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Nanocomplex oscillations as forewarning of fatigue collapse of NEMS

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ABSTRACT

In this paper we demonstrate that complex oscillations precede the fatigue collapse of nano-electromechanical systems. As a prototype of working nano-device, we consider a nanowire-based nanoswitch loaded by a periodic electro-mechanical force. Just before failure, nano-sub-harmonics are abruptly generated in the nano-displacement field. Such a forewarning, found to be larger for smaller systems, could thus be used as a simple binary tool for monitoring the nano-system integrity, atomistic cracks remaining undetectable by current microscopes.

KEYWORDS: complexity, sub-harmonics, non-linearity, dynamics, forewarning, collapse, fatigue, cracks, nano-electromechanical systems

1. INTRODUCTION

Nano-electromechanical systems (NEMS) will probably revolutionize our future technology, due to their extreme miniaturized size. Only recently, some research groups have been able to manufacture nano-systems. For instance, Kim and Lieber [1] developed a nanotweezer; its mechanical capability was demonstrated by gripping and manipulating submicron clusters and nanowires. Likewise, Rueckes *et al.* [2] investigated a carbon nanotube-based nonvolatile random access memory, by considering an innovative bistable nanoswitch based on electrostatic and van der Waals forces; the viability of the concept was demonstrated by the experimental realization of a reversible bistable nanotube-based bit. Furthermore, the first really true nanotube-based nano-electro-mechanical system, fully integrating electronic control and mechanical response, was recently developed by Fennimore *et al.* [3], through the realization of a rotational motor; the authors reported the construction and successful operation of a fully synthetic nanoscale electromechanical motor incorporating a rotational metal plate with a multi-walled carbon nanotube serving as the key motion-enabling element. More recently other NEMS have been built. For example, Ke *et al.* [4], similarly to [1], reported the development of a nanoswitch, as well as of a detailed analytical study on the pull-in voltage required to the on/off transition of the device.

In parallel to this fast acceleration in the development of nano-systems, key analyses on their static and dynamic behaviours have been reported [4-10], mainly devoted to the prediction of the NEMS pull-in voltage. In spite of this, the monitoring of such nano-systems during their fatigue life, still represents a difficult task. Nevertheless, the study of the nonlinear dynamics of nano-systems may represent a powerful tool for damage detection and non-destructive monitoring. The analysis of the dynamic response of a structure to excitation forces and the monitoring of alterations, which may occur during its lifetime, can be employed as a global integrity-assessment technique to detect, for example, the presence of a crack. The damage assessment problem in cracked large structures has been extensively studied in the

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last decade [11-15], highlighting that the vibration based inspection is a valid method to detect, localise and quantify cracks especially in one-dimensional structures. Dealing with the presence of a crack in a beam, previous studies have demonstrated that a transverse crack can change its state, from open to closed and viceversa, when the structure, subjected to an external load, vibrates [13, 14]. As a consequence, a nonlinear dynamic behaviour is introduced, that could be useful for crack detection.

In this paper we consider a nanowire loaded by a periodic electromechanical force and show that strong damage, arising just before failure, abruptly induces sub-harmonics in the nano-displacement field: thus, complex oscillations precede the collapse of nano-systems, and their extreme miniaturized size is found to enlarge this forewarning. Such a finding could thus be used as a simple binary tool for monitoring the NEMS integrity and its eventual substitution in integrated nanostructured architectures.

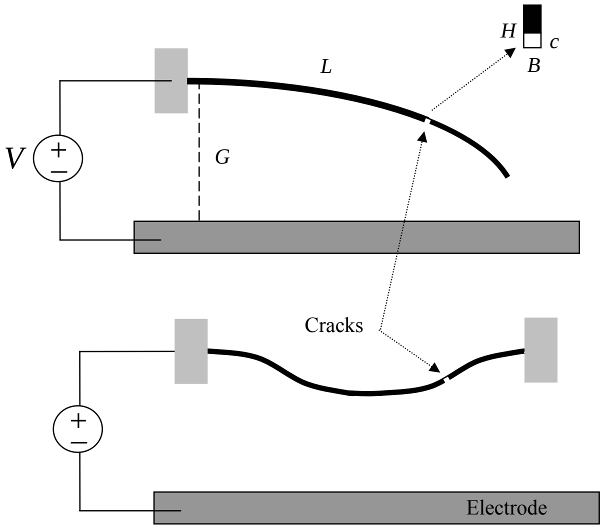

Figure 1. Single- or doubly-clamped vibrating cracked nanowire-based NEMS; V is the applied voltage, G is the gap, L is the length, B and H are the base and height of the cross-section, c is the crack length.

2. Nanocomplexity during fatigue of NEMS

Consider a nanowire of length L, cross-section base B and height H, suspended at a gap distance G over a substrate, from which a difference in voltage V is imposed, Figure 1. We discretize the system with an opportune number of degrees of freedom. The working conditions are simulated by a periodic electromechanical vector of loads (forces/couples) $\{V\}$, mainly a function of the applied voltage. The nano-displacements $\{X\}$ (translations and rotations) must thus satisfy the dynamical equilibrium of the system:

$$[M]\{\ddot{X}\}+[D]\{\dot{X}\}+[S]\{X\}+\{F(\{X\})\}=\{V\} \qquad (1)$$

where $[M]$, $[D]$ and $[S]$ represent respectively the mass, damping and stiffness matrixes of the nano-system, derivable according to the Beam Theory [14], and $\{F(\{X\})\}$ is the nonlinearity induced by the presence of nano-cracks (the dot over the symbols represents the time derivative). It is given by [14]:

$$\{F(\{X\})\}=\sum_i\left[\Delta S^{(i)}\right]f^{(i)}(\{X\})\{X\}$$

$$f^{(i)}(\{X\})=\frac{X_{i_r}-X_{i_l}}{\left|X_{i_r}-X_{i_l}\right|_{\max}} \qquad (2)$$

where $[S]+\sum_i[\Delta S^{(i)}(c_i)]$ is the stiffness matrix of the undamaged nano-system and $[\Delta S^{(i)}(c_i)]$ is half of the variation in stiffness, derivable according to Fracture Mechanics [14], introduced when the ith crack is fully open, a function of the ith crack depth c_i. According to this notation $f^{(i)}(\{X\})$ ranges linearly between −1 and +1 and models the transition between the conditions of ith crack fully-open and fully-closed, depending on the curvature of the corresponding cracked element ($X_{i_{l,r}}$ are the left and right rotations of the ith cracked finite element).

The force vector $\{V\}$ is assumed to have a period $P=2\pi/\omega$. Thus, according to Fourier, it can be developed in the following form:

$$\{V\}=\sum_{j=0}^{Q}\left(\{V_S\}_j\sin\frac{j}{n}\omega t+\{V_C\}_j\cos\frac{j}{n}\omega t\right) \qquad (3)$$

with n=1, where t is the time. Q should be large enough to reach a good approximation. A different from the unity parameter n describes sub-harmonic generation ([16, 17]) and thus complexity, that is a transition towards a deterministic chaos. Thus, assuming as the period of the displacement a multiple n of the period of the excitation (in the experiments [15] $n \geq 2$), and according to Fourier analysis, we can write $\{X\}$ formally as $\{V\}$ in eq. (3) if the substitution $V \to X$ is made (here $n \neq 1$). Introducing this time-dependent $\{X(t)\}$ into the crack function $\{F(X)\}$ and developing according to Fourier analysis yields again the same expansion of eq. (3) if $V \to F$, where $\{F_{S,C}\}$ are known functions of the constants $\{X_{S,C}\}$.

By introducing such expressions for V, X, F into eq. (1) and balancing the harmonics with the same angular frequency, would formally solve the problem, correlating load and displacement. Accordingly, a algebraic system of Q+1 nonlinear equations is derived in the form of:

$$[A(j)]\{X_{SC}(j)\} = \{V_{SC}(j)\} - \{F_{SC}(j)\},$$
$$\begin{Bmatrix} \{Y_S\}_j \\ \{Y_C\}_j \end{Bmatrix} = \{Y_{SC}(j)\} \, \forall Y = V, X, F, \quad j=0,\dots,Q \tag{4}$$

where $[A(j)]$ is a known matrix (see [14,16,17] for details).

The force vector $\{V\}$ acting on the nano-system is the sum of the mechanical $\{V_{mech}\}$, electrostatic $\{V_{elec}\}$ and van der Waals $\{V_{vdW}\}$ loads. The Pauli's repulsion can also be similarly introduced in the model, but it would play a role if and only if nanowire and substrate are in contact. While the mechanical load directly acts on the nano-system (e.g., as in mass nano-sensors), the electric and van der Waals loads can be derived from the related energies $E_{elec,vdW}$ as:

$$\{V\} = \{V_{mech}\} + \{V_{elec}\} + \{V_{vdW}\},$$
$$\{V_{elec,vdW}\} = -\frac{\mathrm{d}E_{elec,vdW}}{\mathrm{d}\{X\}} \tag{5a}$$

$$E_{elec} = \frac{C(\{X\})V^2}{2},$$
$$E_{vdW} = \int_{\Omega_1}\int_{\Omega_2} \frac{C_6 n_1 n_2}{x^6} \mathrm{d}\Omega_1 \mathrm{d}\Omega_2 \tag{5b}$$

where C is the NEMS electrical capacitance, $\Omega_{1,2}$ are the two domains between which we are calculating the van der Waals forces (e.g., nanowire and substrate), having atomic densities $n_{1,2}$, C_6 is a material constant and x is the modulus of the position vector [6].

The fatigue crack growth in a nano-system can be followed by considering our recently proposed quantized Paris' law [18], in dimensionless form:

$$\frac{\mathrm{d}c_i/q}{\mathrm{d}N} = p\frac{\Delta K_i^{*m}}{K_C} \tag{6}$$

where q is the fracture quantum (related to the atomic size of the nano-system), N is the number of load cycles ($\dot{N} = P^{-1}$), ΔK_i^* is the variation of the root mean square of the stress-intensity factor at the tip of the ith crack (of length c_i), K_C is the material fracture toughness, and p,m are the material Paris' dimensionless constants. Thus [$\Delta S^{(i)}(c_i)$] can be accordingly updated during fatigue nano-crack growth.

Coupling eqs. (4-6), the dynamic behaviour of electromechanical nano-systems with propagating fatigue nano-cracks can be predicted. Each of the Q+1 systems in eq. (4) can be solved numerically using an iterative procedure, starting assuming $\{F(j)\} = \{0\}$ and then evaluating $\{F(j)\}$ according to the solutions for $\{X(j)\}$ derived at the previous step, updating the force and damage according to eqs. (5) and (6), until a satisfactory convergence is reached.

Our methodology, taking into account the variable contact between the crack faces, can straight-forwardly be applied also to study the nano-sub-harmonics generated in the dynamics of different small contacts [19].

3. In-silicon nano-experiments

For the sake of simplicity we here assume a large gap G if compared to the maximum nanowire deflection $|\{X\}|_{\max}$, so that the capacitance C becomes independent from $\{X\}$ and the van der Waals energy negligible [6]. For such a case we found a distributed electrostatic force per unit length f_{elec} plus a concentrated force F_{elec} acting at the nanowire tip (if cantilever) in the following form:

$$f_{elec} \approx (1-\alpha)\frac{\varepsilon_0 V^2}{2G^2}, \quad F_{elec} \approx \alpha\frac{\varepsilon_0 V^2 L}{2G^2} \tag{7}$$

where $\varepsilon_0 = 8.85 \times 10^{-12}\,\mathrm{C^2N^{-1}m^{-2}}$ is the vacuum permittivity and α is the charge tip concentration fraction (roughly $\alpha \approx 1$ for singly-clamped or $\alpha \approx 0$ for doubly-clamped NEMS [7,8]).

Moreover, by integrating eq. (6), we derive the following simplified solution (exact for the Griffith's case):

$$\frac{T(c/H)}{T(0)} = \frac{N(c/H)}{N(0)} \approx \frac{(1+q/H)^{1-m/2} - (c/H+q/H)^{1-m/2}}{(1+q/H)^{1-m/2} - (q/H)^{1-m/2}}, \quad m \neq 2 \qquad (8a)$$

$$\approx \frac{\ln\{(1+q/H)/(c/H+q/H)\}}{\ln\{(1+q/H)/(q/H)\}}, \quad m=2 \qquad (8b)$$

where $N(c/H)$ represents the number of cycles needed to reach the fatigue failure of a nano-system containing a nano-crack of relative depth c/H. Thus $N(0)$ is the fatigue life for the undamaged system, whereas $T(c/H)/T(0)$ represents the relative time to failure of the damaged NEMS ($T=NP$). Note the correction imposed by the quantization, whereas the classical Paris' law would correspond to $q/H = 0$ (large systems), giving trivially $N(c/H)/N(0) = \delta_{c/H,0}$.

A cantilever nanowire having size of B=H=10nm, G=100nm and L=1000nm, with a crack at the middle position of length equal to 0 (undamaged case), 3, 6 or 9nm is considered. Assume V=47.5volts (lower than the pull-in voltage), corresponding to a force at the tip of ~1nN (but we note that our model is linear with respect to the force and since we are going to show dimensionless results the applied voltage is here arbitrary), with a frequency P^{-1}=20MHz (~½ of the nanowire fundamental frequency). The Young's modulus be 1TPa and the density equal to 1300kg/m^3 (carbon). We have assumed a modal damping of 10^{-2} and a discretization in 20 finite elements. We compute the amplitudes of the harmonics j/n in the tip displacement, normalized to that of the linear component (j/n=1). We have found that values of n=4 and Q=16 give a good approximation, that is, for larger values of n and Q, substantially coincident solutions are obtained. Thus, 1 offset (j/n=0), 1 linear component (j/n=1), 3 high-harmonics (j/n=2,3,4) and 12 sub-harmonics (j/n different from an integer number) are sufficient to describe the dynamics of our nano-system. In-silicon nano-experiments were performed and are summarized in Figures 2-5. In Figure 2 the high-harmonics and the offset are shown as a function of the crack-depth: a continuous growth is clearly observed, suggesting that such components can help in detecting weak damage [14]. In contrast, in Figure 3 the growth of the sub-harmonics and thus of the system complexity is shown to be extremely discontinuous [16, 17]. A threshold appearance is clearly observed (compare with the offset growth, also reported in Fig. 3); for our system, the complexity abruptly arises at a relative crack-depth of $(c/H)_{complexity} \approx 60\%$, thus nano-sub-harmonics can help in detecting strong damage in NEMS. In Figure 4 the correlation between the crack-depth and the failure forewarning (i.e., $T((c/H)_{complexity})/T(0)$) is depicted

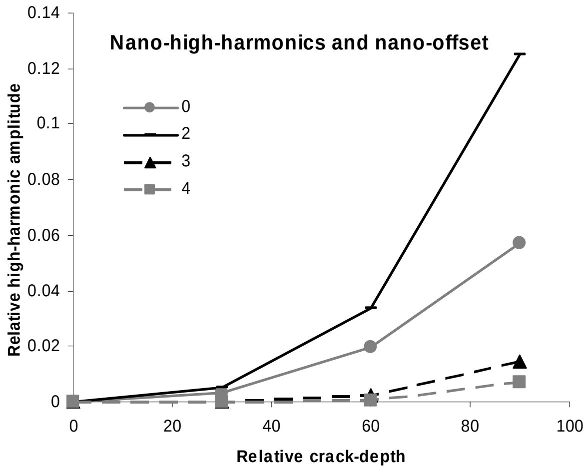

Figure 2. The continuous growth of the nano-high-harmonics by increasing the NEMS damage.

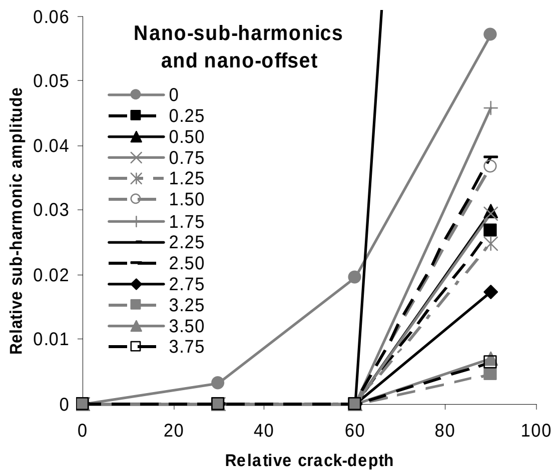

Figure 3. The discontinuous growth of the nano-sub-harmonics by increasing the NEMS damage.

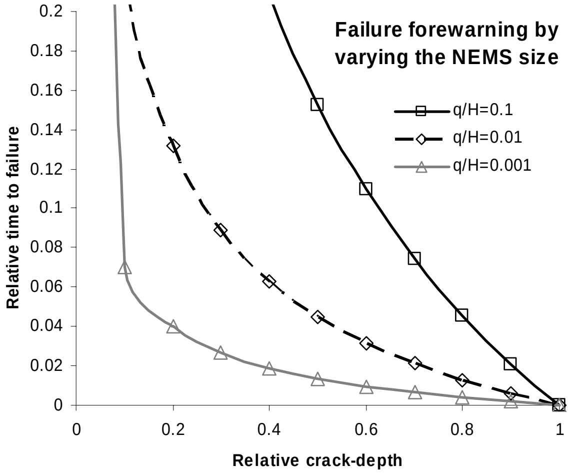

Figure 4. The failure forewarning by varying the NEMS size: it increases by decreasing the system size (m=3).

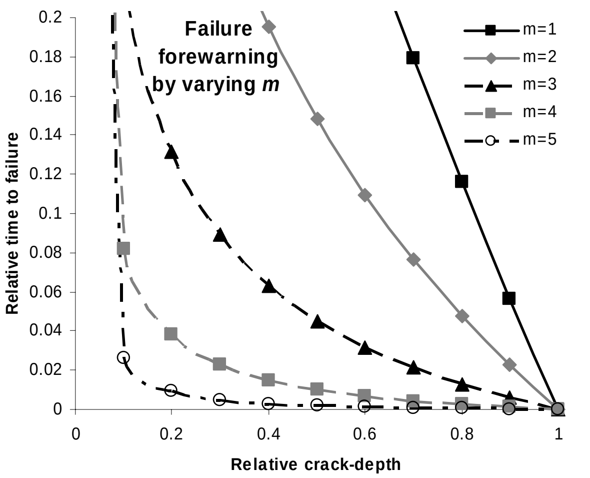

Figure 5. The failure forewarning by varying the Paris' exponent: it increases by decreasing m (H/q=100).

(considering m=3, usually m>2) as a function of q/H, showing that the forewarning is size-dependent. In particular for $(c/H)_{complexity} \approx 60\%$ we have $T((c/H)_{complexity})/T(0)$ of 1%, 3% or 11% for H/q equal respectively to 1000, 100 or 10. Smaller systems are thus more sensitive to the proposed monitoring technique. In Figure 5 (considering H/q =100, plausibly for our system assuming q~0.1nm), the failure forewarning as a function of the crack-depth is depicted by varying the Paris' exponent m: smaller values would help the monitoring.

4. CONCLUSION

Our findings clearly suggest that nanocomplexity abruptly precedes the fatigue collapse of a NEMS and can thus be used as a simple binary innovative tool for monitoring the NEMS integrity.

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