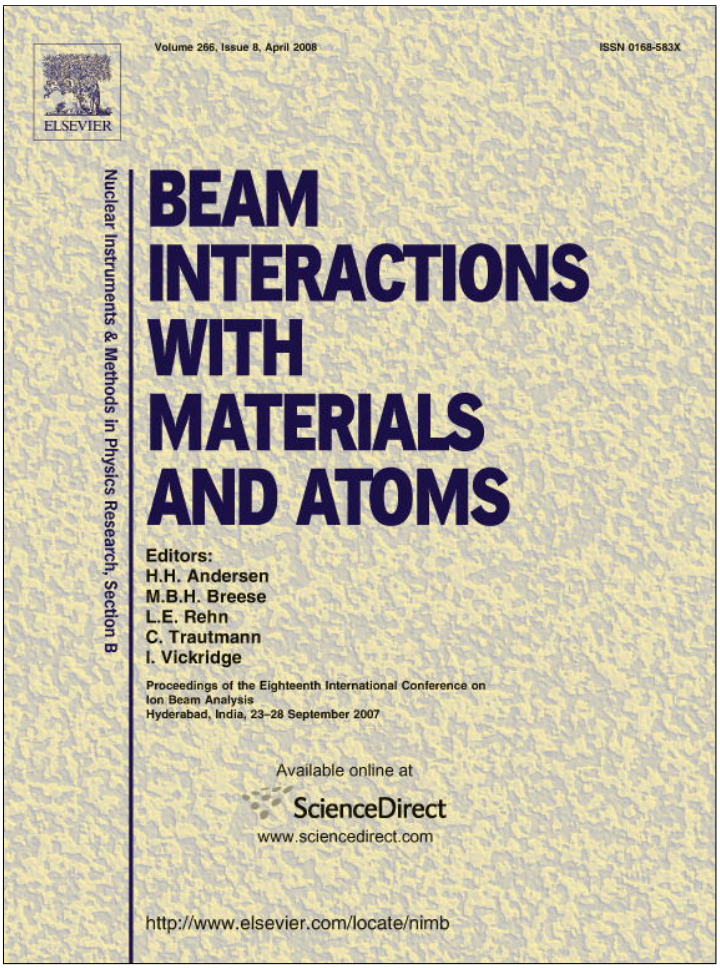

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Molecular dynamics for ion beam analysis

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Abstract

Molecular dynamics (MD) computer simulations, while very extensively used in chemistry and materials physics, have largely been absent in the theoretical treatment of ion beam analysis. Instead the computationally more efficient binary collision approximation (BCA) methods are widely used. In this paper I compare the two methods regarding the level of physical approximation versus accuracy, using a simple model study as an illustrative example. I then show, based on results in the literature, that although in most cases BCA methods are well sufficient for ion beam analysis, there are special conditions where MD methods are required even for keV and MeV kinetic energy processes.

PACS: 61.80.Jh; 02.70.Ns

Keywords: Molecular dynamics simulation; Ion beam analysis; Binary collision approximation

1. Introduction

Ion beam analysis of materials involves, by definition, the passage of energetic ions in matter. Hence to obtain theoretical understanding a capability to simulate the ion movement processes is needed. Although in some cases analytical or numerical transport theory methods are sufficient to obtain the average transport properties, more complex irradiation conditions tend to require the use of methods that explicitly simulate the movement of individual ions in matter.

The by far most used methods to simulate ion beam analysis (IBA) processes are those based on the binary collision approximation (BCA) [1–8,7,9–14]. In this approach, the passage of the ion is treated as a sequence of independent binary collisions, neglecting possible many-body effects. For each collision, the classical scattering integral is solved for a given impact parameter between the ion and a lattice atom. The impact parameter is obtained either completely randomly based only on the composition and density of the solid (corresponding to the irradiation of an amorphous material) or by tracking the position of the ion in a crystalline structure. The easiest approach is to have the collisions occur timewise sequentially, but it is also possible – and sometimes necessary – to treat several collisions which occur simultaneously [3,12,15].

As an aside, I note that the amorphous material approach is in our field often called "the Monte Carlo (MC)" method based on the random selection of impact parameters. However, this usage is quite misleading as completely different kinds of MC methods are in much wider use in other branches of physics [16–18]. Hence the method should be called, e.g. MC-BCA or simply BCA.

In molecular dynamics (MD) methods, the equations of motion for N interacting objects are solved by the numerical integration of the Newton (or Lagrange or Hamilton) equations of motion [17,19] to obtain a simulation of the motion of the N interacting bodies with progressing time. Thus it simulates the full many-body dynamics in an atomic system, and it is well known how to make the method arbitrarily accurate within the interatomic interaction model used [17,19,20], even for high energies [21]. The MD method is extremely widely used in chemistry,

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biochemistry and materials physics (see e.g. examples and references in [22,19,20]). It is also now the primary theoretical tool used for examining the ion beam *modification* of materials [23]. On the other hand, MD methods have not been widely used to examine the ion beam *analysis* of materials. The obvious reason to this is that they demand much more computer capacity than the BCA methods as they involve an iteration over short (fs or less) time steps, and for every time step require the calculation of the interactions between N atoms. This makes conventional, "full MD" calculations entirely impractical for common IBA situations which involve ions passing hundreds of nanometers deep in a material, and hence involve millions of atoms in the collision cascades. However, a variety of MD exist in which only the interactions of the incoming ion with the immediate recoil atoms are treated, termed MD in the recoil interaction approximation (MD-RIA) [21]. This approximation allows for simulating the passage of an ion in matter without simulating the interactions between the lattice atoms, making it possible to simulate even MeV energy ions with statistics within a reasonable time.

In the remainder of this paper I will first present an illustrative comparison of the difference between MD and BCA simulations for a model system, then proceed to discuss cases where both full MD and MD-RIA methods have been used, to give an idea as to when they may be useful. I chose to exclude simulations of sputtering from the discussion. Simulation of sputtering in the heat spike regime [24] and reactive sputtering [25] obviously requires use of MD methods, but these topics are somewhat outside the main scope of the IBA conference.

2. Model study

To illustrate the differences between the various levels of possible approximation to simulate passage of ions in matter, I have carried out simulations of individual trajectories of Ar ions passing through about 2 nm thick Cu foil under channeling conditions. As a starting point I used our full MD code parcas [26], which has special features tailored for the simulations of ion irradiation of materials. The most important of these include the use of high-energy repulsive potentials smoothly joint to the equilibrium ones, an adaptive time step which allows for treating even very high-energy head-on collisions correctly, and inclusion of electronic stopping powers [21].

In the current model study, the Ar ion was placed outside a Cu foil consisting of 5 unit cells of Cu in the face-centered cubic crystal structure, and directed towards it at an incident angle of $\theta = 7°$ off the z axis normal. The Cu cell was initially at 0 K, and the Ar was placed at exactly the same height in the y dimension as one of the lattice planes of Cu, thus ensuring that it will remain in the same y plane throughout the simulation. However, the simulations did also include all interactions outside the y plane. Since the purpose of the model study is merely to illustrate the effect of various levels of approximations on individual trajectories, electronic stopping was for simplicity switched off in the simulations. The main quantity monitored in the simulations was the energy loss of the Ar ion in the Cu foil. The simulations were run for 100 fs, which was a long enough time that for all energies the Ar ion had passed through the foil and was no longer interacting with any atom. The Ar–Cu interaction was the ZBL universal potential [27], and the Cu–Cu one the Sabochick–Lam equilibrium potential to which ZBL universal potential had been smoothly joint at interatomic separations below the nearest-neighbour one [28].

The levels of approximations used were the following. Initially the simulations were run in full MD mode, thus creating a full collision cascade (which did not evolve to the end due to the short 100 fs simulation time, but this does not affect the final energy of the Ar ion). After this, all Cu–Cu interactions were switched off to obtain an MD-RIA simulation. At all energies used in the current MD simulations, the Ar ion was observed to move in the same channel of the Cu lattice. In a BCA code including multiple collisions, this would most likely mean that the ion would be allowed to collide with all atoms along this row of atoms. Hence I made a special modification of the MD inputs, where the atoms right next to the channel where the Ar moves are the only interacting ones (keeping Cu–Cu interactions turned off). This made the MD code mimic a BCA multiple collision one. Finally, to mimic a BCA code without multiple collisions, I determined from the end result of the MD-RIA simulations as to which atoms had received at least 10 eV of kinetic energy from the Ar ion. These atoms (which depending on energy were 2–5 in number) were then made the only interacting ones (still keeping Cu–Cu interactions turned off). I note that although the 10 eV energy criterion is of course somewhat arbitrary, the usual algorithms for choosing which were the atoms that are colliding with the ion in BCA are also somewhat arbitrary. The four levels of approximation used are labeled "full MD", "MD-RIA", "BCA multiple coll." and "BCA".

The results for the case of 10 keV Ar are illustrated in Fig. 1. The Ar trajectories are almost indistinguishable, but careful examination shows that the BCA trajectory does differ somewhat from those of the other cases. The result on the lattice modification in the full MD run is, of course, highly different from that in the other cases.

The results for the energy loss are illustrated in Fig. 2 in the energy range from 4 keV to 1 MeV. Lower energies were not included in the comparison since at 3 keV and lower energies the Ar is not transmitted through the foil. The MD-RIA is in essentially perfect agreement with the full MD result at all energies, and the BCA with multiple collisions differs by only a few percent. However, the plain BCA result differs strongly from the others, even at the very high energy of 300 keV. Inspection of the 300 keV trajectory showed that due to the lack of weak collisions in the BCA, the trajectory of the Ar ion happens to be different enough after the first collision that it leaves the channel,

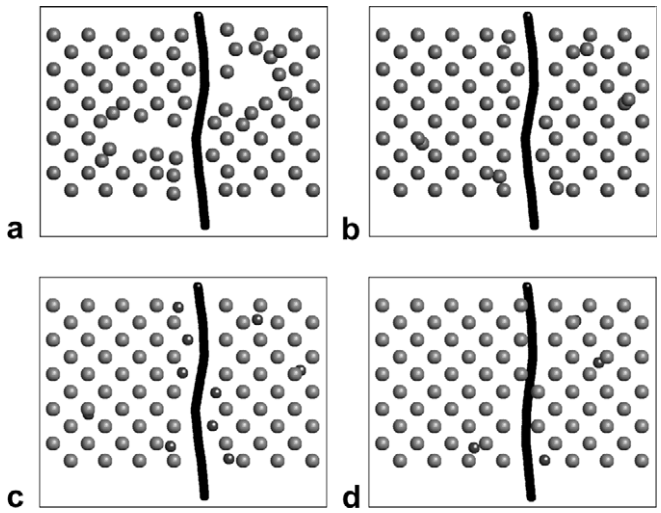

Fig. 1. Illustration of differences between (a) full MD, (b) MD-RIA, (c) BCA with multiple collisions, (d) BCA simulations. In the plots, all positions of the Ar atom while it was passing from top to bottom through the Cu foil are shown, forming the trajectory shown in the middle. For the lattice atoms the positions at 40 fs (when the Ar has already left the plotting region) are shown. In parts (c) and (d) the atoms included as mobile in the MD-mimicked BCA simulations (see text) are distinguished with smaller spheres. In the full MD case it is clearly evident that the primary recoils have started a collision cascade in the material. At all other levels of approximation the cascade is missing. The MD-RIA and BCA multiple collision systems look very similar, while in the BCA case only a few atoms have received a recoil energy.

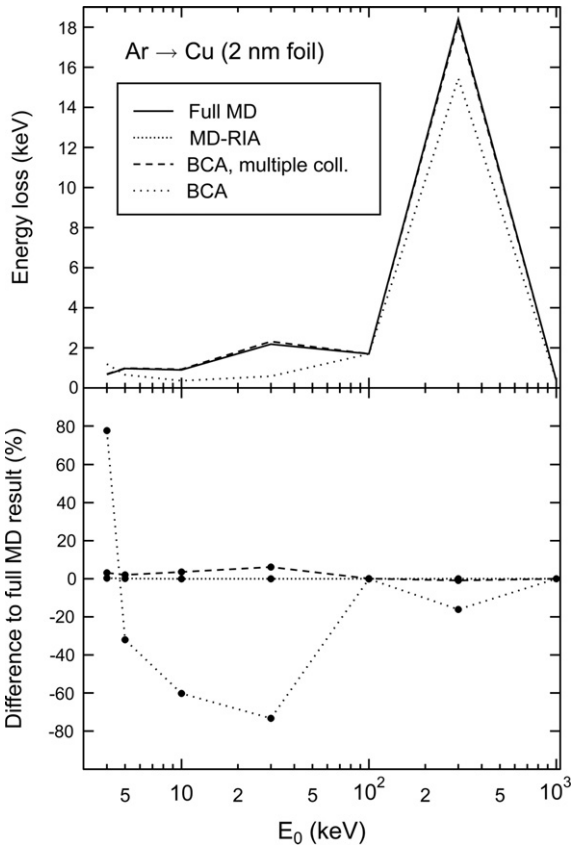

Fig. 2. Comparison of the Ar energy loss in the 2 nm Cu foil for the *individual* trajectory described in the text. The upper part shows the energy loss, and the lower part the relative difference of the MD-RIA, BCA multiple collision and BCA results to the full MD result. Since the full MD and MD-RIA results agree almost perfectly, they are indistinguishable in the upper part of the figure.

and experiences entirely different collisions in the remainder of the run.

I emphasize that the current study is one of the individual trajectories. In a simulation of the average energy loss over a large number of trajectories, and including thermal random atom displacements, the big BCA–MD difference would certainly be much reduced. However, the current results serve well to illustrate the extreme sensitivity of individual trajectories to small perturbations in the atom positions, and also indicate that at least BCA models including multiple collisions can be expected to work well also under channeling conditions. To assess the average accuracy of MD or BCA methods, simulations including statistics over random initial impact points are naturally needed. In the remainder of the paper I will discuss some examples of such studies from the literature.

3. Ion range calculations

The theoretical prediction of the penetration depths of ions in matter is not an ion beam analysis technique *per se*. However, the measurement of ion range profiles is frequently carried out with IBA techniques such as Rutherford backscattering (RBS), elastic recoil detection analysis (ERDA) or nuclear resonance broadening (NRB). Moreover, by combining ion range calculations with measurements of range profiles it may be possible to deduce information about the electronic stopping or sample structure [29,30]. Thus range calculations may in such contexts be considered an indirect method of ion beam analysis, and the same simulation methods used to obtain range profiles can also be used to simulate ion beam analysis. Hence I will consider in this section examples of where MD methods have been used to calculate range profiles.

Although MD methods were used to carry out ion range calculations as early as 1971 [2], their wider use began in the 1990's when computer capacity had advanced enough to enable obtaining good statistics in a reasonable time [21,31]. Although the initial works [21,31] did not carry out a systematic one-to-one comparison of the accuracy of MD versus BCA, they did demonstrate that it was becoming practical to simulate ion penetration with statistics of tens of thousands of events even at keV energies. Moreover, the use of MD does provide some clear advantages over BCA methods. Multiple simultaneous collisions are naturally taken into account correctly, while in BCA there are pitfalls in how they should be treated [32,15]. In MD simulations it is easily possible to take into use attractive potentials [33] and even angular-dependent ones [31]. For instance, for the case of 1 keV As implantation of Si, Chan et al. [33] have shown that using an interatomic

potential with an attractive well clearly gave better agreement with experiment than the purely repulsive ZBL potential.

A systematic comparison of MD and BCA range calculations was carried out by Hobler and Betz [15]. To ensure that the results are directly comparable (i.e. have identical interatomic potentials and electronic stopping powers), they implemented MD-RIA and BCA versions of the same code. By comparing range profiles of H, He, B, Si and As implantation of Si, and using a criterion of 5% difference in the projected range, they obtained an energy limit of validity for BCA in Si as

$$30M_1^{0.55}\ \text{eV} \tag{1}$$

where M_1 is the mass of the incoming projectile. However, it should be understood that this limit applies to the projected mean ranges; if the shape of the tail is of interest, the limit may be higher. This is exemplified in the study by Chan et al. [33], which shows that even though the projected range is essentially the same, the tails of the distribution may be significantly different.

The use of MD methods to simulate range profiles does offer one distinct advantage over BCA. Since the simulation tracks the position of atoms over small steps (<0.1 Å [21]), implementing electronic stopping that depends on the local electron density is straightforward. In the Puska–Echenique–Nieminen–Ritchie (PENR) model, the electronic stopping of an ion is calculated by density-functional theory from the local electron density acting at the site of the atom [34]. The electron density in silicon is highly non-homogeneous, and in particular in the middle of the ⟨1 1 0⟩ channel it is more than an order of magnitude weaker than the average value (<0.05 e/Å^3 in the channel versus 0.7 e/Å^3 on average) [35]. Thus to properly treat the ion movement in a channel, it is important to use a three-dimensional electron density function describing the electron density correctly in the channel. We [36–38] have developed an MD-RIA method using a three-dimensional electron density function that reproduced well the experimental ion range profile data for several ions in Si in both random and channeled directions. Some results of the model are illustrated in Fig. 3.

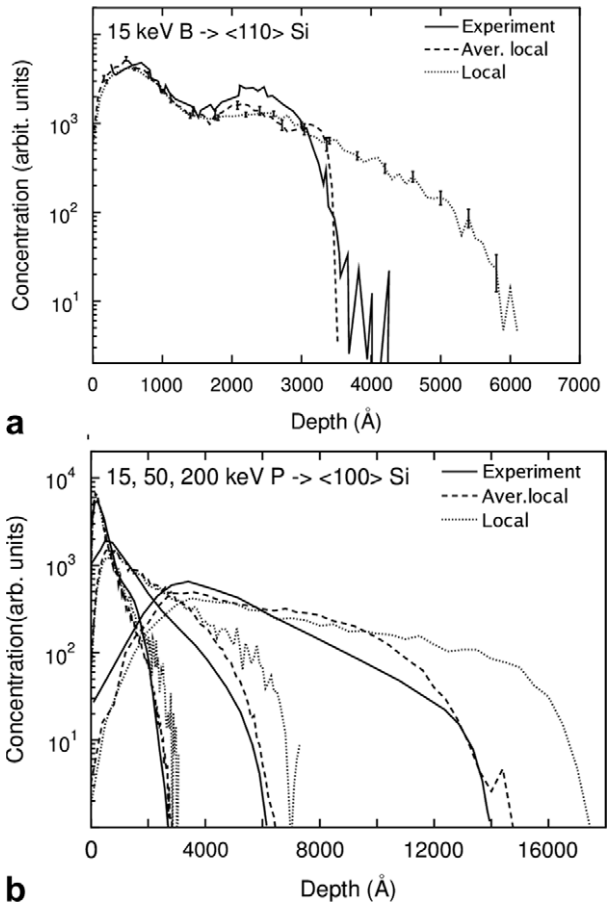

Fig. 3. Ion ranges in silicon calculated with the MD-RIA code MDRANGE [39] model employing a three-dimensional electron density compared to experiment. The "Aver. local" curves signify the a model where the size of the ion moving in the crystal is taken into account, and the "Local" curves signify one where the ion is assumed to be pointlike. For details on the calculations see [38].

4. Cluster ion irradiation

Another case where using an MD model to simulate irradiation is crucial, is in examining cluster ion bombardment of materials. It is well known that cluster ion irradiation often leads to nonlinear effects, in the sense that the outcome of the irradiation of a cluster of N atoms A_N does not lead to the same outcome as when N independent ions A_1 at the same energy/atom irradiate the same material [40–45]. Such effects have been experimentally observed for energies exceeding 1 MeV/cluster [43].

The nonlinearities are due to several physical effects, such as the vicinity of the atoms to each other, which makes it possible for several ions to transfer energy to the same lattice atom. Also the cohesion within the cluster is important, especially in the cluster ion scattering experiments. Such effects can not be modelled within a conventional BCA model (although it might be possible to a limited extent to treat them in a hybrid MD-BCA scheme).

For instance, the experimental observation by Andersen et al. that Au cluster ion irradiation of Cu, but not Si, leads to a strongly enhanced straggling of the ion range distribution [45] was explained by full MD simulations of 1–10 keV ion ranges of Au_1–Au_7 in Cu and Si. The simulations showed that with increasing numbers of atoms in the clusters, the mean range is only slightly increased, but the straggling is increased strongly in Cu, but not in Si [46]. These observations are perfectly in line with the experimental observations [45]. The full MD simulations also showed that the reason to the effect is enhanced movement of the cluster atoms in the heat spike phase of a cascade, an effect which neither MD-RIA nor BCA models could simulate. The reason for the difference between Cu and Si is that heat spikes are very pronounced in dense metals like Cu, but barely exist in Si [47,46] (see Fig. 4).

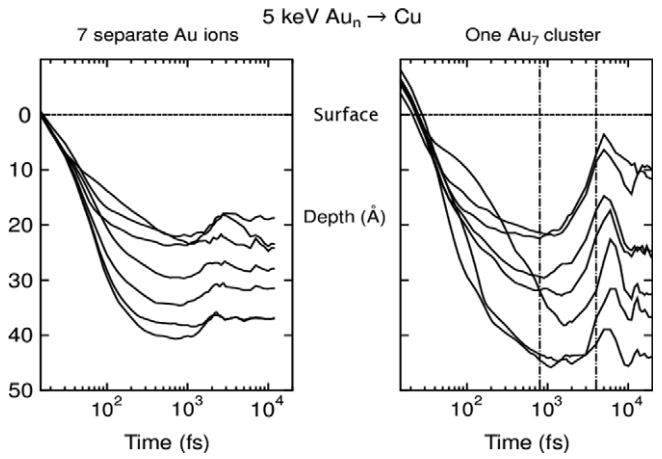

Fig. 4. Development of the z coordinate of Au ions implanted either separately from each other (left), or in a cluster (right). In the cluster case, visual inspection showed that massive heat spikes developed, which lead to a redistribution of atoms. This is reflected in the time dependence of the positions of the Au atoms: in the cluster, but not the single ion, case they are strongly changed after 1 ps in the heat spike phase. For details on the calculation see [46].

Surface scattering by clusters as a tool for analysis and enhanced sputtering is becoming increasingly popular, and further increases the need for MD simulations in the field. Webb et al. [48,49] have studied how fullerene impacts affect the desorption of material from surfaces using MD methods, and shown that using cluster irradiation it is possible to sputter a large fraction of intact molecules from a surface.

5. Elastic recoil detection analysis

All previous effects where MD methods were needed involved keV energies. I end the paper by mentioning a case where even for MeV energies an MD method gave different results from a BCA one. Mayer et al. examined the effects on multiple scattering on typical RBS and ERDA applications by comparing analytical theory with BCA and MD-RIA simulations [50]. Both the BCA and MD codes used the same interatomic potentials and electronic stopping powers. Although the differences between BCA and the MD-RIA calculations were smaller, they were in some cases of the order of 5% regarding the angular and energy spread, which could be experimentally significant. While the differences obviously are related to multiple scattering effects, the exact reason for the differences was not determined. However, the results indicate that even for MeV energy ion beam analysis methods, MD methods might be needed when the highest possible accuracy is desired, either as a stand-alone method or at least to calibrate the parameters of the BCA methods.

6. Summary and conclusions

I have discussed as to when molecular dynamics methods might be needed for ion beam analysis purposes. I first recalled the physical principles underlying the MD and BCA methods at four levels of approximation: full MD, MD-RIA, BCA with multiple simultaneous collisions, and BCA with single collisions. From these principles it is clear that only full MD can completely handle true many-body dynamics, but for high energies MD in the recoil interaction approximation is often enough to treat the ion movement. While BCA methods are almost always good as a first approximation of the true many-body dynamics for single ion irradiation conditions, it is not possible to give a single criterion for when they are sufficiently accurate compared to MD or MD-RIA. Instead the examples of comparisons of MD and BCA I cited showed that the "BCA–MD" limit strongly depends on the case studied and the accuracy that is desired. On the other hand, in some applications (such as the discussed cases of attractive potentials or 3D electron densities) the use of MD methods may be simply motivated by the fact that they may be easier to implement than a corresponding BCA method. While MD methods remain slower than BCA ones, with present-day computer capacity sufficient statistics for, e.g. a range profile can in many cases be obtained in a matter of minutes or hours, which is usually sufficiently fast at least in basic research.

I also pointed out that in the increasingly popular case of examining cluster ion irradiation, nonlinear many-body effects often play a crucial role in the outcome even for energies of the order of MeV's/cluster. Simulating such cluster ion irradiation effects clearly demands the use of MD methods.

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