Physica B 453 (2014) 14–18

Contents lists available at ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Theoretical approach to the phonon modes and specific heat of germanium nanowires

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ARTICLE INFO

Available online 11 May 2014

Keywords:
Phonons
Nanowires
Germanium
Specific Heat

ABSTRACT

The phonon modes and specific heat of Ge nanowires were computed using a first principles density functional theory scheme with a generalized gradient approximation and finite-displacement supercell algorithms. The nanowires were modeled in three different directions: [001], [111], and [110], using the supercell technique. All surface dangling bonds were saturated with Hydrogen atoms. The results show that the specific heat of the GeNWs at room temperature increases as the nanowire diameter decreases, regardless the orientation due to the phonon confinement and surface passivation. Also the phonon confinement effects could be observed since the highest optical phonon modes in the Ge vibration interval shifted to a lower frequency compared to their bulk counterparts.

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1. Introduction

In the last years, there has been extended interest in the research of one dimensional (1-D) semiconductor nanostructures such as nanowires due to their enhanced electrical and mechanical properties compared to their bulk counterparts. Specially Germanium Nanowires (GeNWs) have attracted great attention due to the better characteristics of Ge compared to Si (larger exciton Bohr radius and hole mobility) [1], which make them suitable for applications in transistors for spintronics [2], and as anode material in Li-ion batteries [3]. Hence, there have been extensive theoretical investigations in this material such as the work of Sk and collaborators [4], which focus mainly on the changes on the electronic properties of GeNWs using chlorine and fluorine surface passivation. However the theoretical studies of the vibrational properties in this kind of materials are mostly performed scarcely in Silicon NWs [5], and only a few in GeNWs [6].

The vibrational properties in nanostructures are modified by surface effects and phonon confinement compared to the material in its bulk crystalline forms. A large number of physical properties can be understood in terms of phonons such as the thermal conductance, Raman spectrum, electron–phonon coupling in solar cells, low field mobility, surface roughness and impurities. Also the phonon dispersion could give information of the stability of the GeNWs, because of the occurrence of negative (imaginary) frequencies in the phonon dispersion would indicate mechanical instabilities in the system [6].

Hence motivated by the experimental advances [7,8] we performed a theoretical study of the effect of anisotropy on the vibrational properties and specific heat of GeNWs through the finite displacement algorithm within the density functional theory (DFT), by comparing the phonon band structure, density of states and specific heat of GeNWs oriented in [001], [110] and [111] directions.

2. Model and calculation scheme

The nanowires were modeled using the supercell technique [9,10] by removing atoms outside a circumference with diameter (d) from an otherwise perfect crystalline bulk Ge in the [001], [110] and [111] directions [Fig. 1(a–c)], with system periodicities of a, $a/\sqrt{2}$ and $a\sqrt{3}$, respectively; where a is the lattice parameter of crystalline Ge (5.65 Å). The nanowire diameters were calculated through the scheme detailed by Niquet and co-workers [11], using the following expression:

$$d = 2\sqrt{\frac{N_{Ge}a^3}{8\pi c}} \quad (1)$$

where N_{Ge} is the number of Ge atoms per supercell, a is the lattice parameter of crystalline Ge and c is the periodicity of the nanowires.

The nanowires are placed in simulation cells with dimensions so that the distance between the nanowires and its replica is above 12 Å. The surface dangling bonds were saturated with H atoms,

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http://dx.doi.org/10.1016/j.physb.2014.05.005
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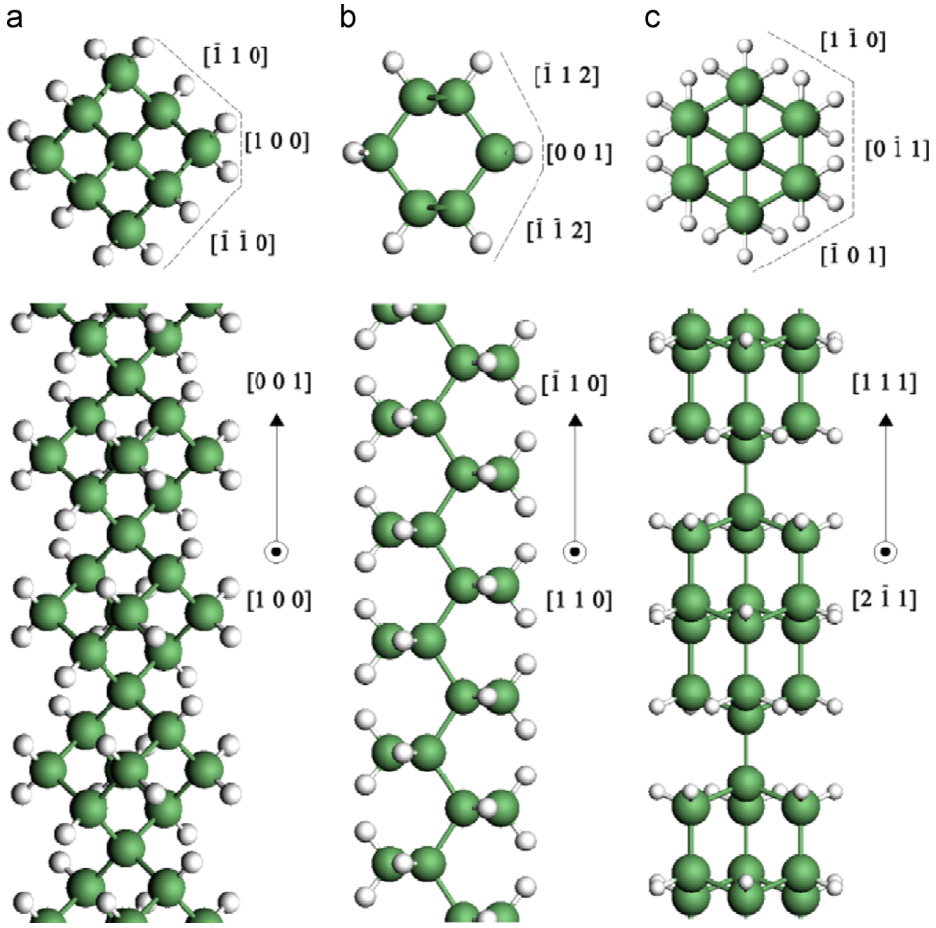

Fig. 1. Model of GeNWs orientated in the a) [001], b) [110] and c)[111] directions. The green and gray spheres represent Ge and H atoms, respectively.

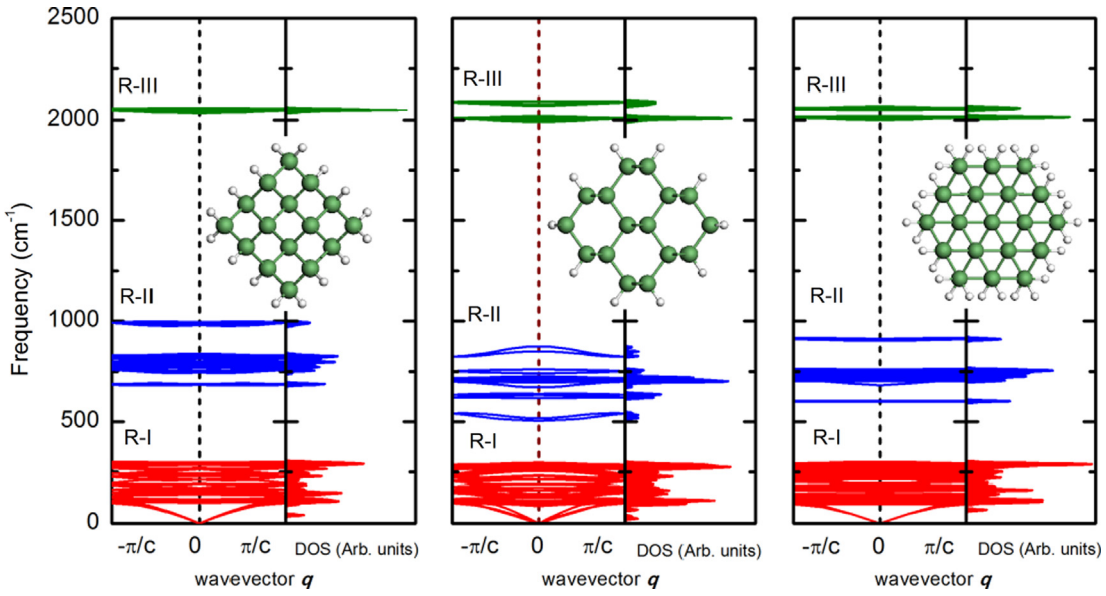

Fig. 2. Phonon band structure and density of states of a) [001], b) [110] and c) [111] nanowires with diameters of 8.90 Å, 10.48 Å and 10.46 Å, respectively.

since there is experimental evidence that H termination can be achieved in the nanowire synthesis [12].

The calculations were performed using the *ab initio* density functional theory (DFT) scheme through the generalized gradient approximation (GGA) using the Perdew–Burke–Ernzerhof Functional [13] and norm-conserving pseudopotentials [14] as implemented in the CASTEP [15] code. The energy cutoff used was of 720 eV with reciprocal space sampling grids up to $1 \times 1 \times 6$ according to the Monkhorst-Pack scheme [16]. All structures were optimized to their minimum energy configurations using the BFGS [16] algorithm. The GeNWs are considered relaxed when all internal forces are less than 0.03 eV/Å. To study the vibrational

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