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Influence of intrinsic strain on irradiation induced damage: the role of threshold displacement and surface binding energies

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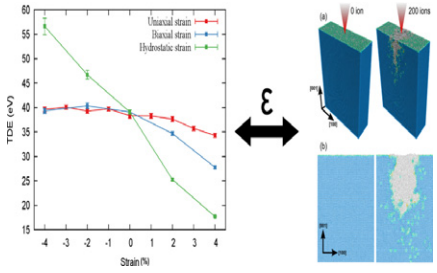
HIGHLIGHTS

- The threshold displacement energy is shown to be strain dependent.
- The strain dependence is related to the anarmonicity of the potential.
- Cascade simulations show strain dependant damage formation and sputter rate.
- Surface binding energy with realistic surface show significant increase compare to the typical idealized situation.

GRAPHICAL ABSTRACT



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ABSTRACT

Focused ion beam (FIB) machining has become a standard tool for sample preparation and in combination with digital image correlation (DIC) for the evaluation of local intrinsic stresses by measuring strain relaxation. However, FIB milling always leads to irradiation damage of the material. Current models for the formation of irradiation damage and the sputter yield are based on two key parameters, the threshold displacement energy (TDE) and surface binding energy (SBE), which are usually determined from unstrained systems with idealized surfaces. Here we use atomistic simulations to determine the TDE and SBE for strained silicon and aluminum and compare the results to full cascade simulations. A clear, material class dependent influence of the strain state on the TDE is observed, and surface amorphisation is shown to significantly increase the SBE of {001} surfaces.

1. Introduction

Over the past few decades, the focused ion beam (FIB) technique has established itself in the material science community as an indespensible tool in the field of micro/nano mechanics [1,2], with typical applications including sample preparation for electron microscopy [3] or atom probe tomography [4] as well as the fabrication of micro- or nano-objects for mechanical testing [5,6]. In this context, the damage induced by FIB irradiation has been extensively investigated, both through experiments [7–11] and simulations [12–14], as well as in studies combining both these approaches [15]. Most of these studies focus on the influence of ion beam energy, incidence angle and ion type on the damage produced within a specific target material. The measurement of local intrinsic stresses through FIB milling of specific geometries and subsequent determination of the relaxation strain through digital image correlation (DIC) has recently emerged as an innovative application of the FIB [16]. The relation between the visible surface strain

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relaxation and the intrinsic stress which existed in the material before FIB milling is, however, not straightforward. Among various factors which might interfere with a proper evaluation of stresses, the interplay of intrinsic stresses and irradiation induced damage is largely unknown. Only recently, Pastewka et al. [13] investigated the influence of ion irradiation with grazing-angles on strained samples through atomistic simulations. Our own recent work has shown a clear influence of strain on the damage induced by FIB [17]. Although relatively large strains of the order of 1–4% were used in these studies, the results are relevant especially for nanostructured materials, which can easily sustain such large strains. For example, Si layers with more than 12% strain were shown to be present in nanoheterostructures [18]. Consequently, a comprehensive study of the relation between intrinsic strain/stresses and the formation of irradiation induced damage would be of primary importance for assessing the reliability of any stress measurement technique involving FIB milling.

The threshold displacement energy (TDE) and the surface binding energy (SBE) are traditionally used to assess the resistance of a material to irradiation damage. Atomistic simulations are uniquely positioned to determine these properties. Pioneering molecular dynamics calculations of the TDE date back to more than fifty years ago [19,20]. The lack of computational power and of sophisticated interatomic potentials, however, confined these studies to consider pair interactions only, leading to plausible albeit imprecise values. With the development of the embedded atom method (EAM) in the 1980s [21], the simulation of many-body interactions became accessible which led to more reliable modeling of displacement cascades [22]. Nowadays, calculations of TDE with even more accurate, DFT-informed interatomic potentials [23,24] and *ab-initio* calculations [25] pursue the comprehensive understanding of the formation of irradiation damage. A similar historical trend is observed for the calculation of the SBE. Early atomistic studies in the 1970s using two-body potentials [26–28] were improved by the consideration of many-body interactions [29–31]. We note here that the calculation of TDE and SBE via atomistic simulations has traditionally been carried out on stress free crystalline structures close to the equilibrium state; the influence of intrinsic strain, to the best of your knowledge, has not yet been considered.

In this work, we address the influence of strain on irradiation damage with a detailed atomistic study of fundamental material properties characterizing the propensity of ion irradiation to induce damage in a material. We present for the first time the computation of the TDE as function of strain using silicon and aluminum as model materials for semiconductors and metals. Furthermore, we compute the surface binding energy (SBE) as function of strain using a statistical approach for amorphized surfaces. These properties are finally correlated with the results of full collision cascade simulations of strained materials.

2. Methods

2.1. Atomistic simulations

A key aspect of atomistic simulations is the modeling of interatomic interactions. In the current work, we use recent semi-empirical potentials which are fitted to data from density functional theory (DFT) calculations to model the interaction in pure silicon and pure aluminum. The Si–Si interactions are modeled with the three-body potential from Stillinger and Weber [32] (denoted in the followoing by *SW*), which has been further optimized by Pizzagalli et al. [33] to better reproduce the mechanical properties as well as the TDE of silicon. The Al–Al interactions are modeled by the embedded atom method (EAM) potential of Pun and Mishin [34], developed for Ni-Al compounds (denoted *Pun* in the following). For the Ga–[Si,Al] interaction in ion irradiation, the Ziegler-Biersack-Littmark (*ZBL*) potential is used [35]. This universal repulsive potential is designed to represent high energy atom collisions, albeit ignoring atomic bonding [13,35].

During a collision cascade, some atoms, in particular the primary knock-on atoms (PKA), have a very high energy. To represent such high-energy interactions, the *SW* and *Pun* potentials are smoothly merged to the *ZBL* potential for short inter-atomic distances following the procedure outlined in Ref. [36,37]. The merging is made for distances between 1.7–2.0 Å and 1.8–2.1 Å for Si and Al, respectively. For details of the joining procedure and the influence of the cutoff, see Nordlund et al. [23]. These authors acknowledge the subjective approach commonly used in the literature and recommended the use of simulations based on the density functional theory to highlight the choice. Such *ab-initio* simulations being out of the scope of the present study, the potential used in the current work is merged based on available literature data on Si [36,37]. Since no previous studies are available for Al, the merging region is defined proportional to the one for Si, based on the nearest neighbor distance in the Al fcc structure.

The present atomistic simulations are performed with the open-source software LAMMPS (version 7 Dec 2015) [38] running on both central processing unit (CPU) and graphics processing unit (GPU) [39–41]. Samples are cut from bulk materials and statically relaxed using the conjugate gradient algorithm. The molecular dynamics (MD) simulations are performed with a default timestep of 1.0 fs. Strain is introduced by homogeneously rescaling the coordinates of the atoms and the simulation box in the periodic directions. For bi-axial and uni-axial applied strain, the other directions are kept stress free, allowing for the corresponding Poisson contraction. This models typical experimental situations, e.g. in strained semiconductor devices [42]. More details on the specific MD simulations are given below.

Atomistic configurations are post-processed and visualized using OVITO [43]. The analysis of irradiation induced damage is performed by using the diamond structure identification method [44] and the common neighbour analysis (CNA) method [45] for silicon and aluminum, respectively.

2.2. Threshold displacement energy

The TDE is an intrinsic property of bulk materials. It corresponds to the energy required to move an atom from its original stable position to a meta-stable position, creating a point defect. This threshold is, however, highly anisotropic. In crystals, it depends on the crystallographic direction and on the thermal noise, which can displace the atoms slightly from their ground state positions. The determination of an averaged TDE can, however, be performed using a statistical approach [25].

In our work, we compute the TDE by using the following scheme, similar to Nordlund et al. [23]. A perfect bulk crystal of 8000 atoms is thermalized at given temperatures (36 K and 300 K) and zero pressure. A velocity $v^{\theta,\phi}$ corresponding to an energy of 2 eV is attributed to a randomly chosen atom in a random direction characterized in a spherical coordinate system by (θ,ϕ), and a MD simulation is preformed in the NVE ensemble for 6 ps. $v^{\theta,\phi}$ is then increased by steps of 2 eV till the detection of a defect, at an energy $E^{\mathrm{TDE}}(\theta,\phi)$. Note that only the formation of Frenkel pairs (as detected by the Voronoi cell analysis [45,46]) is considered here. The averaged TDE value is constructed over $N = 1000$ randomly chosen directions:

$$\langle \mathrm{TDE} \rangle = \left(\sum_{\psi=0}^{2\pi} \sum_{\phi=0}^{\pi} E^{\mathrm{TDE}}(\psi,\phi) \right) \times N^{-1}. \quad (1)$$