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A BCA-MD approach with adaptive volume to simulate high-energy PKAs in materials of interest for Fusion

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Abstract

We present a method combining the Binary Collision Approximation (BCA) and Molecular Dynamics (MD) with adaptive volume to simulate high-energy collision cascades in solids under irradiation. The results obtained with the BCA-MD method with adaptive volume are in very good agreement with those obtained with full MD calculations. The BCA-MD predicts very well in a broad range of Primary Knock-on Atom (PKA) energies the different phases of evolution of the cascade, the number of Frenkel pairs, the fraction of point defects in clusters and their size distribution. The BCA-MD method proposed here achieves a considerable acceleration of MD simulations with a speedup factor that increases with the PKA energy. For a PKA energy of 80 keV in Fe, the speedup measured is higher than 30. For a PKA energy of 0.5 MeV in Fe, by comparison with MD simulations performed by other authors, we estimate that the BCA-MD accelerates MD simulations by a factor 312.

Keywords: Binary Collision Approximation, Molecular Dynamics, Irradiation, Collision cascades, Defect formation

1. Introduction

Nowadays, it is common to find technological environments where materials are irradiated with energetic particles such as space applications exposed to energetic electrons or protons coming from the solar wind [1, 2] or from galactic

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cosmic rays [3, 4], detectors in particle colliders [5, 6], materials in fission or in future fusion reactors [7, 8, 9, 10], materials used in the storage of radioactive waste coming from nuclear power plants [11, 12], materials used as shield in radiation medicine and biology [13], nanopatterning [14, 15] or implantation of dopants in semiconductor for the fabrication of electronic devices [16, 17, 18, 19].

In all cases, the irradiation process results in the initial displacement of an atom in the material, often called the Primary Knock-on Atom (PKA), by interaction with an impinging particle such as an electron, neutron or ion. This displaced atom, in turn, dissipates its initial kinetic energy by collisions with other atoms in the solid, displacing some of them, leading to the so-called collision cascade. At the end of the cascade, some atoms remain displaced from their lattice sites in the material, which gives rise to defects such as self-interstitial atoms (SIA) and their accompanying vacancies (V). Often, these defects can even agglomerate into more complex ones during the time of the cascade [20, 21, 22]. In some cases, the presence of these defects implies a degradation of the performance of the material, which can be detrimental to its proper functioning or even, in some cases, harmful if the safety of human beings is concerned. Therefore, it is essential to accurately predict the formation of defects under irradiation in order to understand how material modifications evolve as functions of irradiation parameters and/or to anticipate when the degradation of material properties will start affecting its performance.

However, investigating the formation of defects in solids under irradiation is a hard task as atomistic mechanisms that come into play take place in timescales in the order of ps and in small volumes in the order of nm^3. For these reasons, in general it is extremely difficult or even not possible to experimentally characterize and follow the evolution of collision cascades. Only *post-mortem* analysis, provided that defects are detectable, can bring some insight, though partial, on what occured during displacement cascades. Therefore, modelling and computational simulations represent valuable tools to investigate and shed some light on such complex phenomena as they enable a detailed analysis of cascades, collision by collision.

To do so, two simulation techniques are commonly used, namely, the Molecular Dynamics (MD) and the Binary Collision Approximation (BCA). MD has been widely used for decades to simulate atomic collisions in materials under irradiation [23, 24, 25, 26]. Given an interatomic potential of interaction between atoms, MD solves numerically the Newton equations of motion of each atom in the system. Since the equations of motion of each atom in the system must be solved at the same time, MD simulations become computationally prohibitive in practice for high kinetic energies of the projectile ($\gtrsim 100\ keV$)[27].

The BCA has also been extensively used for decades [28, 29, 30, 31, 32, 33] to simulate collision cascades in solids under irradiation. Potentials used in the BCA are designed to account for close encounter interactions. Given such a repulsive interatomic potential, the problem of atomic collisions in solids can be reduced to a problem of binary collisions if the kinetic energy of the projectile is significantly higher than the one of lattice atoms. Following this approach, the trajectory of moving particles can be regarded as a series of isolated binary collisions. Between collisions, it is assumed that particles move along straight-line segments. Since the BCA only follows the trajectory of atoms that have been displaced from their lattice site, BCA calculations are much faster than MD simulations. However, as the particles slow down, their kinetic energy reaches a threshold below which they no longer interact with individual atoms of the solid, but instead suffer simultaneous collisions with many atoms. Thereby, below this critical value, the binary collision approximation breaks down.

The idea of combining the BCA and the MD in order to accelerate MD calculations arises thus naturally. In fact, a link between these two methods was first attempted several decades ago by Jaraiz *et al* [26] but the authors only compared trajectories and the number of atoms displaced for very low projectile energies ($\sim keV$), without paying attention to the final state of defects nor to the acceleration of simulations that could be achieved with this technique. In this work, we show that, in fact, such combination of the BCA and MD does not provide a significant acceleration of MD calculations. Therefore, we propose to revisit this technique and improve it in order to achieve considerable

accelerations of MD simulations. The specific materials that were selected for this work are Fe and W, which have an obvious interest as model material to study radiation effects in structural components in future fusion reactors, where the neutron spectrum will include highly energetic neutrons ($\sim$14 MeV). Energetic PKA are thus expected to be produced in Fe and in W and it therefore represents an interesting case where to apply the BCA-MD. The concept of combining the BCA with MD will be explained in detail in Sec. 2. Section 3 will be devoted to describe how the volume of the MD cell can be adapted and optimized using the information obtained with the BCA. In Sec. 4 we shall show that the results obtained with the combined BCA-MD method are in very good agreement with those obtained with full MD calculations in a broad range of PKA energies. Finally, in Sec. 5 we shall calculate the speedup factor achieved by the BCA-MD in comparison to full MD calculations.

2. The BCA-MD method: The concept

The way we propose to combine the BCA and MD differs from that proposed by Jaraiz *et al* [26]. In their work, the authors first simulated the cascade using BCA and, only subcascades of it with a kinetic energy lower than a certain cut-off were placed into a MD cell. In our approach, the dynamics of the whole cascade is calculated using the BCA as long as there are AIMs with a kinetic energy higher than a threshold energy fixed in advance. This threshold energy must be above the energy below which the BCA breaks down (10 eV in Fe). AIMs whose kinetic energy falls below this threshold energy are abandonned during the BCA simulation, i.e., their trajectory is no longer followed. Once the last AIM has reached the threshold energy, the whole cascade obtained with the BCA is transferred as initial conditions into a MD cell to simulate the last stages of the cascade. In this approach, we assume thus that disregarding the time at which each AIM reaches the threshold energy has no effect on the dynamics of the cascade. Indeed, collision cascades are stochastic by nature and not all AIMs reach the threshold energy at the same time during a cascade.

In fact, the time at which the last AIM reaches the threshold energy is very short for all PKA energies. For a PKA energy of 5 keV, the last AIM reaches the threshold energy in average after 84 fs whereas it takes in average 338 fs for a PKA energy of 200 keV. Furthermore, the most probable time at which AIMs stop is even shorter, less than 100 fs, regardless of the initial PKA energy. This is approximately two orders of magnitude lower than the time necessary for the defects to become distinguishable, regardless of the PKA energy. Clearly, in our approach, AIMs are stopped in the early stages of the cascade. On the other hand, Calder *et al.* [34] demonstrated using MD simulations that the formation of large SIA clusters is due to hypersonic recoil atoms that are produced in the early stages of the cascade and that travel individually beyond the main shock front, creating their own shock wave. In particular, Calder *et al.* showed that this process takes place in a few hundred fs. In another work, Sand *et al.*[35] explain that during this time, atoms travel individually penetrating undisturbed areas of the lattice, *before* the pressure wave forms. In our approach, AIMs are stopped during BCA calculations when they still have a hypersonic velocity ($\sim 5 \cdot v_{sound}$) and at similar times than those found by Calder *et al.*. Since AIMs are hypersonic when they are stopped, it is unlikely that a zone of the cascade could interfer with another one during the short time interval considered here, i.e., the time that passes between the first AIM is stopped and the last one. Indeed, by definition, shock waves propagate at the velocity of sound, which is much lower than the velocity of AIMs. According to these arguments, we can disregard the difference in time at which the different AIMs are stopped since it should not affect the subsequent evolution of the collision cascade. Therefore, we can reasonably assume this time interval as sufficiently short and such that all the information obtained with the BCA can be transferred in a single step to the MD simulation as initial conditions. The data that must be passed from the BCA to the MD must be such that the cascade can be reconstructed and resumed without loss of information. We consider that the following information obtained with the BCA contains the data necessary to resume the cascade evolution when used as initial condition

in a MD simulation:

1. Coordinates of each vacancy
2. Coordinates of each AIM
3. Velocity vector of each AIM
4. Velocity vector of lattice atoms that suffered collisions but without displacement from their site

The last data must be transferred to the MD simulation in order to preserve the total energy. Indeed, during a cascade, many collisions are such that the energy transferred to lattice atoms is small and not enough to displace them from their lattice site. If these collisions were not taken into account, a fraction of the initial kinetic energy of the PKA would be missing when the MD simulation starts. This could lead to incorrect and misleading results. In addition to the data transferred from the BCA to the MD simulation, there is another important point that must be adressed when combining the BCA with MD simulations. Indeed, it must be noted that, in the BCA framework, the potential energy is not taken into account and, after a collision, the position of the atoms is determined using their asymptotic trajectories. Hence, when atoms from the BCA cascade are placed into the MD cell, it can happen that some of them ends up much closer to a lattice atom from the MD cell than if it followed the real trajectory taking into account the potential. As a result, the atom feels a strong repulsive force due to the potential energy created by the lattice atom. This force can induce an additional but artificial kinetic energy, which can strongly affect the cascade as a whole. In order to circumvent this problem, when the atoms coming from the BCA simulation are placed into the MD cell, we first proceed to a minimization of their potential energy before they are allowed to evolve according to their initial velocity vector.

3. Adaptation of the MD simulation volume

Once the first stages of the cascade have been calculated using BCA, the cascade must be transferred to a MD cell to simulate last stages of the cascade.

To do so, a MD volume cell must be defined in advance. As for full MD calculations, the simulation volume must be sufficiently large to avoid the cascade reaching the boundaries of the cell. However, often, it is observed *a posteriori* that the volume was unnecessarily large and that, in fact, a significant part of the computational effort was devoted to simulate the vibration of lattice atoms around their equilibrium position but far from the cascade. Thus, if the volume of the MD cell necessary to simulate a cascade could be predicted in advance, the number of atoms in the system could be optimized and the computational effort could be reduced. This can be achieved with the BCA-MD by taking into account that, at the end of the cascade obtained with the BCA, AIMs have a relatively low kinetic energy ($\sim$ a few hundreds of eV) when they are introduced in the MD cell. In other words, when the BCA cascade is transferred to the MD simulation box, it is expected that the volume of the cascade will not significantly increase further since atoms that are in movement will not cover long distances. Thereby, the MD simulation volume–and thus, the number of atoms in the system–that is necessary to simulate the last stages of the cascade can be predicted in advance using the coordinates of the atoms and vacancies obtained by BCA calculations.

For instance, in the case of a PKA energy of 80 keV in Fe, it was found that full MD simulation boxes with sides of $300a_0$ (54 million atoms) were necessary to avoid the cascades reaching the boundaries of the cell. In contrast, with the BCA-MD a MD simulation volume with a parallelepiped shape that adapts to each cascade can be defined using the coordinates of the defects obtained from BCA calculations (see example in Fig. 1). With this method, MD simulation volumes with only 1.26 million atoms in average are necessary, i.e., 42 times less atoms than in full MD simulations. We can thus expect a significant reduction of the simulation time using this optimization of the MD simulation volume.

However, in order to avoid any temperature effect that could alter the formation of defects during the cascade, we check for each cascade that the number of atoms in the optimized MD simulation volume is sufficient and such that the average temperature corresponding to the total kinetic energy of all atoms

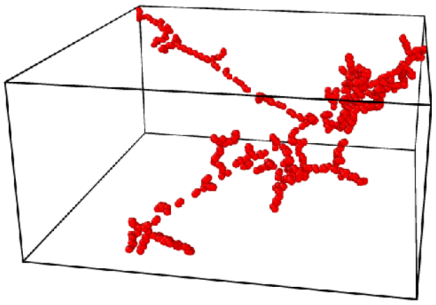

Figure 1: Optimized MD simulation domain defined by the minimum and maximum coordinates of atoms in motion (red balls) in a cascade obtained with the BCA for a PKA energy of 80 keV. For this particular cascade, the MD simulation domain contains 1.24 M lattice atoms (not shown).

(lattice atoms + PKA) is lower than a given maximum temperature defined in advance. When this is not the case, the minimum number of atoms N_{atoms} that must contain the system in order to limit the average temperature during the cascade is determined using the following relashionship:

$$E_{PKA} + \frac{3}{2} N_{atoms} k_B T_{eq} = \frac{3}{2} N_{atoms} k_B T_{max} \quad (1)$$

where k_B is the Boltzmann constant, T_{eq} the equilibrium temperature of the system before the collision cascade and T_{max} the maximum average temperature allowed in the system. Then, the MD volume initially calculated is recalculated by adding extra-cells in all directions and such that the total number of atoms in the system is equal to that obtained using Eq. 1.

4. Validation of the BCA-MD: Comparison to MD calculations

In order to validate the BCA-MD method described in the previous sections, we simulated collision cascades in Fe and W for PKA energies from 5 to 150 keV in the $\langle 135 \rangle$ high-index direction. Results obtained with the BCA-MD were systematically compared to those obtained using full MD calculations.

Different aspects of the collision cascade evolution were considered to validate the BCA-MD, as described in the following sub-sections. For each energy, a set of 30 cascades was simulated using both methods in order to get a sufficiently large statistics. In the case of the BCA-MD, the MD simulation volume was adapted to each cascade allowing a maximum temperature T_{max} =250 K in the system, as defined in Eq. 1. Defects and defects in clusters were analysed using the OVITO code [36]. SIAs and Vs were identified using a Wigner-Seitz cell analysis. Interstitials (vacancies) were considered to belong to the same cluster if they are within a distance of third (second) nearest neighbor.

MD simulations were performed using the LAMMPS code [37]. The interatomic potential developed by Ackland *et al* [38] (A04) was used to describe the interaction between Fe atoms, after being smoothly joined to the Ziegler – Biersack – Littmark (ZBL) universal repulsive potential [30], that is commonly used to describe short-range collisions. In the case of W, the potential developed by Derlet *et al.*[39]. In both cases, the Fe and W crystals were equilibrated at temperature T with a Langevin thermostat with a short relaxation time during 5 ps. The temperature was chosen to avoid defect migration during the cascade, as highly mobile defects form in Fe under irradiation [40]. Cascades were initiated by imparting a kinetic energy E_k to a selected PKA and its evolution was followed until a maximum time of 15 ps with a variable time step with a maximum value of 3 fs. In order to avoid channelling effects, an initial high-index direction [25] $\langle 135 \rangle$ was used for the PKA. The position of the PKA was chosen to be in the middle of the simulation box. During the collision cascade no control of the temperature was performed, i.e., we used the NVE microcanonical ensemble with periodic boundary conditions. The simulation boxes were chosen sufficiently large to contain the cascades within the cell boundaries, avoiding any interference of the cascade with itself by periodic overlap. In each simulation, we observed a slight increase in temperature of the system and can conclude that it did not have any discernible effect on the defect formation generated by the collision cascade. No electronic stopping nor electron–phonon coupling was included in our simulations.

BCA simulations were performed with the MARLOWE-CIEMAT[33] code, a modified version of MARLOWE [28, 29] (version 15b). As in MD calculations, BCA simulations were performed using the ZBL potential for short-range interactions. The binding energy of lattice atoms used in BCA calculations, i.e., the energy necessary to kick off a lattice atom from its site, was set equal to the binding energy predicted by the interatomic potentials used in MD calculations. As is usually done, in this work we used a maximum value for the impact paremater slightly smaller than the first nearest neighbor distance, which in the case of bcc metals, is $a_0\sqrt{3}/2$ (a_0 being the lattice parameter). The temperature was the same as in MD simulations. As in MD simulations, no stopping power was used in BCA simulations and cascades were initiated by imparting a kinetic energy E_k to a PKA along the $\langle 135 \rangle$ high-index direction.

4.1. Stages of the collision cascade evolution

One of the important aspects of the collision cascades that the BCA-MD must predict correctly is the different stages identified with MD, i.e., the ballistic phase, the thermal spike and the colling down phase. To show that the BCA-MD is able to reproduce with a very good agreement these different phases of the cascades, we simulated collision cascades for a PKA energy of 40 keV in Fe with a threshold energy of 1 keV. This threshold energy is well above the threshold below which the BCA breaks down (10 eV in Fe). In Fig. 2 we compare the evolution of the number of displaced atoms (averaged over 30 cascades) as a function of time, obtained using the BCA-MD and full MD. As we can see, the BCA-MD is in very good agreement with full MD calculations. The method reproduces very well the different stages of the evolution of collision cascades from short to long times. We can notice that the curve corresponding to the BCA-MD does not start at the same time as full MD calculations since the time at which the BCA-MD starts corresponds to the average time at which the last AIM is stopped in BCA calculations. The evolution of the number of displaced atoms obtained for a much lower threshold energy, 10 eV, is also shown for comparison. In this case, the BCA-MD fails to correctly describe the evolution

of the collision cascades, as expected, since the BCA breaks down at this energy.

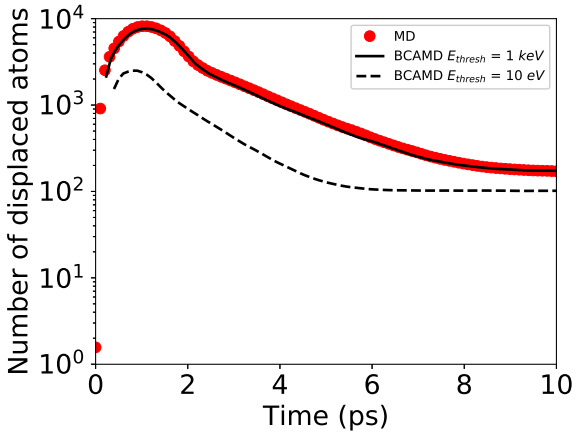

Figure 2: Evolution of the number of displaced atoms with time in Fe for a PKA energy of 40 keV calculated using full MD (red circles), the BCA-MD with a threshold energy of 1 keV (solid line) and the BCA-MD with a threshold energy of 10 eV (dashed line).

4.2. Number of Frenkel pairs and fraction of point defects in clusters

The objetive is to show that the BCA-MD predicts with a very good accuracy the number of defects and the clusters that form during the cascades. Cascades are simulated for a broad range of PKA energies both in Fe and W using full MD and the BCA-MD. In this case of the BCA-MD, simulations are performed using a fixed threshold energy of 250 eV, i.e., well above the range of validity of the BCA in Fe and in W.

4.2.1. Case of Fe

In Fig. 3 we show the average number of Frenkel pairs (FP) along with the standard deviation obtained with the BCA-MD method as a function of the PKA energy. As a reference, the number of FP obtained by full MD calculations is also shown. The figure evidences that the BCA-MD method predicts with an excellent accuracy the number of SIA and V that form during collision cascades in a wide range of PKA energies.

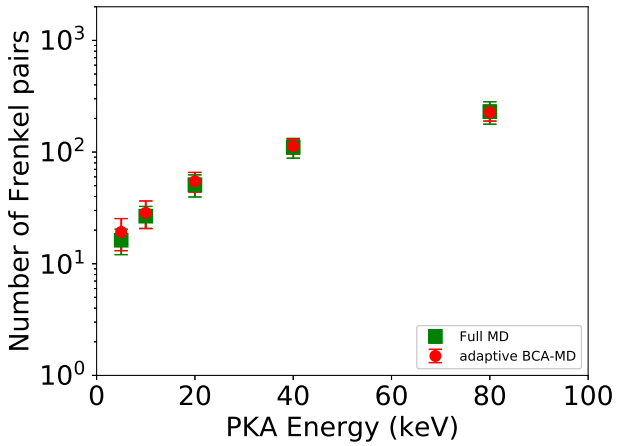

Figure 3: Comparison between the number of Frenkel pairs obtained by the BCA-MD method (red circles) and full MD calculations (green squares) as a function of the PKA energy.

Figures 4 and 5 where we show the fraction of SIAs and Vs agglomerated into clusters at the end of the cascade, demonstrate that the BCA-MD also predicts very well the formation of clusters of point defects during the cascades. Clearly, the agreement between the BCA-MD and full MD calculations is very good.

In addition to the comparisons performed in previous sections, we simulated collision cascades in Fe for a PKA energy of 500 keV in the high-index direction $\langle 135 \rangle$. Since full MD calculations would be prohibitive for this PKA energy, results obtained with the BCA-MD method were compared to data found in the literature. We found that the average number of FPs predicted by the BCA-MD ($n_{FP} = 1565$) for the PKA energy of 0.5 MeV is in very good agreement with the result obtained by Zarkadoula *et al.* ($n_{FP} = 1450$) using full MD calculations for the same energy.

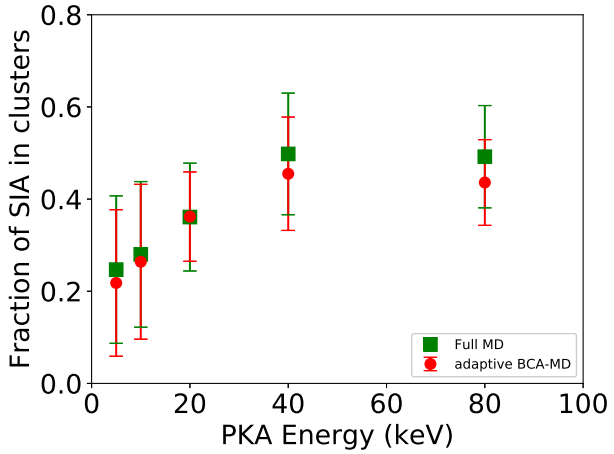

Figure 4: Comparison between the fraction of SIA in clusters obtained by the BCA-MD method (red circles) and full MD calculations (green squares) as a function of the PKA energy.

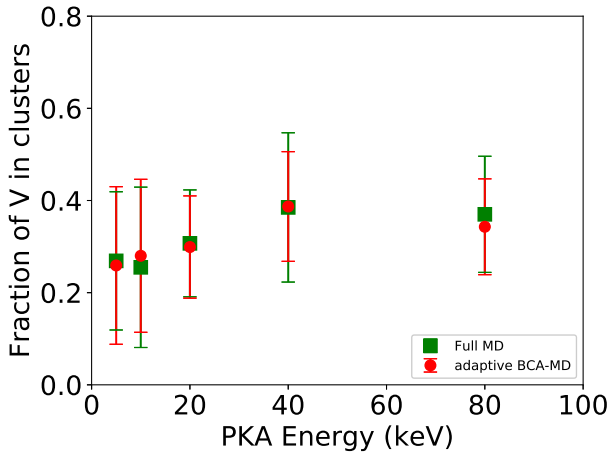

Figure 5: Comparison between the fraction of V in clusters obtained by the BCA-MD method (red circles) and full MD calculations (green squares) as a function of the PKA energy.

4.2.2. Case of W

5. Speedup of MD calculations using the BCA-MD

In the previous section we demonstrated that the BCA-MD method reproduces with a very good accuracy and in a broad range of PKA energies, the

different aspects of the collision cascade evolution in comparison to what is predicted by full MD calculations. In this section, we shall demonstrate that the adaptive BCA-MD method achieves a significant acceleration of MD calculations. To do so, we quantified the speedup factor achieved by the BCA-MD for the different PKA energies as follows:

$$speedup = \frac{\overline{cpu(MD)}}{\overline{cpu(BCAMD)}} \tag{2}$$

where $\overline{cpu(MD)}$ and $\overline{cpu(BCAMD)}$ are the average CPU times achieved by the MD and the BCA-MD, respectively, obtained over 30 cascades. The CPU time necessary to compute each cascade was measured for a physical time of 15 ps. For each PKA energy case, the same number of processors was used in full MD calculations and for BCA-MD simulations to measure the CPU time.

Here, it must be noted that the speedup calculated is not absolute but depends to a certain extent on the number of atoms that were used in full MD calculations, as the speedup is calculated taking as reference (see Eq. 2) the computational effort corresponding to full MD calculations. However, for each PKA energy, the MD cell dimensions are not arbitrary but were chosen for each PKA energy such that the cascades do not reach cell boundaries of the MD box in order to avoid interaction with itself. In particular, in the case of Fe, it is well-known that collision cascades can divide into various sub-cascades[35] oriented in different directions. As a consequence, large MD simulation volumes are necessary to contain the cascades, especially for large PKA energies.

The resulting speedup achieved by the BCA-MD with adaptive volume is shown in Fig. 6 for each PKA energy. As we can see, the higher the PKA energy, the higher the speedup achieved. For instance, for a PKA energy of 80 keV in Fe, the acceleration factor of simulations is already higher than 30 with respect to full MD calculations. These results clearly demonstrate that the BCA-MD method with adaptive volume is especially well-suited to investigate high-energy collision cascades in solids as it considerably accelerates MD simulations.

For comparison, we also show in Fig. 6 the speedup that is achieved by

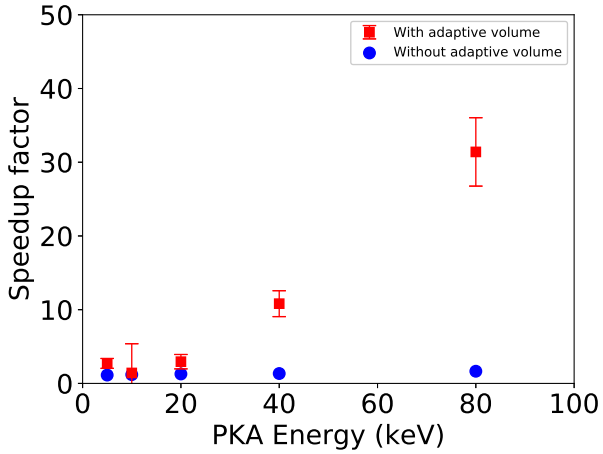

Figure 6: Speedup achieved by the BCA-MD method with adaptive volume as a function of the PKA energy (red squares). The speedup achieved by the BCA-MD without adapting the MD volume is also shown for comparison (blue circles).

the BCA-MD when the MD volume is *not* adapted, i.e., when using the same number of atoms in the system as in full MD calculations. Clearly, the speedup achieved when the cascade obtained using the BCA is simply transferred to a MD cell without adapting the volume, is marginal. This demonstrates that the computational effort saved by simulating first stages of the cascades with BCA, is in fact minor. The BCA-MD method only achieves a significant acceleration of MD simulations when the volume of the MD cell, i.e., the number of atoms in the system, is adapted and optimized using the cascade obtained by the BCA.

For the collision cascades of 0.5 MeV it was not possible to explicitly calculate the speedup achieved by the BCA-MD since simulating these cascades with full MD would have been prohibitive. Indeed, as Zarkadoula *et al.* reported in their work[27], simulating such high-energy cascades in Fe with MD up to a physical time of 40 ps, required in average 24 h of calculation using 60000 cores of the HECToR supercomputer[41]. In the case of the BCA-MD method, each simulation only required in average 96 min of computational effort using 2880 cores of the HPC Marconi[42] to reach the same physical time.

Assuming a similar efficiency between the processors of the HECToR and the Marconi supercomputers, this corresponds to a speedup factor of 312. Clearly, the BCA-MD method with adaptive volume achieves a considerable acceleration of MD calculations to simulate high-energy collision cascades. In addition, the method significantly reduces the number of processors necessary to perform the numerical simulations and hence, the power consumption that is inherent to the functioning of the processors.

6. Conclusions

In this work, we have developed a combined BCA-MD method to accelerate MD simulations in the case of high-energy collision cascades in solids under irradiation. This method simulates first stages of the ballistic phase of the displacement cascade using the BCA. During BCA simulations, each atom in motion is stopped when its kinetic energy falls below a threshold energy fixed in advance. This threshold energy must be larger than the kinetic energy corresponding to the velocity of sound in the material, limit below which the BCA breaks down due to simultaneous collisions that are not accounted for by the BCA. Then, the data obtained by means of the BCA, namely, the coordinates of the vacancies, the coordinates and the velocity vector of atoms in motion and the phononic energy transferred to lattice atoms, are introduced as input in MD, which simulates last stages of the cascade.

We have demonstrated that the cascade obtained with the BCA can be transferred to the MD disregarding the time at which each AIM has been stopped. During this time interval, AIMs have an hypersonic velocity and the shock wave created individually by each AIM does not have time to interfer with the rest of the cascade.

Taking adavantage of the information obtained with BCA calculations, we have developped a method that allows predicting in advance the volume of the MD cell necessary to simulates last stages of each cascade. This is achieved by taking into account that, at the end of the BCA simulation, AIMs have

a relatively low kinetic energy and the volume of the cascade is not expected to significantly increase during MD simulations. The numbers of atoms in the system is thereby strongly reduced and adapted for each cascade, instead of using a large and constant simulation volume as is usually done in full MD calculations. This significantly reduces the number of Newton equations to solve and hence, the computational effort of MD simulations.

The results obtained with the BCA-MD method with adaptive volume are in very good agreement with those obtained with full MD calculations. The BCA-MD predicts very well in a broad range of PKA energies the different phases of the collision cascade, the final number of Frenkel pairs, the fraction of SIAs and Vs in clusters and their size distribution.

By comparison of the CPU time of BCA-MD and full MD simulations at different PKA energies, we have showed that the BCA-MD with adaptive volume achieves a considerable speedup of MD simulations. It has been found that the speedup increases with the PKA energy and a speedup value higher than 30 has been obtained for collision cascades in Fe with PKA energy of 80 keV. By comparison with MD calculations found in the literature, we have determined that the speedup achieved by the BCA-MD with adaptive volume for PKA energies of 0.5 MeV in Fe is approximately 312. MD simulations that required 24 h of calculations using 60000 cores on a supercomputer could be achieved with the BCA-MD in only 96 min with only 2880 cores.

We believe the BCA-MD method with adaptive volume will pave the way towards exploring the formation of defects in solids under high-energy irradiation conditions, which until now was prohibitive to MD calculations. The reduced computational effort needed to simulate high-energy collision cascades in solids with the BCA-MD method with adaptive volume will not only facilitate the investigation of atomistic mechanisms that take place at high energy but will also contribute to obtaining a larger statistics. The database of cascades thereby obtained with the BCA-MD will be useful to simulate the subsequent long-term evolution of defects in solids under irradiation by means of kinetic models based on a kinetic Monte Carlo approach or the Rate Theory. In addition, the

BCA-MD method strongly decreases the number of processors necessary to perform the numerical simulations and the power consumption associated to the functioning of processors necessary.

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8. Data availability

The raw/processed data required to reproduce these findings cannot be shared at this time due to technical or time limitations.

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