Nuclear Instruments and Methods in Physics Research B xxx (2017) xxx–xxx

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

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

Atomistic simulation of ion irradiation of semiconductor heterostructures

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ARTICLE INFO

Article history:
Received 10 December 2016
Accepted 11 April 2017
Available online xxxx

Keywords:
Semiconductor heterostructures
Ion beam mixing
Molecular dynamics

ABSTRACT

Recently the possibility to use ion beam mixing combined with suitable annealing has been suggested as a possible means to synthesize individual silicon quantum dots in a silica layer, with the possibility to function as single-electron transistors. For this to work, it is necessary to have a careful control of the ion beam mixing in $Si/SiO_2/Si$ heterostructures, as well as understand the nature of not only the composition, but also the chemical modification of the SiO_2 layer by the mixing with Si. We describe here a procedure to synthesize $Si/SiO_2/Si$ heterostructures in molecular dynamics, with an energy minimization scheme to create strong and stable interfaces. The created heterostructures are irradiated at energies and fluences matching corresponding experiments. The results show a considerable degree of interface mixing, as expected. They also show some densification of the silica layer due to recoil implantation, and formation of a considerable number of coordination defects. Due to the strong covalent bonding in silicon and silica, the densification is not fully elastically relaxed even in the presence of a nearby surface.

1. Introduction

With more hand-held devices like smartphones, tablets, cameras, etc, connecting to the internet-of-things, power consumption is increasing exponentially. A search for more power-efficient components, which can facilitate the transition to a new era, is natural. The currently available transistors inside integrated semiconductor circuits will soon have reached their limitations [1]. Single electron transistors (SET) are by nature consuming less power [2], due to the limited current needed to send a signal from the emitter to the collector. However, the currently available SETs need cryogenic temperatures to work properly and, hence, are not very practical. A stable performance of a SET at room temperature will create a strong platform for reduction of power consumption by numerous electronic devices in simultaneous use.

The functional principle of the SET is based on formation of a quantum dot embedded in a dielectric matrix. Formation of Si nanocrystals embedded in amorphous silica structure is a straightforward way to achieve the suitable structure in a CMOS compatible manufacturing process.

Earlier it was shown by both experiments and computer simulations that quantum dots can be formed in a-SiO_2) by annealing Si_xO_{2-x}. Such meta-stable mixture can be formed by ion mixing of a Si/a-SiO_2 interface caused by low-energy ion beam irradiation [3–8]. Using kinetic Monte Carlo (kMC) [5,9], the results of annealing process can be assessed quite closely, provided that the initial density profiles of the different components in all layers of the multi-layered structure are well known.

In this work, we present molecular dynamics (MD) simulations of the initial irradiation process of SiO_2/Si layered simulation cell, resulting in the density profiles, which can be used in subsequent kinetic Monte Carlo simulations. The results are discussed and the potential pitfalls for accelerated MD simulations are underlined.

2. Development of simulation approach

2.1. Irradiation condition

The ion fluence needed to achieve sufficient atomic mixing during irradiation is at least 2.5×10^{15} cm^{-2} [10,11], and can be reached with approximately 10,000 ions over the surface of a simulation cell with side lengths of 10 s of nanometers. The simulations of such an amount of ions within reasonable time is computationally very demanding using conventional MD algorithms. Acceleration of the simulation runs by applying suitable

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http://dx.doi.org/10.1016/j.nimb.2017.04.034
0168-583X/

approximations is required. All MD simulations in the current work are performed by using PARCAS [12,13] MD code, which is routinely used to simulate ion cascades in parallel mode on multiple computer cores. Yet, depending on the number of ions and the chosen interatomic potential, the time required for a single series to 10,000 ions amounts to many days of simulations, which is not affordable for systematic industrial process optimization. In the current work, we explore possible ways to reduce the computational costs of high fluence irradiation without affecting the final result dramatically.

As an initial attempt to simulate high fluence irradiation at small computational costs, we simulated multiple impacts of Ne and Si ions on structures consisting of amorphous SiO_2 (a-SiO_2) and crystalline (c-Si) slabs. The ions were selected to investigate two ways of modifying the layered structure: either by using highly focused Ne ion irradiation, available from a Helium Ion Microscope (HIM) [11], or a regular Si ion broad beam.

In the current work, we focus on the details of accelerated MD simulations, which aim to enable realistic evaluation of the ion mixing process for industrially acceptable simulation times. Although MD simulations rely on the choice of interatomic potentials, multi-body interactions as well as the possibility to follow the dynamics of variation of atomic density due to collisional cascades and consequent buildup of stresses due to irradiation, make this type of simulations more attractive compared to the Binary Collision Approximation (BCA) approach [14]. To enable a detailed analysis of ion mixing in the studied structure, we simulate two cases of relatively small cells with two and one interfaces. While the size of the a-SiO_2 slab is kept close to the experimental value of 70 Å, the thickness of the c-Si slab was reduced for efficiency of the current simulations. The lateral size of all cells in this paper was 198 Å. The interactions between the Si–Si and Si–O atoms were given by the Tersoff-like interatomic potential by Munetoh et al. [15]. A schematic view of the regions of the structure can be seen in Fig. 1. To describe high-energy interactions, the ZBL potential [16] was joint to the Munetoh potential at short distances, and was also used to describe the interaction of Ne atoms with Si and O at all distances. More detail on how the irradiations were set up can be found in Section 2.3.

In the following, we describe the construction of simulation cells and formation of a-SiO_2/c-Si interfaces.

2.2. Preparation of heterostructures

The simulation cell is a multilayered structure, consisting of an a-SiO_2 layer embedded inside the c-Si matrix. The dimensions of the simulation cell were defined by experimental conditions, where the a-SiO_2 layer has a thickness of approximately 70 Å. The lateral dimensions are chosen to enclose the entire cascade region to avoid artefacts arising from the periodic boundary conditions (PBC) and the temperature control of the borders on the lateral sides of the cell. The stable a-SiO_2 structure was obtained by relaxation of the initial SiO_2 cell (obtained using the Wooten–Wiener–Weaire method in Ref. [17]) and re-relaxed with Munetoh potential with PBC applied in all directions in the NPT ensemble at 300 K, applying both Berendsen temperature and pressure controls with ($\tau_T = 0.1$ ps and $\tau_p = 0.1$ ps). The surrounding Si at the top and the bottom of the a-SiO_2 was relaxed in crystalline form in such a way that the lateral dimensions of c-Si cell were perfectly matching the lateral dimensions of the SiO_2 cell. This was important to eliminate the concentration of artificial stresses on the sides of the cell, due to the PBC, affecting the results.

To create a multilayered structure, we merged the a-SiO_2 and c-Si structures along the z-direction by compressing the c-Si matrix by 1.5 Å. Placing the compressed Si slabs at the top and the bottom of the a-SiO_2 slab at different distances between the slabs, we could control the quality of the forming interface by monitoring the potential energy of the entire system (see Fig. 2). PBC applied in all directions guaranteed that the stress due to compression relaxes towards the interface rather than at an open surface. The entire cell was allowed to relax for 250 ps. During this time, the Si parts sprung outwards towards their original size, filling the gap between the slabs and hence providing the fuse of the stacked structures. The separation distance d of the slabs resulting in the lowest potential energy of the interface after relaxation was chosen as the most optimal structure (see Inset in Fig. 3, which shows that $d = 1.2$ Å gave the lowest interface energy). In the case of a single interface, the structure was created in a similar manner as described here, however, the atoms around one of the interfaces were removed, and the structure was relaxed again with an open surface at the top and frozen layers at the bottom of the simulation cell. The dimensions of the structures used for irradiation simulations are shown in Fig. 1. In the figure, a) images correspond to

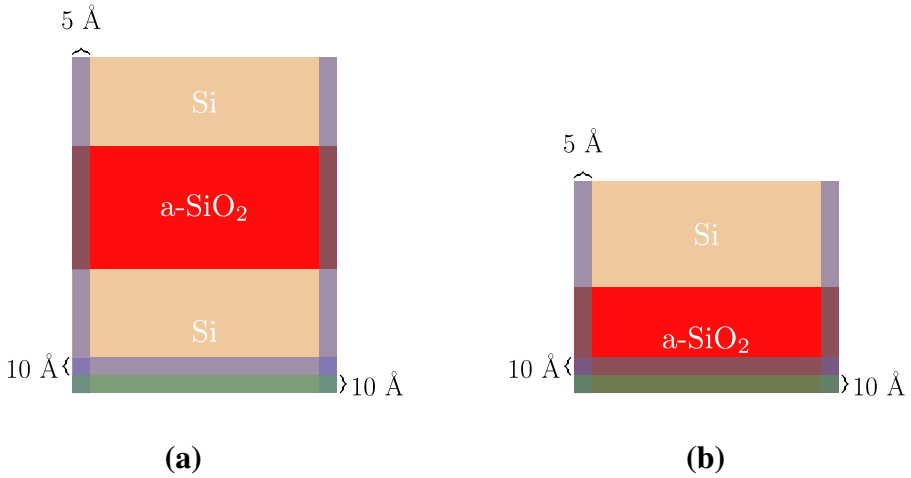

Fig. 1. A schematic view of the simulation boxes with (a) two a-SiO_2/c-Si interfaces and (b) one a-SiO_2/c-Si interface, with corresponding dimensions used in the MD simulations of (a) focused and (b) homogeneous irradiation runs. The regions where the temperature was controlled to 300 K during irradiation runs are indicated in blue. The atoms fixed at the bottom to prevent the shift of the entire cell are shown in green. In case (a) periodic boundary condition in z-direction was enabled, thus control of the temperature was needed on both sides of the fixed atoms.

Please cite this article in press as: C. Fridlund et al., Atomistic simulation of ion irradiation of semiconductor heterostructures, Nucl. Instr. Meth. B (2017), http://dx.doi.org/10.1016/j.nimb.2017.04.034