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Molecular dynamics simulation of silicon nanostructures

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Abstract

A silicon nanowire can be seen as a very small stick taken out of a bulk structure. Recent works show that they can be synthesized experimentally. This work initiates a series of Molecular Dynamics simulation studies of such structures. The first step towards this goal is the choice of the potential best suited to represent the physics of such a system. We have compared the two most popular potentials for bulk silicon: Stillinger–Weber and Tersoff. Our calculations show that the latter potential seem to represent better the reconstruction of the nanowire surface.

Keywords: Molecular Dynamics; Silicon; Irradiation

1. Introduction

A nanowire consists of a rod which can have a length of thousands of atoms while its width can be less than ten atoms. The atoms that build up the nanowire follow a crystallographic pattern and the axial direction can be parallel to any direction in principle. In the case of a silicon nanowire the atoms present the same structure as bulk silicon, e.g., the diamond structure. Such systems have recently been studied both experimentally and theoretically [3,4].

Due to the small dimensions involved, silicon nanowires seem very promising on the engineering of very small gears that could be used, for example, in the production of nanomotors. Cui et al. [3] used laser catalyst growth to produce silicon nanowires at controllable sizes and orientations. Doping by implantation with boron or phosphorous could alter the electronic properties and produce a p or n-type semiconductor, respectively. Moreover, in the case of high doping the system exhibits a metallic behavior. These observations open the possibility of producing in the same wire regions having different electronic properties which could give origin to nanodiodes or nanotransistors. The ion implantation, a common technique to introduce dopants into

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materials seems to be very useful also in nanoscale systems [5,6].

Wu et al. [4] synthesized via chemical vapor deposition silicon nanowires of several nanometers wide. Gold was used as a catalyst for the sylane vapor. High resolution microscopy helped on the identification of the geometries formed. The preferred orientation depends strongly on the nanowire diameter. For the smaller diameters, up to 10 nm, 95% of the nanowires were found to orient themselves along the $\langle 1\,1\,0\rangle$ direction. As the diameter increases the nanowire tend to follow the $\langle 1\,1\,2\rangle$ direction reaching the $\langle 1\,1\,1\rangle$ direction for diameters between 20 and 30 nm.

Electron microscopy can identify the nanowire orientation as well as its diameter. However, it is not possible to localize the exact position of each particle in such system. The Molecular Dynamics approach can fill this gap left by the experimental technique. Starting from an initial configuration which can be inferred from the experimental evidences one can follow the evolution of the atomic positions of the system. Therefore, this technique can foresee surface reconstruction as well as the system response to irradiation. As it is well known, the computing time depends strongly on the number of particles; the larger the system the more cpu time is required. In order to avoid long simulation runs we decide to start with the smallest kind of silicon nanowires observed by Wu et al. [4] which are those aligned along the $\langle 1\,1\,0\rangle$ direction.

The present contribution describes the details of simulation procedure and discusses the pertinence of the use of the usual potentials to simulate Si nanostructures. In Section 2 we briefly explain the details of the simulation technique. Right after we present our results and their implications. The last section presents our conclusions.

2. Simulation details

The Molecular Dynamics approach consists in solving the coupled equations of motions of all particles. In order to proceed with simulations we used a standard code which contains time saving techniques as a cutoff radius as well as neighbor list. The Verlet integrator and a time step of 1 fs were used. Periodic boundary conditions were used along the main nanowire axis while the other two directions were kept free. Since we have chosen to simulate the $\langle 1\,1\,0\rangle$ nanowire, periodicity happens along this direction. The main simulation cell has 1820 atoms. Fig. 1 shows our prototype nanowire before any run has been performed. Starting with this configuration we let the system relax over some thousands of time steps. In order to reduce the system temperature down to zero we performed a simulated annealing. After the first relaxation run we scale all velocities to a lower value and let the system relax again. This procedure is repeated several times until the desired temperature is reached.

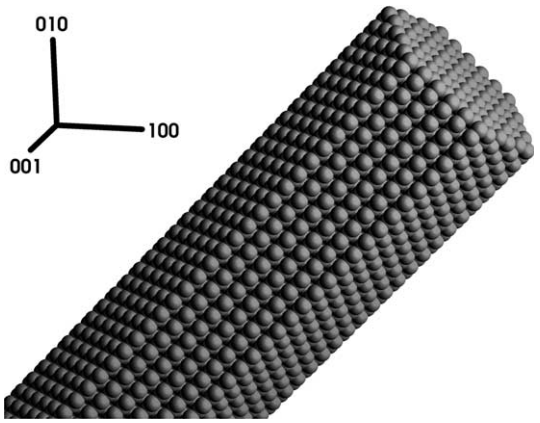

Fig. 1. Prototype nanowire structure. The main structure is parallel to the crystallographic $\langle 1\,1\,0\rangle$ direction.

3. Results and discussion

A Molecular Dynamics simulation depends strongly on the choice of potential which rules out the interaction of each particle. There are several potentials which have been developed with the purpose of describing bulk silicon. We decided to compare the two most popular ones: Stillinger–Weber [1] and Tersoff [2]. Both potentials have been extensively studied regarding bulk properties. The main criterion we use in order to decide which potential works better will be the surface behavior. A good potential must describe accurately the surface properties, since this kind of system has a high