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Vibrational properties of Cu nanowires

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ABSTRACT

We have calculated local vibrational density of states (LDOS) of a center atom (CA) of a rectangular Cu nanowire with the axial orientation of ⟨100⟩, using a real space Green's function approach with force constants extracted from interaction potentials based on the embedded atom method. The LDOS of a center atom of a strained nanowire is found to exhibit quite distinctive characteristics as compared to that of a strain-free nanowire, the most striking feature of which is the existence of high frequency modes above the bulk band even for small strain of 2.5%. We further find that these high frequency modes are shifted to even higher frequencies when the nanowire is exposed to an increasing axial strain.

1. Introduction

The properties of materials with high surface to volume ratio, such as nanorods, nanotubes and nanowires, have been the focus of a broad range of both experimental and theoretical works as these low dimensional materials exhibit quite distinctive characteristics compared to the corresponding bulk or surface systems [1]. For example, electronic properties of carbon nanotubes are strongly modulated by varying size of diameter and the helicity of the tubes. Thermal conductivity is expected to decrease for nanowires with diameters less than the bulk mean free path of heat carriers. Due to enhanced surface effects, the difference in the mechanical properties between nano-scale and large-scale components is established to be quite large. Thus, in any attempt to effectively use nano-structured materials in emerging technologies, a thorough understanding of their properties is essential.

Except for a few studies [2], most theoretical works, ranging from molecular dynamic simulations to first principle electronic structure calculations, are devoted to determination of elastic, electronic, and structural properties of metal nanowires. On the other hand, the vibrational characteristics of nanowires, specifically in the radial direction, are expected to be altered compared to the bulk system for symmetry reasons. In addition to the issue of unavoidable size effect, the vibrational characteristics are likely to differ from those of bulk system and of a strain-free nanowire when the nanowire is under a strain. We thus aim to show in this paper, through reliable and accurate calculations, that vibrational properties of a rectangular Cu nanowire change significantly when the nanowire is exposed to an axial strain and that these varying characteristics can be traced to the changes in bond-lengths and force constants between the atoms while recognizing that there is no simple relation between the local density of states and modifications of specific force constants due to the collective nature of the vibrational modes in a solid and to the many body nature of the interactions.

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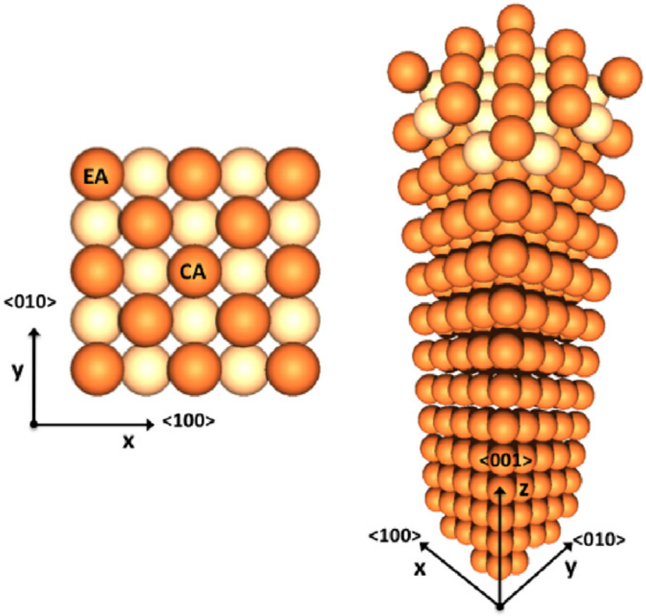

Fig. 1. Cross-sectional (on the left) and perspective view (on the right) of the $\langle 100\rangle$ axially oriented nanowire with 5 × 5 number of atoms along the diagonals. The darker and lighter yellow spheres show the atoms in A and B type stacking of Cu(100) crystal. Here CA and EA, respectively, stand for center and edge atom of the cross-sectional plane.

2. Geometry and computational details

In this report, we are interested in rectangular nanowires with $\langle 100\rangle$ axial orientation that can be fabricated by cutting the (100) slab through the (100) walls of a square. As indicated in Fig. 1, in this specific type of nanowires the cross-sectional area is determined by the number of atoms along the diagonals, namely by $n \times n$. Here, we have investigated the 5 × 5 type Cu nanowire. In our calculations, we have taken the x and y axis to lie in the cross-sectional plane and z being along the axial direction of the wire. In the simulations, periodic boundary condition is applied along the axial direction to simulate an infinitely long nanowire, while no such constraint is imposed along the directions parallel to the cross-sectional plane.

To describe the interactions between the atoms in model systems, we use potentials obtained from the embedded atom method (EAM) [3]. It has so far proven to be reliable for examining the energetics, structure and dynamics of low-coordinated surfaces and nano-structured materials of the six fcc metals Ag, Au, Cu, Ni, Pd and Pt, and their alloys [3–6]. The method exploits two findings associated with the total energy of a system of interest at ground state: (1) the ground state of an interacting electron gas is a unique functional of the total electron charge density [7]. (2) The energy of an impurity in a host is a functional of the electron density of the unperturbed host electron density [8]. That is to say $E = F_{z,R}(\rho_h)$, where $\rho_h(R)$ is the electron density of the host without impurity at R, the position where the impurity is to be replaced, and Z the type of the impurity. So the method views each atom in a solid as an impurity embedded in a host consisting of all other atoms and thus its energy is given by

$$E_i = F_i(\rho_i(R_i)) + \frac{1}{2}\sum_j \varphi(R_{ij}) \tag{1}$$

where ρ_i is the electron density of the host without atom i and defined as a superposition of f_j, the electron density of atom j as a function of distance from its center

$$\rho_i = \sum_{j\neq i} f_j(R_{ij}), \tag{2}$$

while R_{ij} is the distance between atoms i and j, $F_i(\rho_i)$ is the energy to embed atom i in electron density ρ_i, and φ is a short range electrostatic pair potential between atom i and j. Hence, the total energy of a solid is simply a sum over all atoms in the solid and given by

$$E_{tot} = \sum_i F_i(\rho_i(R_i)) + \frac{1}{2}\sum_{i,j} \varphi(R_{ij}). \tag{3}$$

It is further assumed that the electron density ρ_i is given by a linear superposition of the electron densities of the constituent atoms which is taken to be spherically symmetric. The EAM functions for the 6 fcc metals, Ag, Au, Cu, Ni, Pd, and Pt, and their