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Atomistic simulations of focused ion beam machining of strained silicon

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ABSTRACT

The focused ion beam (FIB) technique has established itself as an indispensable tool in the material science community, both to analyze samples and to prepare specimens by FIB milling. In combination with digital image correlation (DIC), FIB milling can, furthermore, be used to evaluate intrinsic stresses by monitoring the strain release during milling. The irradiation damage introduced by such milling, however, results in a change in the stress/strain state and elastic properties of the material; changes in the strain state in turn affect the bonding strength, and are hence expected to implicitly influence irradiation damage formation and sputtering. To elucidate this complex interplay between strain, irradiation damage and sputtering, we perform TRIM calculations and molecular dynamics simulations on silicon irradiated by Ga^+ ions, with slab and trench-like geometries, whilst simultaneously applying uniaxial tensile and compressive strains up to 4%. In addition we calculate the threshold displacement energy (TDE) and the surface binding energy (SBE) for various strain states. The sputter rate and amount of damage produced in the MD simulations show a clear influence of the strain state. The SBE shows no significant dependence on strain, but is strongly affected by surface reconstructions. The TDE shows a clear strain-dependence, which, however, cannot explain the influence of strain on the extent of the induced irradiation damage or the sputter rate.

1. Introduction

Over the last decades, focused ion beam (FIB) techniques have become widely used in the material science community [1]. Typical applications include imaging [2], sample preparation for electron microscopy [3] or atom probe tomography [4], the fabrication of micro or nano scale specimens for mechanical testing [5], and its combined application with digital image correlation (DIC) to determine intrinsic stresses [6,7]. FIB milling has, however, been known to induce irradiation damage in the machined material; the influence of irradiation-induced defects on the material properties is a major drawback of the method [8]. The damage induced by FIB irradiation has been extensively studied, both by experiments [9–12] and simulations [13–15], as well as using combined approaches [16]. In these studies, the authors usually focus on the influence of the ion beam energy, incidence angle, ion type *etc.* on the sputter process and irradiation damage in different target materials. In particular for materials like silicon, which upon irradiation exhibit structural amorphization, this damage induces stress and strain, as shown by atomistic simulation [13] and experiments [17]. Materials undergoing irradiation can furthermore exhibit intrinsic stresses up to 1.5 GPa [18], as those used in strain engineering [19,20] or in the case of multi-layer structures [18,21]. Only a few atomistic studies have looked into the relation between the intrinsic stress state and low-energy irradiation processes in silicon [13,22,23]. A thorough understanding of the complex interplay between the stress or strain state and irradiation induced damage and sputtering process is, however, still lacking. This fundamental question is of particular concern for so-called FIB-DIC techniques which combine FIB milling with DIC in order to measure the intrinsic stress from the release of surface strains. In this context, residual stresses up to 6 GPa have been determined previously in the literature [6].

Here, we present a detailed atomistic study of FIB milling on strained silicon using gallium ions. The manuscript is organized as follows: We first present the particular methods we use for the classical atomistic modeling of ionic irradiation. The results for samples with and without strain are then described and discussed in the light of the calculation of the threshold displacement energy (TDE) and the surface binding energy (SBE) of strained silicon.

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2. Simulation methods

2.1. Sample geometry

Most of the previous work on FIB induced damage in silicon used slab-like samples (corresponding to an infinitely extended surface) to study the influence of the beam incidence angle and the ion dose [13,15,24–26] on the sputter process and the resulting damage. Only few studies considered other sample geometries, like lamella [27].

In the present study, we choose two sample geometries. The first is a slab-like geometry (Fig. 1a) similar to the ones used in the aforementioned studies. It consists of one (001) free surface and an ion beam with a normal incidence angle $\theta^{[001]} = 1^\circ$, with θ being the angle between the ion beam and the normal to the targeted (001) surface. This small deviation of 1° is chosen to reduce ion channeling. The second geometry consists of two orthogonal {001} free surfaces and an ion beam centered at the common corner of these two surfaces (Fig. 1b). The (001) surface is hence irradiated under normal incidence with $\theta^{[001]} = 1^\circ$, whereas the (100) surface is irradiated under an extreme grazing incidence with $\theta^{[100]} = 89^\circ$. Note that the {001} family of surfaces chosen in this study is typical for experiments on silicon wafers [10,28–30]. The sample dimensions are chosen to strike a balance between the large volume required for correct stress–strain relaxation and reasonable computational times: $60 \times 20 \times 74$ a_0 ($33 \times 11 \times 43\,\mathrm{nm}^3$) in the x, y and z directions, respectively, with $a_0 = 0.5431$ nm being the lattice parameter at 0 K of the chosen Si potential [31]. This results in initial samples with approximately 0.7 million atoms. Periodic boundary conditions (PBC) are only applied in the y-[010] direction (Fig. 1a and b). The boundary conditions in the z-[001] and x-[100] are either free or 2D-tethered. Tethered boundary conditions (TBC) do not prohibit but rather restrain the displacement of atoms. The displacement restriction is controlled by a spring which links a particle to its original position (here we used a stiffness of $k = 10^9\,\mathrm{N\,m^{-1}}$). Note that in the case of 2D-TBC, the tethered atoms can still move freely in the plane of the corresponding surface to allow the dilatation/contraction of the whole sample.

2.2. Interatomic potentials

For the Ga–Si interaction, the Ziegler–Biersack–Littmark (ZBL) potential is used [32]. This universal repulsive potential is designed to model high energy atomic collisions, when the influence of the chemistry becomes negligible. After the collision cascade, the chemistry of the Ga^+ ion should, however, be considered and suitable inter-atomic models for Si–Ga and Ga–Ga interactions used. Since currently no well-tested binary potentials exist, the Ga^+ ions are usually kept inside the sample with an approximated interaction model ignoring atomic bonding (e.g. the ZBL potential), or they are removed from the system after the end of the collision cascade. The latter approach was chosen in this work, since it has been previously shown to not significantly influence the defect formation in comparison to retaining the Ga^+ ions with ZBL interactions [13].

We use a recent parametrization of the Stillinger–Weber potential (SW_m) to model the Si–Si interaction [31]. This parametrization improves the description of defect-related properties in silicon, in particular the TDE which is a critical quantity for irradiation cascades simulations. The properties of the amorphous phase, often observed in irradiation simulations, are also improved [31]. During a collision cascade, some Si atoms, particularly the primary knock-on atoms (PKA), will have a very high energy. To represent such Si–Si interaction at high energies, the SW_m potential is smoothly merged to the ZBL potential for short inter-atomic distances [27]. The two potentials are merged over a distance between 1.7 and 2.0 Å; the details of the joining procedure are described in [33].

2.3. Molecular dynamics simulations

The MD simulations presented in this work are performed with the LAMMPS software (version 7 May 2015) [34], using the Verlet algorithm with a default timestep of 1.0 fs. Simulations in the NVT and NPT ensemble use Nosé-Hoover thermostat and barostat [35,36]. Samples are cut from the bulk material and statically relaxed using the conjugate gradient algorithm. The structures are then homogeneously scaled to fit the lattice parameter at 300 K, and thermalized at 300 K by using successively the NVE and NVT thermodynamic ensembles for a total time of 20 ps. Successive cascade simulations were finally run from this initial structure.

During a collision cascade, the heat spike regime requires sufficient energy dissipation without perturbing the trajectories of the high velocity particles. The kinetic energy provided by the fired ions is dissipated using a thermostatted region of 2 nm thickness, parallel to the ion beam and placed as far as possible from the initial position of the fired ion (Fig. 1a and b). Consequently, the position of the thermostatted layer is different for each collision cascade. In this layer, the temperature is controlled by a Berendsen thermostat [37]. Even if the thermostatted region acts as a barrier for the ion propagation, the influence on the effective damage formation is negligible and a similar scheme has also been successfully used previously [27].

The position of Ga^+ ions is randomly determined at a distance of 2 nm from the (001) surface by following a normal distribution with a standard deviation of 2 nm typical for atomistic simulations [24,27,26]. Fig. 1c shows an example of such a distribution with 500 ions. A velocity corresponding to a kinetic energy of 5 kV in the direction of the beam is attributed to the ion. An MD simulation – the collision cascade – is then performed for a maximum time of 15 ps with a variable timestep to ensure that no atoms will be displaced by a distance larger than 0.01 nm during one MD step. Because of the high energy involved, sputtering can occur. An atom is considered as sputtered and then removed from the simulation if it leaves the simulation box, i.e., the distance between the atom and the closest surface of the original sample being larger than two times the cutoff of the potential. For all ions, the collision cascade is finished by the end of these 15 ps, with a final global temperature below 400 K. A final MD simulation is performed for 15 ps to slowly cool down the system from the current temperature to 300 K, and obtain the structure ready to run the next collision cascade.

As reference, silicon bulk samples with amorphous structure are obtained by the classical melt-quench procedure. A bulk crystalline Si sample is melted and quenched to 300 K at a quench rate of 10^{13} K/s, typical for atomistic simulations [31,38,39]. This amorphous structure is maintained at 300 K for 60 ps, with a barostat ensuring a globally stress free sample within the NPT thermodynamic ensemble.

2.4. Calculation of threshold displacement energy and surface binding energy

The TDE is an intrinsic material property. It corresponds to the energy required to move an atom from its original stable position to a meta-stable position, creating a point defect [40]. The TDE is a critical input parameter for simulations of collision cascades in, e.g., the binary collision approximation (BCA) framework [31,41]. In crystals, this threshold is highly anisotropic. In addition to the crystallographic direction it also depends on the thermal noise which slightly displaces the atoms from their ground state. In this context, the determination of an average TDE can be performed by using a