Conversion of mechanical noise into useful electrical energy using piezoelectric 2D materials

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I. INTRODUCTION

Understanding energy conversion processes at the nanoscale has become crucial for the future development of energy aware ICT technologies[1]. In a new scenario where computing energy consumption is pushed to the fundamental limit[2], proposals oriented to power such a future *zeropower* ICT devices using the energy harvested from ambient sources have started to make sense. Vibration energy harvesting (VEH) technology has demonstrated to be a real alternative to standard electrochemical battery technology for powering portable devices from ambient mechanical energy in the form of vibrations, but only few large scale examples have shown to be useful in real applications[3]. Among all the challenging topics identified in VEH technology, enhancement of the harvested energy density and widening of the frequency response are two of the most intensively investigated. In previous works[4,5,6], we have demonstrated that both challenges can be simultaneously addressed by miniaturizing at the nanoscale the VEH transducers and engineering the non-linearity of their mechanical properties. Nanoelectromechanical structures (NEMS) based on piezoelectric 2D materials have been proposed for this aim. In particular, it has been theoretically demonstrated that tuning the bistable non-linearities of suspended h-BN monoatomic ribbons by a compressive strain induced buckling allows, from one hand, maximizing the energy harvested from wide band Gaussian vibration noise and, from the other, getting power density levels above the state of the art[7]. However, the problem of converting the energy of ambient mechanical noise into useful electrical energy by means of NEMS based on piezoelectric 2D materials is still open. To solve this problem it will be necessary to provide experimental evidence, currently lacking, but previously, a good model for the electromechanical processes involved in the conversion mechanism has to be developed. In this contribution we will present our last theoretical results of the dynamics of one atom thick h-BN suspended nanoribbons. Two computational procedures have been followed: (i) From one hand, we have obtained the deformation potential energy by first performing ab-initio calculations and then we have calculated the dynamics by solving numerically a Langevin type equation. (ii) Alternatively, we have treated also the dynamic part of the problem at the atomistic level by means of molecular dynamics calculations.

II. STATIC CALCULATIONS

Suspended h-BN nanoribbons along the x direction in a clamped-clamped configuration are brought under a compressive strain ε by bringing closer the two clamped ends as depicted in Fig. (1). Eventually, the structure is buckled and, consequently, two symmetric stable states are induced around the plane defined by the uncompressed configuration.

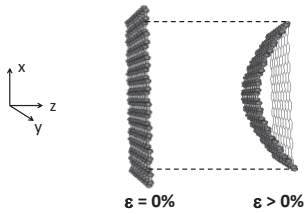

FIG. 1. Schematic representation of 1-atom thick h-BN clamped-clamped suspended nanoribbon in a non-compressed state, ε=0% (left) and a compressed ε>0% state (right).

The elastic potential energy, E, and the 2D longitudinal polarization P_{2D}, have been calculated using DFT as implemented within the SIESTA package[8] in order to have a purely atomistic description and an electronic structure obtained from first-principles. Fig. (2) shows the change in the elastic energy, ΔE, with respect to the ground state energy defined as the energy of the flat and non-compressed ribbon, i.e. $E_{0,0}=E(z=0,\varepsilon=0)$, as a function of the deformation amplitude, z, corresponding to a h-BN nanoribbons 17 nm long and 1 nm wide.

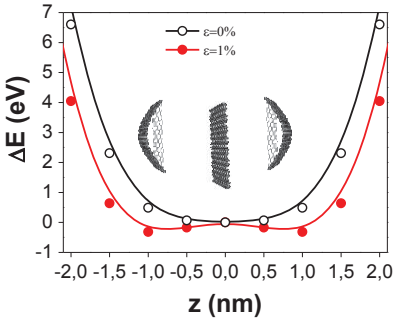

FIG. 2. Elastic energy change, ΔE, with respect to the ground state, $E_{0,0}$ (as defined by the energy of the flat, z=0, non-compressed, ε=0, ribbon) as a function of the vertical static displacement, z, of the central atoms of the h-BN ribbons. Dimensions are in all cases 17 nm long and 1 nm wide.

At a certain compression between 0% and 1%, h-BN ribbons relax the compression energy by buckling their structure and a bistable non-linearity is induced, which is characterized by two energy wells (around z=±1nm) and an energy barrier which separation and height grow with compression[5,6].

III. DYNAMIC CALCULATIONS

The h-BN structures have been excited by an external force with a WGN (white Gaussian noise) spectrum of F_{rms}=5pN of intensity. In these particular conditions, a Langevin equation coupled to a piezoelectric transduction equation have been solved for different compression values from 0% up to 1%. For ε=0% and low compression values, the structure randomly vibrates around z=0 by the action of the noisy external force, since bistability is still not well defined. When compression increases (for ε>0%), the two energy wells start to influence the dynamics of the system and the structure start to eventually jump from one energy well to the opposite one. Such inter-well excursions grow in amplitude when compression increases, since inter-well distance also increases. However, energy barrier height also grows as compression increases and, consequently, when the compression reaches a certain value the barrier is too high and the structure gets stuck into one of the wells, where it vibrates in a similar random way as in the low compression regime.

Those three regimes can be identified in the z_{rms} curve of Fig. (3) (black open circles) and the corresponding P_{rms} curve (red filled circles): the z_{rms} value is larger in the inter-well jumping regime (around ε=0.3%) than in the low and high compression states, where no inter-well excursions are produced.

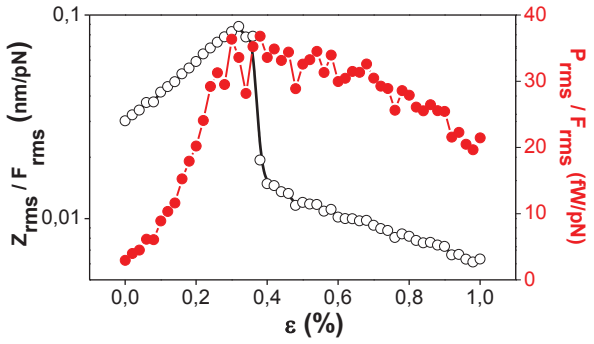

FIG. 3. Response normalized to the excitation force versus compression ε of the rms vertical position of central atoms, z_{rms} (black curves, left axis), and of the rms power delivered to the optimal load* (red curve, right axis). Quality factor is supposed to be Q=100. *The h-BN nanoribbon is electrically loaded by a R_L=240 kΩ resistor, which maximizes the electrical power transferred from the 2D piezoelectric transducer.

Similar results as those obtained by solving the Langevin equation (see Fig. (3)) can be derived by means of molecular dynamics (MD) simulations performed with the LAMMPS code[9]. Thermal excitation is considered in this case as the external vibrational source of noise and temperature is used as the control magnitude of the noise intensity. However, MD gives additional information about the modes of vibration of the nanoribbons and, more specifically, about the dynamics of the transitions between the two fundamental buckled states. In Fig. (4), three representative snapshots of the dynamics of a 100.8 nm x 7.5 nm nanoribbon with a compression of 1.5 % are shown. An excited mode (snapshot b) with a node in the middle of the nanoribbon usually shows up between two fundamental modes (snapshots a and c) associated to the buckled states.

FIG. 4. Snapshots sequence of the dynamics of a 100.8 nm x 7.5 nm h-BN nanoribbon subjected to a compression of ε=1.5 % and thermally excited at T=300K.

With the aim of improving the accuracy of the dynamic model of the compressed piezoelectric h-BN nanoribbons, we are currently introducing the effect of the non-linear damping terms associated to the ripples of the structure. Such instabilities have been previously attributed to the quality factor dependence on the compressive strain level, which has been experimentally observed in suspended nanoribbon structures made of other 2D materials. Additional relevant information derived from this non-linear damping effect is expected to provide new insights to advance on solving the problem of converting the energy of ambient mechanical noise into useful electrical energy.

ACKNOWLEDGEMENTS

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