Surface Science 651 (2016) 100–104

Contents lists available at ScienceDirect

Surface Science

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

Quantitative assessment of molecular dynamics-grown amorphous silicon and germanium films on silicon (111)

Peter Käshammer [a], Nikolai I. Borgardt [b], Michael Seibt [c], Talid Sinno [a,*]

[a] Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA, 19104, USA
[b] National Research University of Electronic Technology (MIET), 103498 Moscow, Russia
[c] IV. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

ARTICLE INFO

Article history:
Received 3 March 2016
Received in revised form 5 April 2016
Accepted 6 April 2016
Available online 8 April 2016

Keywords:
Molecular dynamics
Physical vapor deposition
Amorphous-crystalline interface
Silicon
Germanium

ABSTRACT

Molecular dynamics based on the empirical Tersoff potential was used to simulate the deposition of amorphous silicon and germanium on silicon(111) at various deposition rates and temperatures. The resulting films were analyzed quantitatively by comparing one-dimensional atomic density profiles to experimental measurements. It is found that the simulations are able to capture well the structural features of the deposited films, which exhibit a gradual loss of crystalline order over several monolayers. A simple mechanistic model is used to demonstrate that the simulation temperature may be used to effectively accelerate the surface relaxation processes during deposition, leading to films that are consistent with experimental samples grown at deposition rates many orders-of-magnitude slower than possible in a molecular dynamics simulation.

© 2016 Elsevier B.V. All rights reserved.

1. Introduction

The amorphous-crystalline (a/c) interface in silicon (Si) plays an important role in various aspects of silicon processing. For example, high-dose ion implantation of crystalline Si wafers leads to the formation of amorphous regions within the crystal that must be recrystallized by thermal annealing [1]. Epitaxial silicon wafers, in which a thin, high quality crystalline silicon layer is deposited on an existing wafer, are widely used as substrates for device fabrication. Such layers are frequently deposited at low temperature in an amorphous state, and then crystallized by thermal annealing via solid-phase epitaxial growth (SPEG) [2,3]. Although less extensively studied, the closely-related SiGe a/c interface also is of technological interest, for example as related to SPEG of epitaxial Ge layers on silicon wafers, or Ge ion implantation.

The difficulty in characterizing experimentally at high resolution the structure of the a/c interface region in Si, as well as its technological importance, has motivated a wide range of computational studies. These studies have been largely based on molecular dynamics (MD) simulations with empirical potential descriptions of the atomic interactions. The most commonly employed potentials for simulating the a/c interface in Si are the Stillinger–Weber (SW) potential [4] (e.g., see Refs. [5,6]), the Tersoff T3 (T3) potential [7] (e.g., see Ref. [8]), and the Biswas–Hamann (BH) potential [9] (e.g., see Ref. [10]). Some studies have employed bond-order (BO) [11] or tight-binding (TB) [12] potentials for interface relaxation to increase accuracy. Most computational studies of the a/c interface in Si either prepare a bulk amorphous phase separately that is then joined to a crystalline region along the desired orientation [5,8,13], or begin with a fully crystalline domain that is partially melted and solidified to create the amorphous phase 'in situ' [5,11,12]. In both cases, the amorphous phase is generated by first melting a Si crystal and then quenching the liquid rapidly to prevent crystallization. Realizing a high-quality amorphous phase is not straightforward because of the balance needed between healing defects, such as dangling bonds, and preventing crystallization. For example, in the popular approach of Luedke and Landman [14], one of the parameters in the SW potential [4] is adjusted to promote four-fold coordination during the quenching phase — once the solidification is complete the parameter is reset to its original value and the amorphous solid further relaxed. A different approach for creating an amorphous layer on a crystalline substrate is to simulate a physical vapor deposition process (e.g., molecular beam epitaxy, or MBE). Here, a thin crystalline Si substrate, commonly with either a (111) [10,15,16] or a (100) [17] surface orientation, is first equilibrated and then sputtered with 'vapor phase' atoms. Careful control the thermal energy is important to ensure that sufficient atomic relaxation can take place without completely crystallizing the film [16,18].

The preceding computational studies have collectively established that it is possible to systematically vary the nature of the deposited

* Corresponding author.
E-mail address: talid@seas.upenn.edu (T. Sinno).

http://dx.doi.org/10.1016/j.susc.2016.04.002
0039-6028/© 2016 Elsevier B.V. All rights reserved.

layers between crystalline and amorphous, even at artificially high MD deposition rates. They have also established that the amorphous films generated by direct simulation of deposition exhibit some ordering near the a/c interface region, in qualitative agreement with experiment. However, it has been difficult to make more quantitative connections to experiment because of the aforementioned difficulties in imaging the interface. Recently, high-resolution transmission electron microscopy (HRTEM) combined with iterative image matching has been employed to analyze (111)-oriented a/c interfaces that result from MBE deposition of amorphous Ge [19,20] and Si [21] on atomically flat crystalline Si substrates. The resulting data provides a quantitative view of the region near the a/c interface in the Si-on-Si and Ge-on-Si cases.

Here, we use HRTEM-derived data to investigate the ability of empirical potential-driven MD deposition simulations to reproduce the details of the near-interface regions in Si-on-Si and Ge-on-Si systems. The Tersoff T3 potential is employed throughout the present study; this choice is largely based on the extensive validation of the potential offered by previous studies. In particular, there are two questions that we seek to answer: (1) how well can the T3 potential represent the a/c interface in Si and SiGe? and (2) is it possible to use MD simulations of deposition, which are necessarily carried out at artificially high deposition rates, to construct realistic interface configurations?

2. Methods

Molecular dynamics simulations of deposition were conducted by directing Si or Ge atoms onto a (111) crystalline Si substrate. The substrate was initially relaxed by annealing for 0.05 ns at the desired deposition temperature within the N**s**T statistical ensemble (constant number of particles, stress, and temperature) in order to establish the correct lattice parameter at zero applied stress (i.e., $\sigma_{xx}=\sigma_{yy}=\sigma_{zz}=0$). The simulation cell (Fig. 1) was subjected to periodic boundary conditions in the x–y plane. The initial crystalline Si slab, which consisted of 9216 atoms distributed over twelve (111) Si monolayers, was terminated by free, (111) surfaces in the $+z$ and $-z$ directions. The crystal slab dimensions used for all deposition simulations were 10.8 nm (in the x direction) by 9.3 nm (in y) by 1.7 nm (in z). After the initial relaxation step, the volume of the simulation cell was fixed and the subsequent deposition simulations were carried out in the NVT ensemble (constant number of atoms, volume, and temperature). All MD simulations were carried out with the LAMMPS software package [22].

Deposition simulations were performed by sequentially introducing single atoms with random (x,y) coordinate at a height of 5 nm above the substrate surface and assigning them an initial downward velocity of 0.7 nm/ps. Note that the energies initially assigned to the atoms do not influence the deposition process because atoms are quickly thermalized to the overall system temperature. The vapor phase and substrate atoms (the topmost six (111) layers) were thermalized together using a Nosè-Hoover thermostat to control the system temperature. The lowermost six (111) layers of the substrate were held fixed during the deposition runs. The thermostatting approach described here corresponds to the limit of infinitely fast heat conduction within the substrate. Each deposition simulation was performed at a constant temperature in the range between 0.2 and 0.95 T_m, where T_m(T3-Si) = 2550 K. The deposition flux, F_{dep}, was varied between 2×10^{26}–1×10^{30} atoms/m^2 s, which corresponds to deposition rates, r_{dep}, of one particle per 10–5000 simulation time steps (the MD time step was fixed at 1 fs). Deposition simulations were carried out until at least 1.8 nm of material was deposited, corresponding to approximately 0.5–50 ns of total simulation time. At the end of each simulation, the simulation cell was subjected to constant-volume energy minimization using the LAMMPS conjugate-gradient minimization algorithm. The final deposited amorphous films were 1.8–4.0 nm thick, corresponding to about 6000–21,000 atoms.

One-dimensional density profiles for the a-Si/c-Si and a-Ge/c-Si systems were generated by summing over the atomic density in the x–y plane and projecting the result onto the interface-normal direction, z. The z-projected density was binned into intervals of width 0.00586 nm and the atomic count in each bin normalized by a factor of $(768 * 0.00586\ \text{nm})^{-1}$ so that integration of the one-dimensional density profile over the width of a (111) monolayer resulted in a value of unity. This procedure was chosen to correspond to the one used to process the experimental one-dimensional profiles [19,20]. Briefly, a-Ge or a-Si was deposited by room temperature MBE on specially selected (111) c-Si substrates with a miscut below 0.1° from (111). HRTEM image series were obtained in cross-section geometry. An iterative digital image series matching procedure was used to fit a suitably parameterized two-dimensional atomic density distribution describing near-interfacial partial ordering of the respective amorphous material close to the c-Si substrate. Finally, the one-dimensional density profiles used in this paper were calculated by projection along the interface. As discussed in detail in Refs. [19 and 20], this approach provides a robust procedure for quantifying crystal-induced ordering in amorphous materials, and includes a full statistical analysis that provides confidence limits on the atomic density function.

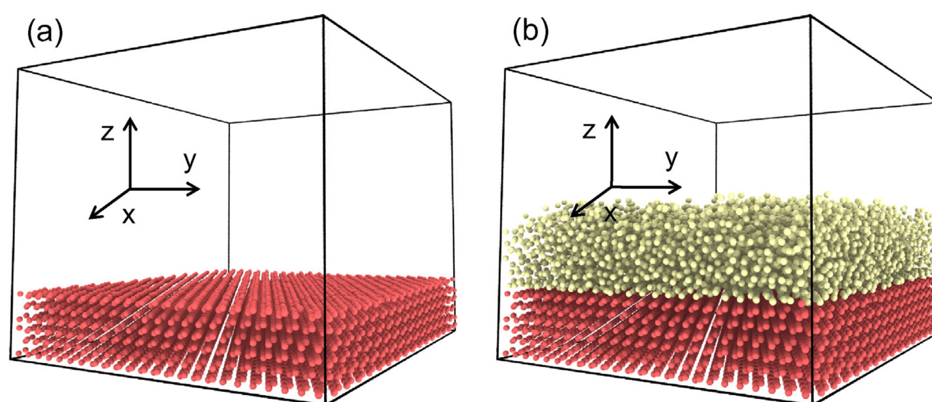

Fig. 1. Simulation cell configuration (a) prior to and (b) during deposition of Ge on a (111)-oriented Si substrate. Red spheres denote Si atoms that comprise the relaxed crystalline slab prior to deposition; yellow atoms denote deposited Ge atoms. The dimensions of the simulation cell are 10.8 nm (x) by 9.3 nm (y) by 8 nm (z), with an initial crystalline substrate thickness of 1.7 nm. Images rendered using the OVITO software package [23]. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Download English Version:

https://daneshyari.com/en/article/5421218

Download Persian Version:

https://daneshyari.com/article/5421218

Daneshyari.com