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Surface morphology and interface chemistry under ion irradiation – Simultaneous atomistic simulation of collisional and thermal kinetics

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ABSTRACT

A novel program package has been developed which allows for the simultaneous treatment of atomistic kinetics in collision cascades caused by energetic ion impacts and thermally activated relaxation and diffusion. In this 3D program named TRIDER (TRansport of Ions in matter with DEfect Relaxation) the collision cascades treated in the framework of the Binary Collision Approximation has been combined with kinetic lattice Monte-Carlo simulations of the atomistic relaxation and diffusion. TRIDER simulations allow a more realistic description of ion-induced surface patterning because subsurface defect kinetics can be included in the simulations, which is demonstrated for low-energy Ar^+ ion irradiation of silicon. A deeper understanding of ion beam mixing of bimetal interfaces can also be achieved: it is shown that the conventional Gaussian mixing profile is changed substantially for immiscible metals due to precipitation and for chemically active metals due to formation of intermetallics of different stoichiometry.

1. Introduction

Several simulation techniques have been applied in the literature to model ion-induced interactions phenomena. The most accurate and detailed way to describe the collision cascade is achieved by molecular dynamics (MD) calculations. However, due to large spatiotemporal requirements for computational resources one can only simulate small scale effects [1]. A much more efficient approach is a combination of different simulation techniques, e.g., MD with kinetic Monte-Carlo (KMC) [2–4], where the information about distribution of atomic relocations calculated with MD is used as an input to KMC. Alternatively, combinations of the Binary Collision Approximation (BCA) and KMC approaches have been proposed by Koponen et al. [5] for two-dimensional simulation of surface sputtering and Kellerman et al. [6] for bulk and surface defects generation and diffusion. Atomistic simulation used for modeling the evolution of surface morphologies and interface mixing under ion irradiation have been less developed in recent years. Ballistic interactions have been there usually simplified by a random removal of atoms from the surface [7–9] or by surface defect creation around the site of ion incidence [10]. Moreover, BCA simulations have been exploited to extract positions of sputtered atoms and to handle redeposition [11,12] as well as bulk defects created during the collision cascade [6]. All these simulations use KMC treatment of defects either restricted to two-dimensional Solid-on-Solid (SOS) model [7,11,9] or three-dimensional lattice KMC [6,10]. However, Kellerman et al. [6] simplified the KMC defect kinetics neglecting nearest neighbor (NN) interactions. Here, a new simulation technique ("TRIDER" – TRansport of Ions in matter with DEfect Relaxation), which combines BCA and three-dimensional lattice KMC, has been developed and applied. It allows for a full 3D description of radiation damage formation, atomistic relaxation and diffusion, which delivers a more realistic predictions of the evolution of surface morphologies and interface mixing profiles under ion irradiation.

Below, irradiation of Si surface with single and multiple Ar^+ ions, as well as Al/Pb and Pt/Co bimetal interfaces with He^+ ions, will be demonstrated and discussed: (i) single ion impact on Si demonstrating the simulation procedure by showing creation of vacancy and interstitial defects during the collision cascade and their migration during the relaxation phase; (ii) multiple ion impacts on Si result in surface modification and formation of broadly known ripple patterns [13,14] and (iii) multiple ion impacts on bimetals result in interface mixing followed by phase separation and precipitation in Al/Pb, and in intermetallic compound formation in Pt/Co.

In Section 2 the principles of TRIDER and its operation will be described. As two examples of application, Section 3 will address the evolution of surface and interface topography under multiple ion irradiation.

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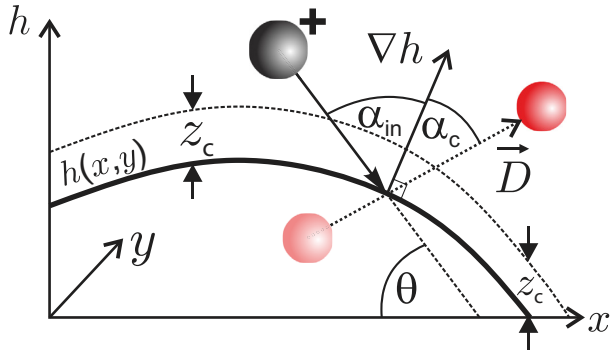

Fig. 1. Cut through the surface $h(x,y)$ plotted by a thick line. An accelerated ion hitting the surface is shown in gray, whereas the light red and dark red circles represent the initial and a later position of a target atom sputtered from the surface. α_{in} and α_c are the incidence angle and sputtering angle relative to the local surface normal ∇h, respectively, whereas θ is the global ion incidence angle. The direction of the sputtered atom is additionally marked by the unit vector $\vec{D}$. z_c is a the maximum distance of atomic interactions. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

2. The simulation method: TRIDER

TRIDER provides a full three-dimensional atomistic treatment of collisional and diffusional phenomena being based on many-body interactions. It can be applied to very large systems (more than 10^8 lattice sites), as it combines a fast BCA code with a bit-coded Cellular Automaton [15] (CA), which is used for KMC simulation. The bit-coding allows for an optimum use of random access memory.

In TRIDER, the processes of *damage formation* and *atomistic relaxation* as well as *diffusion* have been connected. Damage formation includes processes like: vacancy and interstitial creation, sputtering, impurity implantation and surface roughening. Defect relaxation involves defects including vacancies, interstitials, surface vacancies, ad-atoms, impurities and antisite defects, as well as their clustering. As the result of the simulation, information about the atomistic features, e.g., vacancy and defect creation and annihilation, ion erosion of surfaces, bulk and surface diffusion, ion-induced or thermal inter-mixing and concentration profiles in the bulk (especially at interfaces), can be obtained.

The simulation principles of BCA and KMC are generally known and will not be re-addressed here. Only modifications of these methods will be detailed as well as their combination.

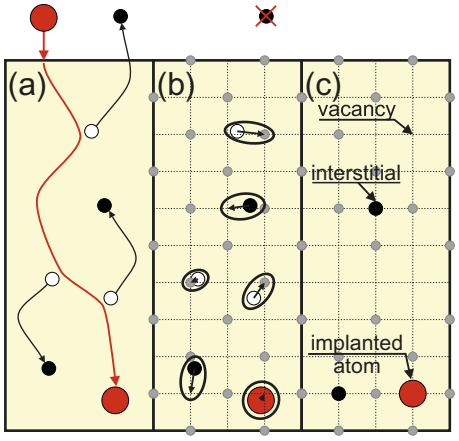

Fig. 2. Scheme describing the mapping of a continuous defect distribution as created by BCA simulations, onto a discrete lattice used in KMC simulations: (a) the incident ion (red sphere) displaces target atoms resulting in vacancies (white spheres) and interstitials (black spheres), with coordinates of real numbers as obtained by BCA simulations; (b) to perform lattice KMC simulation, each vacancy and interstitial is "shifted" to the nearest KMC lattice position or interstitial sublattice position, respectively. (c) The discrete lattice with vacancies, interstitials and impurities (implanted atoms) as used for the KMC simulations. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

2.1. BCA simulation

The current version of TRIDER is based on the sputter version TRIM.SP [16] of the TRIM [17] simulation code, which uses the BCA to describe the transport of ions and recoils in matter due to ion irradiation. Technically, the dynamic relaxation section of TRIDYN [18,19] has been replaced by the KMC algorithm of Strobel and Heinig [10]. The BCA stage of the simulation considers a continuous distribution of atoms in an amorphous substance with coordinates of real numbers. The resulting atomic positions are mapped onto integer numbers of the KMC lattice used by the KMC stage of the simulation (as depicted in Fig. 2). The on-lattice KMC algorithm considers a uniform lattice over the whole system. For this purpose, the most frequently occurring `fcc` lattice is used. The atomic coordinates are stored as occupancy numbers in an `sc` lattice, which is the underlying structure for the regular `fcc` lattice with only half of the available lattice sites being occupied. The other half is used as host for interstitial atoms, being denoted as `fcc` sub-lattice in the following.

For the present purpose the TRIM-type BCA simulation has been modified as follows. The impact position of each incident ion is selected randomly on the surface of the bombarded target. The surface is extracted from the three-dimensional lattice system used for the KMC calculation as a height function $h(x,y)$, with lateral coordinates x and y, where $h(x,y) = 0$ denotes the bottom of the computational volume. In contrast to the normalization of pseudo-projectiles, used previously in TRIDYN to accelerate the computation, in TRIDER each incident ion in the simulation represents one real atom. Every ion trajectory starts externally at the surface $h(u_x, u_y)$, where u_x and u_y are random real numbers uniformly distributed between 0 and the system size in the lateral x and y directions, respectively. In order to correct for the local flux distribution on a corrugated surface an acceptance condition for incoming ions is applied according to

$$R_u \geqslant \cos\alpha_{in}, \tag{1}$$

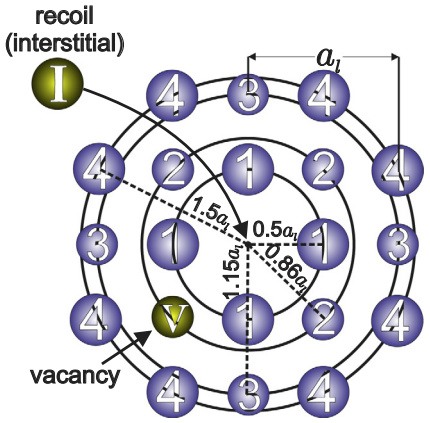

Fig. 3. Scheme of a recombination process in TRIDER. An empty lattice position (vacancy V) with respect to the position of an interstitial atom (I) is searched. Different recombination radii for `fcc` crystal are indicated by the circles, which contain an increasing number of NN shells.