega_0^2\langle u_c^2\rangle$ is the maximum resonator drive energy at constant amplitude $\langle u_c^2\rangle$.[4] The corresponding limit to mass sensitivity $\delta M\approx(2M_{\rm eff}/\omega_0)\delta\omega_r$ Ref. 5 is given by

$$\delta M_{\rm rou}=2M_{\rm eff}(E_{\rm th}/E_C)^{1/2}(\Delta f/\omega_0Q_{{\rm gas},f})^{1/2}\times\left\{\int_0^{+\infty}du(\sqrt{1+\rho^2u})e^{-u}\right\}^{1/2}, \quad (3)$$

where $\delta M_{\rm flat}\sim2M_{\rm eff}(E_{\rm th}/E_C)^{1/2}(\Delta f/\omega_0Q_{{\rm gas},f})^{1/2}$.[5] Figure 3 shows calculations of $\delta M_{\rm rou}$. The latter increases with respect to that of a flat surface $\delta M_{\rm flat}$ with increasing surface roughness (decreasing exponent H and/or increasing ratio w/ξ). Also similar is the behavior in Fig. 4 with increasing roughness amplitude w.

In conclusion, the influence of random self-affine surface roughness on the quality factor $Q_{\rm gas}$ of nanoresonators lim-

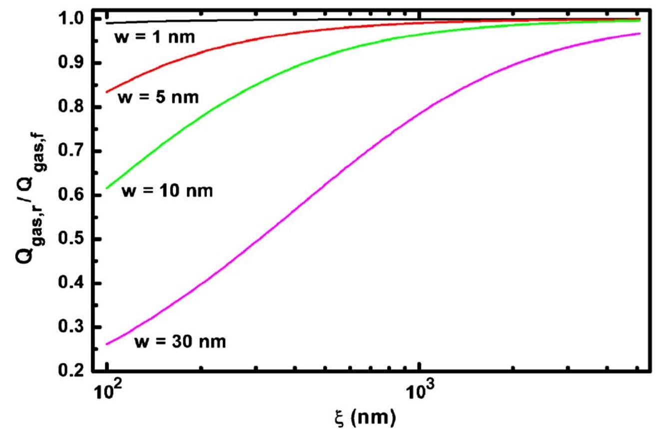

FIG. 2. (Color online) Calculations of the quality factor ratio $Q_{{\rm gas},r}/Q_{{\rm gas},f}$ due to gas dissipation as a function of the correlation length ξ for $H=0.7$ and various roughness amplitudes w.

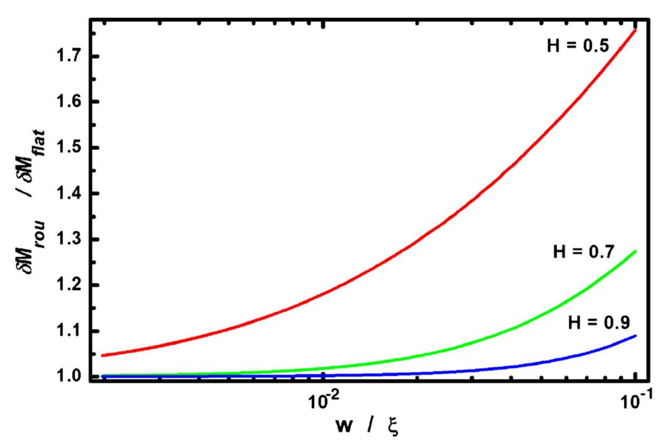

FIG. 3. (Color online) Calculations of the limit to mass sensitivity ratio $\delta M_{\rm rou}/\delta M_{\rm flat}$ due to gas dissipation as a function of the long wavelength roughness ratio w/ξ for $w=10$ nm and various roughness exponents H.

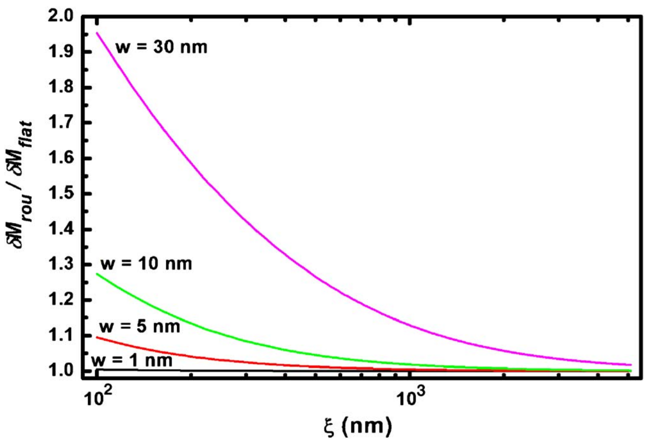

FIG. 4. (Color online) Calculations of the limit to mass sensitivity ratio $\delta M_{\mathrm{rou}}/\delta M_{\mathrm{flat}}$ due to gas dissipation as a function of the correlation length ξ for $H=0.7$ and various roughness amplitudes w.

ited by gas damping within the molecular regime was investigated. It is shown that surface roughening at short lateral wavelengths (decreasing exponent H) and/or long lateral wavelengths (increasing ratio w/ξ) leads to significantly lower quality factors and thus to lower sensitivity to external perturbations. In addition, the corresponding limit to mass sensitivity δM_{rou} is shown to increase significantly with increasing roughening, indicating a necessity for better control of the surface morphology of resonating systems.

The author would like to acknowledge useful discussions with K. Ekinci and H. Craighead.

[1]M. L. Roukes, Phys. World **14**, 25 (2001).
[2]A. N. Cleland and M. L. Roukes, Appl. Phys. Lett. **69**, 2653 (1996).
[3]A. Cleland, *Foundations of Nanomechanics* (Springer, New York, 2003).
[4]K. L. Ekinci and M. L. Roukes, Rev. Sci. Instrum. **76**, 061101 (2005).
[5]K. L. Ekinci, Y. T. Yang, and M. L. Roukes, J. Appl. Phys. **95**, 2682 (2004); A. N. Cleland and M. L. Roukes, *ibid.* **92**, 2758 (2002). For Eq. (1), see also K. Kokubun, M. Hirata, M. Ono, H. Murakami, and Y. Toda, J. Vac. Sci. Technol. A **5**, 2450 (1987); F. R. Blom, S. Bouwstra, M. Elwenspoek, and J. H. J. Fluitman, J. Vac. Sci. Technol. B **10**, 19 (1992).
[6]K. C. Schwab and M. L. Roukes, Phys. Today **58**(7), 36 (2005).
[7]V. Sazonova, Y. Yaish, H. Ustunel, D. Roundy, T. A. Arias, and P. L. McEuen, Nature (London) **431**, 284 (2004).
[8]A. B. Hutchinson, P. A. Truitt, K. C. Schwab, L. Sekaric, J. M. Parpia, H. G. Craighead, and J. E. Butler, Appl. Phys. Lett. **84**, 972 (2004).
[9]D. W. Carr, S. Evoy, L. Sekaric, H. G. Craighead, and J. M. Parpia, Appl. Phys. Lett. **75**, 920 (1999); L. Sekaric, J. M. Parpia, H. G. Craighead, T. Feygelson, B. H. Houston, and J. E. Butler, *ibid.* **81**, 4455 (2002).
[10]S. Evoy, A. Olkhovets, L. Sekaric, J. M. Parpia, H. G. Craighead, and D. W. Carr, Appl. Phys. Lett. **77**, 2397 (2000).
[11]K. Y. Yasumura, T. D. Stowe, E. M. Chow, T. Pfafman, T. W. Kenny, B. C. Stipe, and D. Rugar, J. Microelectromech. Syst. **9**, 117 (2000).
[12]M. L. Roukes, Phys. World **14**, 25 (2001); in *Technical Digest of the 2000 Solid State Sensor and Actuator Workshop*, Hilton Head, SC, 4 June 2000.
[13]K. Y. Yasumura, T. D. Stowe, E. M. Chow, T. Pfafman, T. W. Kenny, and D. Rugar, *Proceedings of the Solid-State Sensor and Actuator Workshop*, Hilton Head Island, SC, 1998 (IEEE, New York, 1998), p. 65.
[14]J. Yang, T. Ono, and M. Esashi, Appl. Phys. Lett. **77**, 3860 (2000).
[15]X. M. H. Huang, C. Zorman, M. Mehregany, and M. L. Roukes, Nature (London) **421**, 496 (2003).
[16]K. L. Ekinci, Y. T. Yang, X. M. Huang, and M. L. Roukes, Appl. Phys. Lett. **81**, 2253 (2002).
[17]M. L. Roukes, Physica B **263**, 1 (1999).
[18]X. Liu, J. F. Vignola, H. J. Simpson, B. R. Lemon, B. H. Houston, and D. M. Photiadis, J. Appl. Phys. **97**, 023524 (2005); H. E. Bömmel and R. Dransfeld, Phys. Rev. **117**, 1245 (1960); C. Zener, *ibid.* **53**, 90 (1938).
[19]X. M. H. Huang, Ph.D. thesis, California Institute of Technology, 2004.
[20]J. Krim and G. Palasantzas, Int. J. Mod. Phys. B **9**, 599 (1995); P. Meakin, Phys. Rep. **235**, 1991 (1994); Y.-P. Zhao, G.-C. Wang, and T.-M. Lu, *Characterization of Amorphous and Crystalline Rough Surfaces: Principles and Applications*, Experimental Methods in the Physical Science Vol. 37 (Academic, New York, 2001), Chap. 3.
[21]R. B. Bhiladvala and Z. J. Wang, Phys. Rev. E **69**, 036307 (2004).
[22]V. B. Braginsky, V. P. Mitrofanov, and V. I. Panov, *Systems with Small Dissipation* (The University of Chicago Press, Chicago, 1985).
[23]B. N. J. Persson and E. J. Tosatti, J. Chem. Phys. **115**, 5597 (2001).
[24]G. Palasantzas and J. Th. M. DeHosson, Phys. Rev. E **67**, 021604 (2003).
[25]G. Palasantzas, Phys. Rev. B **48**, 14472 (1993); **49**, 5785 (1994).
[26]S. K. Sinha, E. B. Sirota, S. Garoff, and H. B. Stanley, Phys. Rev. B **38**, 2297 (1988); H. N. Yang and T. M. Lu, *ibid.* **51**, 2479 (1995).
[27]G. Palasantzas, Phys. Rev. E **56**, 1254 (1997).
[28]R. Lifshitz and M. L. Roukes, Phys. Rev. B **61**, 5600 (2000).
[29]G. E. Uhlenbeck and S. Goudsmit, Phys. Rev. **34**, 145 (1929).