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Computer Simulation of the Sputtering Process

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Abstract. Sputtering is caused by a series of atomic collisions between the incident projectiles and target atoms and between the target atoms themselves. These collision cascades can be followed with computer programs and with the Boltzmann transport equation. The two main approaches with computer programs are the binary collision approximation (BCA) and molecular dynamics (MD); they are both based on classical dynamics. Programs based on BCA describe sputtering by a sequence of independent binary collisions between atoms, whereas MD simulates the time evolution of the multiple interaction of each moving atom with all the atoms in some surrounding. The BCA approach can be regarded to be based on 'sequential event logic', whereas the MD approach is based on 'multiple interaction logic' according to *Harrison* [1]. Both approaches have advantages and disadvantages [2,3].

1 Programs based on the Binary Collision Approximation

Monte Carlo Programs based on the binary collision approximation were already developed at the end of the 6th decade of the 20th century. *Bredov* et al. [4] used such a program to investigate the penetration of ions in solids, and *Goldman* et al. [5] applied such a program to sputtering. Robinson's program MARLOWE [6] was intended to investigate ranges of energetic atoms in solids, which lead to the discovery of channeling in single crystals [7,8]. This success increased the understanding of energetic ions in solids and made the computing approach more trustworthy. Another widely distributed program is TRIM, which was also devised for the study of ranges of ions in solids by *Biersack* devised for the study of ranges of ions in solids by *Biersack* [9]. An extension of this program, TRIM.SP, allowed the investigation of sputtering [10]. Many other programs have been written at several places [2].

In these programs it is assumed that the collisions between atoms can be approximated by elastic binary collisions described by an interaction potential. It is further assumed that the energy loss to electrons can be handled separately as an inelastic energy loss.

1.1 The binary collision

In a binary collision between a moving atom with a single atom at rest the conservation of energy and momentum determines the elastic energy loss of the moving atom and the energy transferred to the recoil. The conservation of angular momentum allows to determine the scattering angle of the moving atom and the recoil angle of the atom set in motion. The scattering angle, ϑ , in the center-of-mass system is determined by an integral, if the impact parameter, p , and the interaction potential, $V(r)$, between the two colliding atoms is known:

$$\vartheta = \pi - 2p \int_R^\infty \left[r^2 / \sqrt{1 - \frac{V(r)}{E_r} - \frac{p^2}{r^2}} \right] dr \quad . \quad (1)$$

r is the distance between the two colliding atoms, and R is the apsis (closest distance) of the collision [2,11]. Collisions are regarded for impact parameters smaller than a maximum value. The BCA procedure implies that the trajectories are approximated by their asymptotes between collisions. In principle, the collision between two moving atoms can be handled, too, but it is not used in most computer programs because it takes much more effort in the mathematical formulation with minor consequences.

In an actual program a sequence of binary collisions is considered. For sputtering the incident projectiles and the recoils generated in collisions are followed three dimensionally until their energy falls below some threshold. A target atom is sputtered, if its energy normal to the surface is larger than the surface binding energy, and if its distance from the surface is large enough, that it will not interact with other target atoms. For the development of the cascade the structure of the solid, crystalline, polycrystalline, and amorphous (randomized or structureless), is important. This leads to the distinction between Monte Carlo (MC) and lattice codes. In the case of a crystalline target the impact position on the target surface has to be chosen randomly; after this choice the cascade is completely determined. In an amorphous target the next collision is chosen randomly after a given mean free path. A crystal program has the advantage, that it can choose all three kinds of target structures by appropriate changes of the sequence of crystal cells. In contrast to crystal codes, where only the impact point is chosen randomly, the programs using an amorphous target are often called Monte Carlo programs because every collision (the impact parameter, azimuthal angle etc.) is chosen randomly. MARLOWE [6] is the best known example for a lattice code (using a crystalline target), TRIM.SP [10] for a Monte Carlo program (using an amorphous target).

1.2 The interaction potential for BCA

One important problem is the use of an appropriate interaction potential. These potentials are generally screened Coulomb potentials, i.e. the Coulomb

potential multiplied by a screening function, which is mostly represented as a sum of exponentials. These potentials are purely repulsive, and they depend only on the internuclear distance. For screened Coulomb potentials the determination of the scattering angle affords a numerical integration, which is the most time consuming part of a program based on the binary collision approximation. The mostly applied potentials are the Molière potential [12], the WHB (Wilson-Haggmark-Biersack) or KrC potential [13], and the ZBL (Ziegler-Biersack-Littmark) potential [14]. These potentials are adjusted to the different collision partners by the screening length, which depends on the nuclear charge of the individual atoms. The WHB and ZBL potentials are mean potentials determined from a number of individual potentials based on Hartree-Fock-Slater (HFS) atoms in the ground state. Therefore, these mean potentials have not the same quality for all different atom-atom combinations. The application of the Molière potential often asks for a correction factor to the screening length for several ion-target combinations in order to get better agreement with experimental data. Nakagawa and Yamamura used a different screening function; their interaction potential is based on relativistic Dirac-Hartree-Fock-Slater (DHFS) atomic charge distributions. The individual constants for this potential are tabulated in [2,15]. The use of screened Coulomb potentials is convenient, because it can be applied to all atomic species, on the other hand it does not care about the shell structure of the atomic element or changes due to the collision.

1.3 The inelastic (electronic) energy loss

The energy loss of a moving atom to target electrons can be dealt with as an inelastic energy loss, which has to be applied additively to the nuclear energy loss. This effect is smaller than the elastic energy loss at low energies but becomes dominant at high energies. This energy loss process reduces the energy of the moving atom, but does not change the direction of a moving atom. At low energies two theoretical models are applied: the Lindhard-Scharff model [16] and the Oen-Robinson model [17]. The Lindhard-Scharff proposal is a friction model, in which the energy loss depends on the atom velocity, an idea already proposed by *Fermi* and *Teller* [18]. In contrast to this continuous energy loss between collisions, the Oen-Robinson energy loss is a local model based on a model proposed by *Firsov* [19]. It is dependent on the impact parameter of the collision, and it also depends on the velocity of the moving atom. The Oen-Robinson energy loss is smaller than the Lindhard-Scharff loss in the keV range and below, but is adjusted to the Lindhard-Scharff loss at higher energies. At high energies, where the electronic energy loss has a maximum and then decreases according to the Bethe-Bloch formula [20,21], the data tables for hydrogen and helium by *Andersen* and *Ziegler* [22,23] are the best choice.

1.4 The surface binding energy

The surface binding energy, U , describes the binding strength of surface atoms to the target. For sputtered atoms a planar surface potential is assumed, which causes an energy loss normal to the surface and a refraction towards the surface. The reason is, that the planar surface potential results in an energy distribution of sputtered atoms with a maximum at about half the surface binding energy in agreement with experimental data; for an isotropic surface potential the maximum would be at zero energy. The most common choice is to use the heat of sublimation for the surface binding energy. This value varies between 0.72 eV for Cs and 8.68 eV for W. It should be mentioned, that projectiles may experience a binding to the surface as for example hydrogen on C or in the case of selfbombardment. The surface binding energy should depend on the surface structure. To remove a target atom from a flat surface should need more energy, for example, than to remove it from an extended position above the surface. The application of the heat of sublimation is a good mean value for the surface binding energy, because these heats have been determined experimentally although for a not well-defined surface. In compound targets the surface binding energy is usually not known; therefore, an interpolation according to the composition is assumed.

1.5 Problems of the concept of BCA

The binary collision approximation is based on some critical assumptions. A serious point is the assumption that at low energies a moving atom collides only with one single target atom. In TRIM.SP this problem is mitigated by including simultaneous weak collisions, but strictly in the binary collision approximation. Another problem is the concept of asymptotic trajectories, which is not a good description at low energies. This does not mean a sudden breakdown of the concept, but it worsens with decreasing energy. As discussed in [2] it starts at about 30 eV for the most unlikely process of a head-on collision; the energy depends also on the species of the colliding atoms. Both of these weaknesses seem not to be very serious, because otherwise the reasonable agreement between calculated and experimental results would be hard to explain.

1.6 Dynamic Monte Carlo programs

In many cases projectiles are implanted in a target leading to a composition change with depth, and this composition changes with the incident fluence. The implanted atoms modify the cascade and as a consequence sputtering and backscattering. Similar effects occur in bombardment of multi-component targets. This problem is taken care of by dynamic programs, which make an update of the target composition after each fluence step. Then the bombardment proceeds until some maximum fluence or equilibrium is reached. An example of such a program is TRIDYN [2,24] and its newest version SDTrimSP

[25], which combines TRIM.SP and TRIDYN. SDTrimSP is devised to run on all platforms (sequential and parallel).

1.7 Advantages of BCA programs

BCA programs allow besides sputtering also the determination of backscattering, transmission, and radiation damage. This includes yields, reflection coefficients, their dependence on incident energy and angle of incidence as well as energy and angular distributions of sputtered and reflected atoms and even more detailed information. A big advantage of programs based on the binary collision approximation is the speed of calculations, which is about four to five orders of magnitude faster than for molecular dynamics programs.

2 Programs based on Molecular Dynamics

The method of molecular dynamics simulation is based on the simple strategy of following the time evolution of a system of particles by solving Newton's equations of motion for the system. It has been used early when the calculation power of computers has been introduced to solve physics problems [26]. Indeed, one of the first applications of molecular dynamics in physics was a radiation damage problem [27]. Since then, the method has been used in many areas of science, such as the physics of liquids, of materials, of biomolecules, etc. Both the method and its applications are described in textbooks [28–33]; and also the issues of ion-solid interaction, radiation effects and, in particular, sputtering have been made accessible in monograph or review form [3,34,35].

2.1 Physics input: forces

The task of solving Newton's equations of motion needs as physical input the knowledge of the forces acting on the particles. For the issue of ion-solid interaction, and sputtering physics, one needs to know the interatomic forces between the projectile and the target atoms and between the target atoms themselves. These are assumed to be given by the interatomic potentials, and by the coupling of the atoms to the electronic system.

The role of quantum-mechanical phenomena in the field of sputtering physics appears to be small; it hence appears justified to use classical molecular dynamics simulation to study this phenomenon.

2.1.1 Interatomic potentials

The calculation of appropriate interatomic potentials is a fundamental issue in solid-state physics [36]. During ion bombardment, however, the atom positions, and hence also the electronic states, deviate strongly from equilibrium;

hence interatomic potentials far away from equilibrium are needed. In principle, these potentials can be calculated by quantum chemistry or density functional theory. Due to the quick time evolution of a collision cascade, such an ‘ab initio’ potential calculation would best be performed at each time step of a molecular dynamics simulation; however, this solution is computationally too complex in large-scale simulations. Instead, as a rule, approximate parametrizations of the potential are used; their regimes of applicability have been assessed over the years.

At high interaction energies, above 100 eV relative energy, say, a collision between two atoms can be assumed to be binary. Then the repulsive potentials described in 1.2 above can be used. At small interaction energy, kinetic energies corresponding to < 1 eV, say, potentials taken to describe the equilibrium structure of solids or liquids at thermal temperatures can be used. These potentials differ for each class of materials – and the corresponding chemical bonding type – studied. Thus, for condensed rare gases, binary potentials of the Lennard-Jones type are appropriate. For metals, many-body potentials are necessary which are often used as parametrized in the embedded-atom-method (EAM) potentials [37,38]. Covalent bonds need three-body potentials to describe the bonding geometry correctly [39–41]. In ionic solids the long-ranged Coulomb forces between anions and cations need to be included. The energy gap between the high- and low-energy regimes described above is usually filled by interpolation. Ideas of how to include physical knowledge – e.g. on displacement energies – to fill this gap are non-trivial to implement [42].

These few words may suffice to point out that the inclusion of appropriate interatomic potentials is a non-trivial task. However, as a benefit for sputtering and other radiation damage calculations, the appropriate binding energies (surface binding, adatom binding, etc.) and defect formation energies are directly included in the potentials.

2.1.2 Electrons

By the interaction with target electrons, swift atoms may be slowed down. This stopping force is implemented as an external force in the molecular dynamics routine. The schemes used are analogous to those described in Sect. 1.3 above.

At lower energies, the electron-atom interaction is better described as the electron-phonon interaction in a material. Several recipes exist of how to include this interaction into a molecular dynamics study [43–48]. A number of issues are still unsolved here: How to describe the electron-atom interaction in a ‘hot’ strongly disordered configuration such as in the centre of a collision cascade or a spike; how the band structure of the material (insulator or metal) enters; how to describe the interaction with hot, possibly non-thermal electrons.

2.2 Technical considerations

In spite of the conceptual simplicity of a molecular dynamics algorithm, a number of more or less technical issues need be considered in order to perform reliable simulations [3].

2.2.1 System size

The number N of target atoms to be included in a simulation cannot be arbitrarily large – simulations with several million atoms are considered big nowadays. This constraint essentially limits the impact energy for which sputtering can be calculated to the order of several 100 keV at the most [49].

2.2.2 Boundary conditions

In order not to study the entire target material used in experiment (containing of the order of $N = 10^{23}$ atoms) only that subvolume is studied by molecular dynamics simulation in which the phenomena of interest occur. This subvolume – containing between 10^3 and 10^7 atoms, say – needs to be given the adequate boundary conditions to mimic the interaction with the surrounding material (energy and momentum exchange). This issue is particularly important for longer (> 1 ps, say) simulations, such as they are relevant under thermal-spike conditions or for cluster impact [50]. In the most refined simulations, the environment of the simulation volume is modelled by a finite-element-method (FEM) algorithm, which solves the elastic and heat conduction equations in the surrounding [51]. Simpler approaches employ energy-damping boundaries or provide for Langevin dynamics at the boundaries [52]. In cases where the question of how the surrounding material reacts is considered irrelevant, free boundary conditions (the simulation volume is considered as a free cluster in vacuum), fixed boundaries vacuum), fixed boundaries (in which in particular the bottommost target atom layer is kept at fixed positions), or laterally periodic boundary conditions (where in reality an infinite multitude of simultaneous projectile impacts are considered) are used.

2.2.3 Initial state

Ion-surface interaction presents an example of chaotic dynamics in the sense that slight variations in the initial conditions lead to large variations in the results, i.e., the sputtering yield [3,53]. In experiment, it is unknown at which exact position (on a femtometer scale) the projectile impinges on the surface. Rather, the typical experiment measures the average over many projectile impacts at random positions. In the simulation, this average is analogously calculated, i.e., by considering a large number of trajectories which are randomly distributed over a representative surface zone (a surface elementary

cell in the case of a crystalline target). The simulation results then allow to provide besides the average quantities detected also an estimate of the statistical error of this quantity.

In the case where temperature effects in the target are considered important (e.g. where projectile channeling is an issue), statistics need to include impacts upon the target in different micro-realizations at this temperature.

2.2.4 Sputtering

The seemingly trivial question of when a target atom can be considered sputtered has to be approached carefully, in particular for cases where the surface is rough or becomes rough during sputtering (e.g. by crater formation). The sputtered-particle detector implemented in the code must make sure that atoms have no chance of being redeposited on the surface. More trivial questions include the detection of sputtered clusters as such, and to exclude atoms which are emitted sideways from the simulation volume (this may happen for free boundary conditions).

2.2.5 Simulation time

While in a BCA code the simulation may terminate when no atom has a kinetic energy larger than the surface binding energy, the situation is more complex in molecular dynamics, since here moving atoms collide. In cases of high energy densities, i.e. in a thermal spike where part of the simulation volume is highly above the melting temperature, sputtering may proceed until 100 ps after projectile impact, or longer [54,55]. Here a definite criterion of when to terminate the simulation is hard to find, and one may resort to analyzing the time dependence of sputtering instead.

2.3 Reliability

Let us assume that the technical issues discussed above – and those not discussed like the numerics of the ordinary differential equation solving routine applied – have been adequately mastered.¹ Then, the simulation results will be as realistic as the physics input is – the interatomic potential and the electron-atom coupling. The experience attained from molecular dynamics simulations of sputtering in the last two decades or so gives us an optimistic picture. In many cases of disagreement between experimental and simulation results, the origin may be surmised to lie in the incomplete understanding of the experimental conditions, such as the geometric and stoichiometric characterization of the surface. However, the two caveats mentioned

¹ Research on the influence of these technical issues on sputtering calculations continues until today, e.g., on the influence of the system size [56] or on strategies of how to choose the ion impact points [53]

above – the role of the electron-atom interaction and the complexities of the interatomic potential in the energy regime important for sputtering – remain an important field of investigation for the future.

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