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Historical review of computer simulation of radiation effects in materials

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ABSTRACT

In this Article, I review the development of computer simulation techniques for studying radiation effects in materials from 1946 until 2018. These developments were often closely intertwined with associated experimental developments, which are also briefly discussed in conjunction with the simulations. The focus is on methods that either deal directly with the primary radiation damage generation event, or with such defects or phase changes that typically occur due to radiation. The methods discussed at some length are, in order of historical appearance: Reaction rate theory or rate equations (RE), Monte Carlo neutronics calculations (MCN), Metropolis Monte Carlo (MMC), Molecular Dynamics (MD), Binary Collision Approximation (BCA), Kinetic Monte Carlo (KMC), Discrete Dislocation Dynamics (DDD), Time-Dependent Density Functional Theory (TDDFT), and Finite Element Modelling (FEM). For each method, I present the origins of the methods, some key developments after this, as well as give some opinions on possible future development paths.

Contents

1. Introduction

In this Article, I review the development of computer simulation techniques for studying radiation effects in materials. The topic of

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"radiation" is in this article understood as ionizing radiation or atomic collision processes, i.e. effects of particles with energies high enough to cause ionization and/or permanent defect production in solid materials (i.e. effects of visible light radiation are excluded). In general, the study of radiation effects of course predates the existence of electronic computers and even mechanical computers. The first report of scientific study of radiation effects can be considered to be from Grove in 1852 [1], and the history of modern physics was closely related to the development of radiation effects science [2–7].

Study of radiation effects also had a profound influence on the much broader field of computational science, as the very first computer simulations ever performed in any field of science, were on radiation effects. Also, the developments on radiation effect simulations were often closely intertwined with experimental developments, and relevant experiments are also briefly mentioned in conjunction with the simulations.

The focus of this article is on methods that either deal directly with the primary radiation damage generation event, or with such defects or phase changes that typically occur due to radiation, but less often in near-equilibrium materials processing. General introductions to computer simulation methods in physics are given in several books, e.g. Refs. [8–10], however, in this article we focus on radiation-relevant methods. For this topic, also several books have been previously written (e.g. Refs. [8,11,12], however, these did not deal with all of the methods discussed in this review article.

Each method is presented in a separate section, organized as follows. At first I give a very brief summary of the basic idea of the method is given, with references to review articles or books where much more detail is given. Then I present the origins of the method are given, with an attempt to provide the original scientific reference to each method. After this, instead of an attempt at a comprehensive review, I present a few key milestones in the method development, up to the present date. I also give a personal, and necessarily partly subjective, opinion on the outlook for the use of the methods in the future. For those methods which are typically run with a few well-established computer codes, I also mention these.

The methods discussed at length are, in order of historical appearance: Rate theory or rate equations (RE, section 3), Monte Carlo neutronics calculations (MCN, section 4), Metropolis Monte Carlo (MMC, section 5), Molecular Dynamics (MD, section 6), Binary Collision Approximation (BCA, section 7), Kinetic Monte Carlo (KMC, section 7), Discrete Dislocation Dynamics (DDD, section 9), Density Functional Theory (DFT, section 10), Time-Dependent Density Functional Theory (TDDFT, section 11), and Finite Element Modelling (FEM, section 12).

While preparing the article, I also considered the crystal plasticity (CP) [13] and phase field modelling (PFM) [14] methods. The number of works on these methods and irradiation using the same search criteria as for the other methods was, however, relatively small, so that I considered it premature to include them separately in a historical review (some of the CP works are included in the FEM statistics, as the methods are related). Their use and importance for studies of radiation effects is, however, likely to increase in the coming years.

It is important to realize that many of these methods are in much wider use outside the radiation effects community. In particular, molecular dynamics is used very extensively in the general chemistry and biophysics communities, and density functional theory both in chemistry and materials physics. The finite-element method is again very widely used in continuum mechanics and engineering. As a simple numerical comparison of the relative importance of radiation effect studies, in 2017 about 14 000 Web of Science-indexed publications were published related to either molecular dynamics or density functional theory. Out of these, about 500 were also related to radiation effects (purely coincidentally, in 2017 the numbers are about the same for both methods). In other words, for these methods, the radiation effects studies are only about 3.5% of the total.

I note that the topic of the origin of these simulation methods is interesting not only for radiation effects specialists, but also for the development of computational physics and numerical mathematics in general. Examples of this are given for some of the methods below.

In the remainder of the article, for the methods listed above, I give a very brief description of how the method works is given; for each of the methods, there are textbook-length treatments available, so giving a comprehensive description is not possible in a limited-length review article. For each method, my best knowledge of their history is given, followed by some highlights of their development over the years. The total number of publications underlying the data on the methods and radiation in Fig. 3 is 19600, and I do not attempt a comprehensive review of this vast body of work.

At the end of the article, there is also a general discussion about how the use of the methods has developed over the years, and some general outlook for the future.

2. Overview of physics and methods

In an attempt to give a reader a view how the different methods relate to each other, I first give a very brief overview of radiation effects, linking the physics stages to different simulation methods. Other articles in this anniversary volume discuss the physics of the different stages in greater detail. Radiation effects physics is also discussed at much wider extent e.g. in Refs. [12,15–17]. This section is organized as the frames in Fig. 1, which are referred to in the following with uppercase letters A-F. The methods relevant to each stage are mentioned briefly with the abbreviations here, while the detailed method descriptions are given in the following Sections 4–12.

A) In the bulk, a radiation damage event is initiated by a passing high-energy particle. This may be a high-energy (100's of keV's or MeV's) ion, neutron or electron. The passing particle occasionally collides strongly with an atom in the material. If the energy transfer to this *primary knock-on atom* (PKA) exceeds the threshold displacement energy [18,19], it starts moving ballistically between other lattice atoms. It will in turn collide with other atoms (secondary knock-on atoms), and so on. The sequence of collisions is called a *collision cascade*. This initial stage is not a thermodynamic system, since the time scale of the high-energy collisions $\sim$ 10 fs) is much shorter than the lattice vibration frequency of solids $\sim$ 300 fs [20]).

The motion of the high-energy particle can be treated with the MCN method, if it is a neutron, and the BCA or MD if it is an ion. The energy loss to electronic excitations (*electronic stopping*) can be treated with either traditional empirical electronic stopping theories or tabulations [21–23] or with TDDFT methods. The collision cascade itself can be treated by BCA or MD simulations.

B) After about 0.2 ps, both BCA and MD simulations show that all the recoiled ions have slowed down to kinetic energies below the threshold displacement energy, $\sim$ 10 eV. At this stage, two outcomes are possible. In case the material has a low density [8,24], the knock-on atoms move largely independent of each other. In this case, the damage remaining is

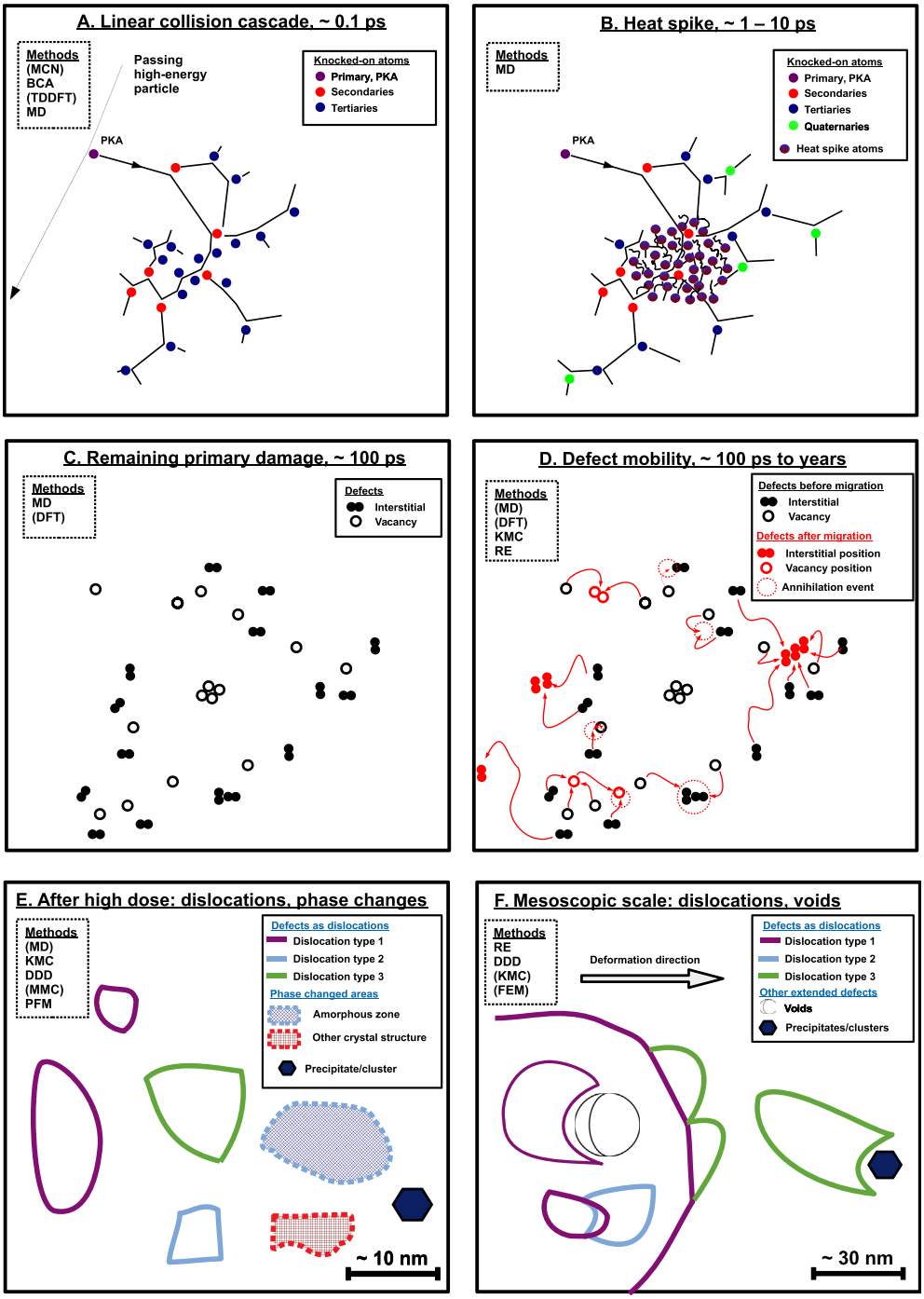

Fig. 1. (Color online) Schematic description of the time scales and physical processes occurring during irradiation of bulk materials. Frames A-C indicate a single primary damage process, D the ensuing defect mobility. E-F illustrate high-dose damage, i.e. what may happen when multiple primary damage events overlap. The dashed boxes indicate which simulation methods are relevant to model which time scale. Abbreviations are MCN = Monte Carlo neutronics calculations, MMC = Metropolis Monte Carlo), MD = Molecular Dynamics, BCA = Binary Collision Approximation, KMC = Kinetic Monte Carlo, DDD = Discrete Dislocation Dynamics (DDD), DFT = Density Functional Theory, TDDFT = Time-Dependent DFT, RE = Rate equations, FEM = Finite Element Method, PFM = Phase field modelling. When the method is in parenthesis, this indicates that the method can describe only some aspect of the problem, as discussed more extensively in the main text. Figure is original work for this article. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

mainly single vacancies and interstitials, or small clusters of these. In dense materials, however, the sequence of collisions typically occur so close to each other that after about 1 ps, there are regions of atoms with kinetic energy around ~ 1 eV right next to each other undergoing complex many-body collisions.

MD simulations have shown that the kinetic energy distributions of these atoms is a Maxwell-Boltzmann one, i.e. the system can be considered to be in a thermodynamic liquid-like state [25]. This state is called a *heat spike* or *thermal spike* or *displacement spike*. Because the system is clearly out of thermodynamic equilibrium, and the processes are so rapid that thermal equilibration

with the surroundings does not have time to occur, the only correct way to treat the system is by MD simulations in the microcanonical thermodynamic ensemble. In other words, MD should be ran as direct solution of the equation of motion without any temperature or pressure control in the collisional region.

C) After about 10–100 ps (depending on thermal conductivity of the material), any collision cascade has cooled down to the ambient temperature, leaving behind some damage.

The same MD simulations that can be used to describe the cascade in stage 2 will somehow describe also the damage formation. However, there are major methodological uncertainties in what the exact form of the damage produced is [26] due to uncertainties in how well the interatomic potentials describe the defect energetics. DFT is much more reliable in this regard, and hence can be used to calibrate or discriminate interatomic potentials.

D) After the single *primary damage event*, i.e. stages A)-C), the defects produced are mobile on some time scale. This mobility is determined by equilibrium thermodynamics (except if an additional cascade happens to hit the same region of the material).

In practically all cases, MD is too slow to describe this mobility, however, either DFT or MD can be useful in determining the diffusivity of individual defects. Both methods can be used to determine the migration energy barrier (typically using the nudged elastic band (NEB) method [27]) for both point defects and also extended defects, at least if these are not too complicated. Also the migration prefactor can be determined, either from analysis of vibration modes [28] or by dynamic simulations [29]. After the migration properties of all relevant defects are known, either KMC or RE methods can be used to simulate their diffusion.

E) In many cases of practical interest, the radiation fluence is so high that any given region in the material is affected by several recoils. In non-amorphizable metals, the damage after a high dose almost invariably is in the form of dislocation loops [30], and sometimes also voids [31]. In semiconductors, even a single recoil event can produce disordered ('amorphous') zones [32,33]. Hence, under prolonged irradiation it is natural that these build up to for increasingly large amorphous zones, which may lead finally to complete amorphization [34–36]. In some ceramics, also phase transitions from one crystalline phase to another have been observed [37].

The formation of dislocations and amorphization due to damage buildup can be readily simulated with MD [38,39]. For longer time scale damage buildup, KMC or RE's are appropriate tools, and for the dislocation mobility, DDD. The MMC method may be useful for examining relative phase stability.

F) After really prolonged irradiation, or if the irradiated system is also under a mechanical load, in metals the dislocation structures tend to grow, and under stress may be mobile. The only method that can certainly simulate dislocation mobility explicitly on the mesoscale is DDD, although also KMC after extension with elastic interactions may give this possibility in the future. FEM or RE's with suitable parametrization of materials properties that depends on dislocation concentration can be used to simulate a material with dislocation in an averaged manner. The RE approach can also be very useful for simulating void and He bubble growth.

3. Reaction rate theory or rate equations (RE)

The term 'reaction rate theory' or 'rate equations' is in general used to mean solving continuum differential equations of defect densities to simulate their diffusion. Thus the method is in principle as old as diffusion theory itself, dating back to the 1850's [40]. The rate theory approach [41–44] has the advantage that it can span very large time, spatial, and energy ranges, from defect production in cascades to changes in macroscopic properties. The disadvantage is that it only gives average defect concentration information. In principle the KMC approach (section 8) could do the same including descriptions of each individual defect. However, the RE approach is, at least if limited to a one-dimensional space description, many orders of magnitude more efficient than KMC, and hence remain still in use. The methods do share the common characteristic that the inputs to RE's can be the same experimental, MD or DFT data as to KMC.

The approach has been used under several different terms, since solution of differential equations for diffusion can be done and called by many names. The publication statistics in Fig. 3 is shown for the terms "rate theory" or "rate equations", but is likely an underestimation due to the naming differences. For defects in solids, rate theory was used without electronic computers for instance by Cottrell to examine how carbon atoms form the "Cottrell atmosphere" around dislocations to slow them down [45]. Somewhat later, in 1957, Waite used rate equations to examine diffusion under a radiation boundary conditions [46], and the following year Dienes and Damask used it to examine radiation enhanced diffusion [47]. Dworschak considered in the 1960s different kinds of trap models with analytical solution of rate equations [48].

The origin of the use of rate theory *computer* modelling specific to radiation effects occurred around 1970, according to a review article by one of the pioneers in the field, Brailsford [42], who cites a paper from 1970 by Wiedersich as the original computer simulation one [49]. Also from other sources, it is clear that the field had a surge of activity starting in 1970–1971, see Ref. [41] and references therein. This was mainly motivated by the desire to understand the recently discovered phenomena of void swelling and radiation induced segregation in structural alloys (for proposed fast breeder reactor cladding/duct applications).

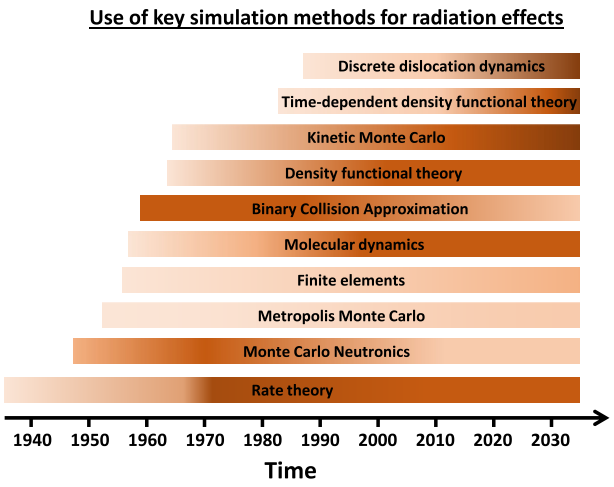

Fig. 2. (Color online) Schematic description of the development in time of the use of some key methods in radiation effects, The bars start at the very first use of the method in any field of science. The color (gray) shading strength are a subjective view by the author on the relative importance of the method in radiation effects studies. Figure is original work for this article. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

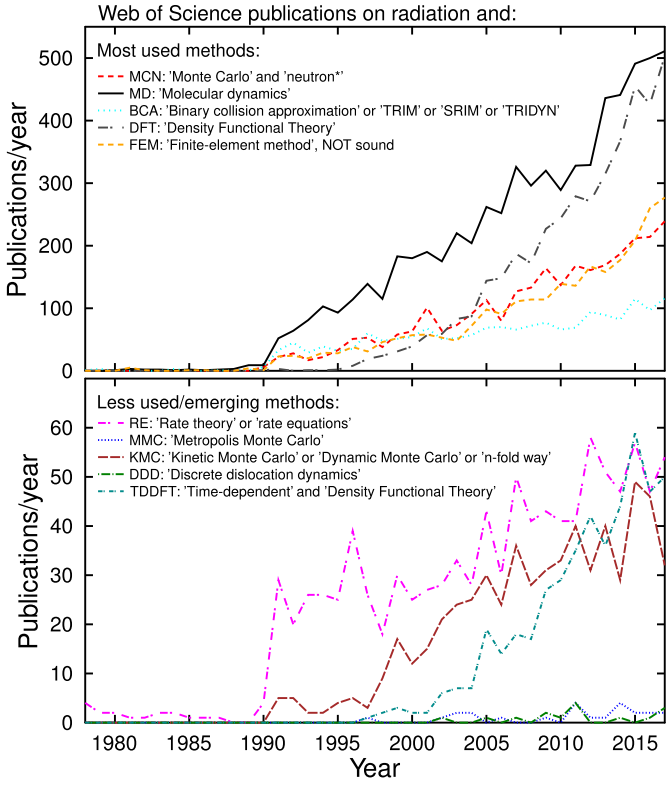

Fig. 3. (Color online) Publication statistics on the usage of different simulation methods with respect to radiation effects. The data is obtained as a search on publication mentioning each method (without the abbreviation) and the key words 'radiation* OR irradiation* OR sputtering* OR cascade*' in a Web of Science topic search on Sep 3, 2018. Note that some publications may not be exactly on ionizing radiation, e.g. the key word radiation may also give articles on solar radiation. However, a manual checking of the titles of the most recent publication indicated that at least most papers found with these keywords are related to some sort of ionizing radiation. The FEM statistics is to a large extent on light radiation, however. Note also that due to variations in naming conventions, especially some early work is missing. The data and figures are original work for this article. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

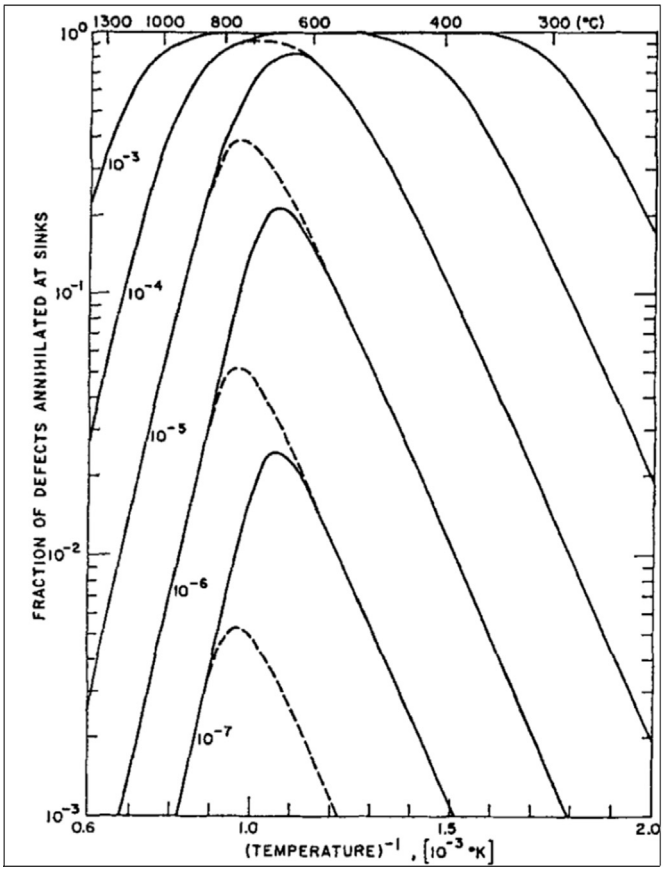

Fig. 4. Fraction of radiation defects that are annihilated at sinks as a function of temperature, as modelled by rate equations in 1972 with a model that did not include defect clustering. The different curves are different sink annihilation probabilities. From Ref. [50]. Copyright Taylor and Francis (1972).

A key point in rate theory is which defects to include and what the trap (sink) strengths are. The results are naturally sensitive to which defects are included, what the associated sink strengths are, and how they are treated [51,52]. Already in 1972, Wiedersich simulated the fraction of defects which are annihilated at sinks in Ni using rate theory as a function of the sink annihilation probability, see Fig. 4. In this early work, defect clustering was neglected. Later on, around 1990 Wiedersich considered also the role of defect clusters formed directly in cascades, and showed that if these are formed in a cascade, they become under many circumstances the dominant sinks for mobile defects [43]. In 1981 Brailsford and Bullough presented a thorough mathematical theory for how to treat the sink strengths of non-saturable defect sinks [52]. Around 2000, Gan et al. used rate theory to model loop formation in light-water reactor steels using [53]. They found that agreement with experiments was obtained only when the possibility of in-cascade interstitial cluster formation was included in the model. Similarly, the results of Katoh et al. [54] also point to the importance of cascade clusters for microstructure evolution, and more recently for Zr by Barashev et al. [55]. Singh et al. considered also the possibility that clusters produced in cascades decorate grown-in dislocation so that they cannot act as dislocation courses [56]. These results are well in line with MD simulations that show direct cluster formation in cascades (cf. section 6).

Trinkaus developed a rate theory for the nucleation of multi-component precipitates, although this was not specific to radiation effects [57].

A rate theory approach to ordering and pattern selection was developed by Walgraef et al. [58]. This approach allowed to predict the formation of ordered vacancy loop microstructures under irradiation. Brailsford and Mansur used in 1977 a rate theory approach to analyze void swelling for comparison of ion, electron and neutron irradiation conditions, concluding that one should use caution when comparing ion and neutron irradiation results [59]. Here it is worth noting that still in 2018, forty years later, the extent to which ion irradiation can be used to mimic neutron ones is being debated. Miller considered in 1979 in detail how dislocation bias (a measure of the preference for interstitial absorption at dislocations [60]) is related to the point defect relaxation volumes, and hence swelling [61].

Odette et al. used in 1988 a rate-theory approach in an attempt to explain the low swelling of ferritic martensitic steels compared to austenitic ones, and attributed it to high self-diffusion and low helium generation rates [62]. It is interesting to compare this result with the MD one cited in 9, where the high radiation hardness of these steels is attributed to Cr slowing down dislocations [63]; it is not obvious whether these effects are complementary or in contradiction to each other. Golubov et al. compared void swelling in fcc and bcc metals, highlighting that differences in 1D diffusion of defect clusters can have an important effect on the reaction kinetics [64].

The rate theory approach can also be very useful for studying He

effects. In 1983 Ghoniem et al. examined He migration in Ni using analytical methods and rate theory, and raised the possibility that He migration is enhanced by migration in a He-divacancy complex. Stoller et al. implemented in 1985 a helium bubble equation of state into rate theory and calculated swelling due to the He in stainless steel based on this [65]. Somewhat later, Katoh et al. [66] studied the effects of He to dpa ration on bubble number density in stainless steels. The swelling was found to be a complex function of irradiation temperature, He/dpa ration and displacement rate. The authors concluded from this, that simple extrapolation of fission reactor damage results to fusion reactors is unlikely to be accurate.

For studying the diffusion of defects and impurities, rate theory and KMC are in principle complementary. A very thorough comparison was presented in Ref. [67], which showed that the RE and OKMC agree well for irradiation conditions that produce a high density of defects (lower temperature and higher displacement rate) and for materials that have a relatively high density of fixed sinks such as dislocations, see Fig. 5.

Rate equations are also widely used to simulate the fusion reactor plasma-material interactions [68–71].

As a final note on rate theory, we mention that the formation of ordered nanostructure arrays on surfaces ("ripples") [72–75] has been described with an differential equation approach mathematically somewhat similar to the defect rate theory. This was first done by Sigmund [76] and later Bradley and Harper for sputter-induced ripple formation [77]. More recently, strong evidence has emerged that at least in amorphous materials, ripple formation is in fact dominated by atom redistribution [78–81].

4. Monte Carlo neutronics calculations (MCN)

The MCN method is very interesting in that its development was a milestone in all of electronic computing; the very first computer simulation ever was a neutronics calculation done by Fermi in 1946. The first declassified publications on the topic appeared in 1948 and 1949 [82,83], but a much later historical paper by Metropolis revealed the first calculations were already done in 1946 on the first electronic computer, the ENIAC [84]. The calculations were about following neutron passage in fissile matter based on random initial positions and collecting statistics. This approach still is the basis of Monte Carlo neutronics calculations.

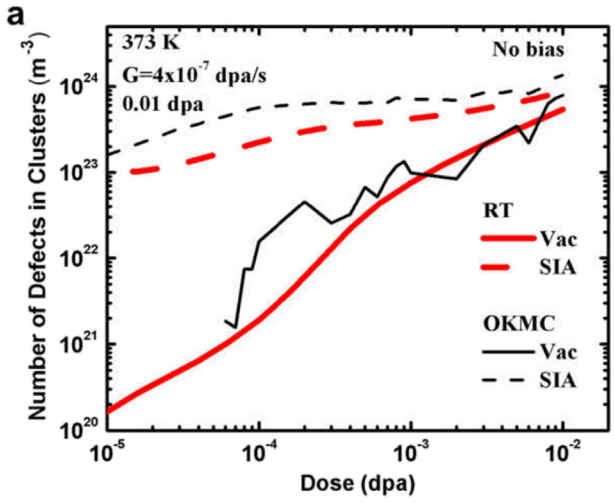

Fig. 5. Number of vacancies (vac) and self-interstitials (SIA) in clusters as a function of irradiation dose in dpa as predicted by rate theory and object kinetic Monte Carlo simulations. From Ref. [67]. Reprinted with permission from publisher. Copyright Elsevier (2008).

The same historical paper [84] also reveals the origin of the peculiar name 'Monte Carlo' for using random numbers in computer simulations. Obviously this name does not have any motivation in physics terminology. Instead, it was coined by Metropolis due to an uncle of Stanislav Ulam apparently having a gambling affliction, and the most famous casino in the world being Monte Carlo in the Principality of Monaco [84]. I note that the more scientific term "stochastic" could very well be used to describe any simulations employing random numbers, and appears to be the dominant term in mathematics. Physicists seem to prefer the term 'Monte Carlo', presumably because of no other reason than the more exciting mental images it may conjure.

After its early origins, the MCN methods have developed to be a routine and key method in design and optimization of nuclear fission power plants, with still expanding use, see Fig. 3. The publication numbers are, however, a severe underestimation of the width of the use of the method, since much of the routine MCN work in fission power plants is not published (not to mention the likely use of the approach in design nuclear device for military purposes). I do not attempt here a comprehensive review of the long history of the MCN method, but merely refer to a few highly cited papers and important codes in the field.

The first paper on MCN simulations in a regular journal were published in 1950 by Kahn, who used the method to address neutron attenuation [85]. About a decade later, Kalos introduced the use of importance sampling to speed up neutronics calculations; this method is now a standard approach in all kinds of MC simulations. Around 1970, MCN simulations were also taken into use in medicine [86].

At first, the calculations only dealt with the neutron motion, but later were extended also to be able to provide the recoil energies the atoms received (PKA in stage A in the schematic Fig. 1), thus setting a basis for calculations of neutron damage in materials [87–89]. Very recently, the damage calculations have been extended to deal with complex geometries and multiple stages of neutron transmutation [90,91].

As the MCN field matured, the solutions were incorporated into a few codes that have become dominant in the field. The likely most used code is the MCNP code developed at Los Alamos. The development of the code can be traced back to 1957 [92], and it has been updated ever since, the latest version being released in 2018 when this article is being written [93]. Another code still under active use and development is the TRIPOLI code developed most recently by Petit et al. [94]. The PHITS code by Iwase et al. is interesting in that it can also handle passage of other heavy elements developed [95]. Recently, the entirely new SERPENT code has attracted interest due to its modern speedup algorithms [96]. Many neutronics codes are only available to scientists in OECD member countries via the OECD Nuclear Energy Agency code database. MIT does publish a modern open source code OpenMOC [97].

5. Metropolis Monte Carlo (MMC)

The same Metropolis who coined the name Monte Carlo, developed together with two Rosenbluths and two Tellers in 1953 a completely different random number method for thermodynamic calculations [98]. In this approach atoms in a system are given random displacements one at a time, and the potential energy difference associated with the shift is determined. If the shift is negative (energetically beneficial), it is always accepted, and if it is positive, the shift may still be accepted with a probability decaying as a Boltzmann factor [98]. This approach leads the atomic system to an equilibrium canonical (NVT) ensemble [99]. The potential energy is obtained from interatomic potentials [100–102].

The original use of this method was to simulate melting of hard

spheres, see Fig. 6. However, the great value of the approach was that it showed that an appropriately selected weighted random sampling can be used to simulate any interacting atom system in the NVT thermodynamic ensemble [99]. Moreover, an even greater value of the approach came from the fact that the same approach can be very useful for searching for global minima of in principle any system, that can be characterized with a continuous variable to be optimized, and a temperature-like variable that characterizes the system state. This starts from an analogy with annealing in materials processing: a real system can be driven to a low-energy equilibrium state by starting with a high temperature and then slowly cooling it down to 0 K, which will optimize the $E(T)$ function. Since the Metropolis MC method simulates the *NVT* ensemble, the annealing can readily be done on a computer by letting $T \rightarrow 0$. If then any other system simulated on a computer can be characterized by something analogous to E and T, it can also be optimized with the MMC annealing approach. This has given the generalised version of the MMC method extremely wide use in statistics, where it is mostly known as Markov chain Monte Carlo [103].

For simulating radiation effects, the MMC method is by contrast used relatively little, see Fig. 3. This is because as an equilibrium simulation method, it cannot be used to simulate the highly nonequilibrium cascade conditions. However, it can be useful in simulations of materials driven first into a nonequilibrium states by irradiation, where MMC can be used to examine the phase stability and aging when these materials are driven back towards equilibrium (frame E in Fig. 1). An important example of such a case is the study of the phase diagram of FeCr, which is the key model alloy behind ferritic stainless steels. For this system, electron irradiation speeded up aging was used to show that the standard textbook phase diagram is wrong [104]. MMC simulations have been used to examine this phase stability for different interatomic potentials [105,106] (for a more detailed discussion of this specific case, see Ref. [107]).

MMC has also been used to study the stable atom configurations on sputtered surfaces [108], the balance of Cr atoms and vacancies in FeCr alloys [109], and segregation of atoms at grain boundaries [110].

6. Molecular dynamics (MD)

Molecular dynamics simulations are a way to simulate the motion of atoms in molecules or solids [111–113]. The crucial physics input to the method are the forces acting between atoms. These can be obtained either from an analytical interatomic potential (which may be the same as for the MMC method) or from a quantum mechanical calculation method, such as DFT.

Molecular dynamics was initially developed to simulate vibrations in diatomic molecules by Alder and Wainwright in 1957 [114,115], and its widest usage area is in fact in molecular and biophysics [112,116,117]. Very soon after 1957 the method was taken into use also in radiation physics. In 1960, Gibson et al. used it to simulate collision sequences in copper, and already in this very first work, found the effect of "recoil collision sequences" (RCS), see Fig. 7. This is still recognized as one of the mechanisms by which interstitials and vacancies can become separated to form stable Frenkel pairs (later works have shown that it is by no means the only one [24,118]). Very soon afterwards, MD simulations were used to examine the threshold displacement energy surface [119,120]. As a special historical observation, I note that the first paper in the Journal of Nuclear Materials with the words "computer simulation" in the title was a paper on MD simulations of threshold energies in Cu from 1978 [121].

In those days, computer capacity was of course very limited. Hence the early simulations involved only a couple o hundred atoms, had the outer atoms forced inwards, and were run with purely repulsive interatomic potentials. By current standards, this kind of simulations would be considered completely unphysical. In this regard, it is amusing to note that the MD simulation value for the average threshold energy in Fe obtained in 1964 by Erginsoy et al. of 40 eV appears to be the source of even an official ASTM standard [122]. There were several experimental values on the threshold in Fe for specific crystal directions [123–125] around 20–30 eV, but Lucasson chose in Ref. [18] to cite the MD value of 44 eV for the average. Moreover, due to this value being cited as an

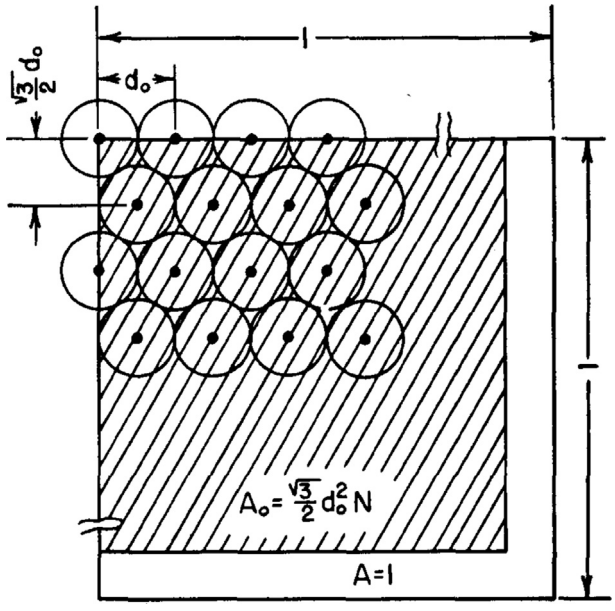

Fig. 6. Image describing simulation setup for the first MMC simulation of melting of a hard sphere system. From Ref. [98]. Reprinted with permission from AIP publishing. Copyright (1953) the American Institute of Physics.

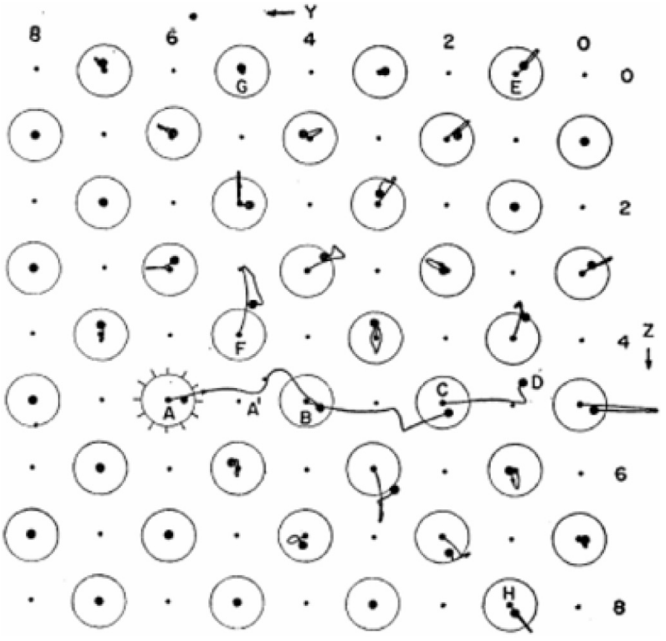

Fig. 7. Image describing the motion of atoms from the first MD simulation of radiation effects [144]. Reprinted figure with permission from [J. B. Gibson et al., Physical Review 120, 1229 (1960)] Copyright (1960) by the American Physical Society.

entry in a table that did not clearly specify the method (Table 2 in Ref. [18]), it is sometimes even confused to be an experimental value.

On the other hand, analytical potential MD simulations with much more advanced modern simulation methods actually give an average threshold that is very close to 40 eV [19]. However, DFT-MD simulations, which should be clearly more reliable than any classical potential, give a value of about 30 eV, indicating that the old value of 40 eV is in fact an overestimation [126].

The computer capacity limitation to a few hundred atoms prevented use of MD simulations for studying radiation effects by higher-energy ions for a couple of decades. However, in the 1980's computers started to become efficient enough to simulate radiation effects also at higher energies. In the early 1980's, Webb, Harrison, Garrison, and coworkers managed simulations of a couple of thousand of atoms, which was enough to simulate sputtering and pit formation at surfaces [127–129]. This lead to a long line of studies of sputtering, first in simple metals and elemental carbon [130–132], and later to more complex systems such as fullerene bombardment [133,134] and sputtering of complex organic molecules [135]. Later on, as interatomic potentials became more advanced such that they could describe chemical bonds in a reasonable way [101,136], MD simulations also started treating chemical sputtering [137–143].

When computers in the 1990's became efficient enough to simulate first tens of thousands, and later millions, of atoms, the surface simulations also could model explosive emission of atoms of atoms and cratering [145–150]. The cratering studies raised the obvious question of whether the craters formed form by the same mechanism as those on planets and moons. Aderjan and Urbassek first showed in 2000 that craters produced by single ions do not form by the same mechanism [151], but rather by flow of a heat spike liquid to the surface [146]. Slightly later, Samela and Nordlund showed that when the projectile size is increased from a single atom to an atom cluster with more than 10 000 atoms, the cratering mechanism does become the same as the macroscopic one, i.e. explosion of a high-pressure zone formed under the projectile to the surface and vacuum [152].

In 1987 Diaz de la Rubia et al. made a breakthrough for understanding bulk radiation effects, when they were able to simulate a system of more than 10000 atoms. This enabled simulating the full development of 5 keV collision cascades inside a material [153], which showed that a heat spike has an underdense core and a overdense shell, just as conceptually envisioned by Brinkman already in 1954 [154], see Fig. 8. Since this work, a large amount of work has been done on understanding bulk heat spikes in metals by MD (see e.g. Refs. [25,155–165]), basically giving all the insights on their nature described above in Section 2. However, it is important to point out that there is also direct experimental evidence for the existence of heat spikes [37,166–168].

Out of the many historical developments in defect production by heat spikes in metals, I only mention one development in more detail. The issue of how dislocation loops form has been studied to a great extent. Experiments show that at least vacancy-type stacking fault tetrahedra can form directly in collision cascades [169,170]. In 1999 Nordlund and Gao reproduced this effect in MD [171], and slightly later Nordlund et al. showed that the SFT production is strongly enhanced near surfaces [172]. I 1991, Diaz de la Rubia et al. claimed to have observed the production of interstitial dislocation loops directly by loop punching in a cascade [156], however, in 1996 the same lead author admitted that this observations was an artefact of a too short analysis time [173]. More recently, new systematic experiments of irradiated W have shown that in this very dense material, at least vacancy-type dislocation loops can form directly in collision cascades, and that simulated and experimental

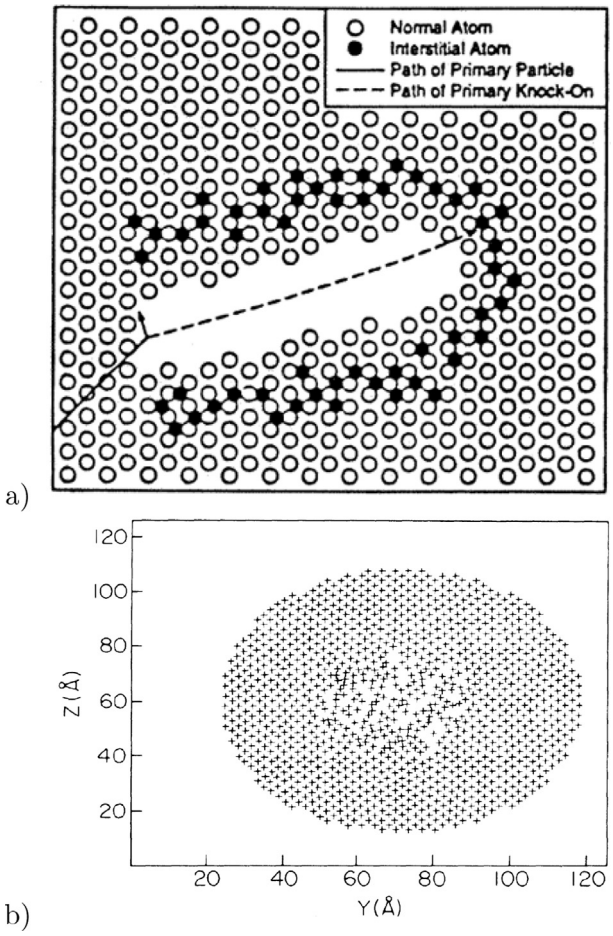

Fig. 8. Top (a): Original conceptual picture of a heat spike from 1954 by Brinkman et al. [154]. Bottom (b): first image showing underdensification in a heat spike in MD simulations by Diaz de la Rubia et al. [153]. a) Reprinted from Ref. [154] with permission from the American Institute of Physics. b) Reprinted figure with permission from [T. Diaz de la Rubia et al., Physical Review Letters 60, 76 (1987)]. Copyright (1987) by the American Physical Society.

cluster size distributions agree well with each other [168], see Fig. 9.

The inclusion of electronic effects (electronic stopping [21,22] and electron-phonon coupling [174]) in the MD simulations has a somewhat curious history. Some of the very first MD simulations did already include electron-phonon coupling [175,176], and several groups have routinely included at least electronic stopping since the mid-1990's [24,177–185] in numerous materials. However, for some reason the groups working on damage in Fe have generally not included electronic stopping [118,159,186]. At high energies, comparison of range profiles with experiments [183,187–189] show that the electronic stopping can be very well treated as a frictional force (how to include a frictional force can be included in MD is well established [113]). For lower ion energies, the electronic excitations start to couple to the phonons and one enters the electron-phonon regime. It is perfectly possible, and even relatively straightforward to include also lower-energy electronic effects in heat spike simulations. However, the exact way how the electron-phonon coupling should be done, and/or what the associated parameters in the model should be, remains unclear in the heat spike regime to this day [190–193]. The TDDFT method holds great promise for giving further insights on this (cf. section 11).

MD simulations of radiation effects have of course not been solely related to metals. Numerous studies have been performed on

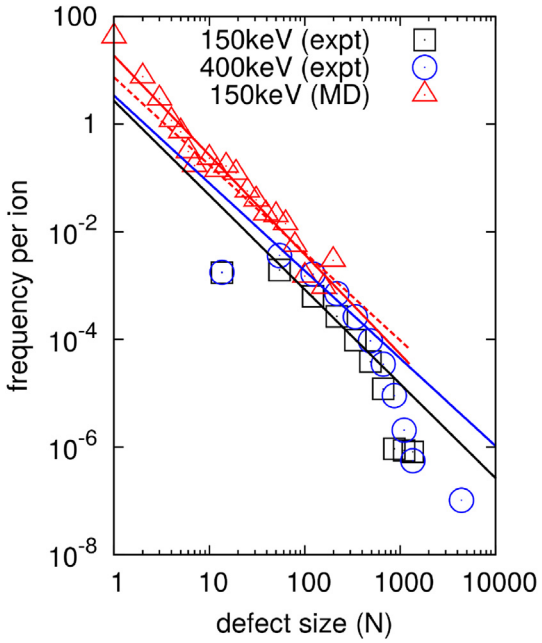

Fig. 9. Good agreement between experimental and simulated cluster size distribution scaling power law exponents for 150 keV and 400 keV W ion irradiation of W thin foils [168]. The *y* axis shows the frequency of occurrence of defect clusters of the given size. Reprinted with permission to be obtained. Reprinted with permission from publisher. Copyright (2015) IOP publishing.

cascade damage in Si, Ge, and other semiconductors [194–201]. These generally all reproduce the key difference between damage in metals and semiconductors: while elemental metals remain crystalline, irradiation of semiconductors leads to production of first amorphous pockets [202] and later on full amorphization [38,203]. The basic reason to this dramatic difference in behaviour is the much higher recrystallization velocity of elemental metals [24,204].

Radiation effects in ceramics have also been examined extensively by MD, see e.g. Refs. [205–217]. These generally show that the behaviour is complicated and somewhere between metals and semiconductors: some ceramic materials amorphize readily, while others do not [210,211].

The early MD simulations cited above were, out of rather obvious reasons, considering either bulk materials, or a smooth surface. However, as nanoscience became the rage in the 2000's, a large amount of MD simulations studies have also considered irradiation of nanostructures. Due to the large fraction of surface in these, their response to radiation can be quite different from that in the bulk. The damage is naturally enhanced at the surface [218], and the sputtering yield can lead to truly massive nonlinear enhancement of sputtering yields [219].

In carbon nanostructures such as graphene and nanotubes, the defects may be very different from those in a bulk material [220,221]. It is interesting to note here that many of the radiation effects in carbon nanotubes were first predicted in simulations and then confirmed by experiments. For instance, MD simulations predicted that there are no proper interstitials in carbon nanotubes, but a 2-fold bonded adatom is a rapidly-moving defect analogous to the interstitial in bulk [222]. This prediction was confirmed by experiments observing rapidly moving surface atoms in graphene [223].

Extensive reviews of radiation effects in nanostructures are available e.g. in Refs. [224–226] and we refer the reader interested in more details on irradiation of nanostructures to these.

A fairly recent development is the MD simulation of high-dose irradiation effects by simulating numerous overlapping cascades. In Si, Ge, GaAs and SiO_2 such simulations are in good agreement with the experimental amorphization doses and damage buildup [38,203,214]. Also the amorphization of Ge nanoclusters embedded in silica matrices have been well reproduced [227]. However, for GaN such MD simulations fail in describing the complex experimentally observed 3-stage amorphization behaviour [199]. In metals, simulations of overlapping cascades can reproduce fairly well the experimentally observed difference between elemental Ni and Ni alloys [228,229]. These good agreements are remarkable considering that the overlapping damage MD simulations overestimate the experimental dose rates by many orders of magnitude.

Due to its versatility, MD based on either classical or quantum mechanical interactions, will certainly remain a key method of radiation effect studies for a long time to come. Accelerated MD schemes have already extended the time scales that can be handled to also cover defect migration partly (part D in Fig. 1) [230–236]. The uncertainties with interatomic potentials will likely be reduced significantly by machine-learning potentials [237–240]. However, we note that their current construction schemes do not include short interatomic distances, and hence their development needs to be extended to the repulsive potential region before they can be reliably used in radiation effect simulations.

For a long time, the radiation effects MD simulations were carried out with a wide range of different codes that were developed with one group, or a few collaborating groups. These include e.g. the SPUT code developed by Harrison, Garrison et al. [241,242], the MOLDY suite of codes developed by Finnis et al. originally at HARWELL [243,244], the MOLDYCASK code based on MOLDY developed by Diaz de la Rubia et al. at LLNL [245], the DYMOKA code by Becquart et al. [246] and the PARCAS code by Nordlund et al. [247]. Since about 2010, the dominant MD code for simulations of hard condensed matter in general has started to be the LAMMPS code developed at Los Alamos [248]. Although originally the code was not particularly well suited for radiation effects, more recent versions do support high-energy repulsive potentials and have a combined electronic-stopping-electron phonon coupling model. Hence it seems that LAMMPS is becoming the dominant MD code also for radiation effects studies.

6.1. MD in recoil interaction approximation (RIA)

The recoil interaction approximation (RIA) is a special variety of MD for simulating ion penetration profiles efficiently. In this approach, all interactions of an ion or recoil with lattice atoms are treated according to the molecular dynamics algorithm, but lattice atom-lattice atom interactions are not calculated. Moreover, the lattice is always generated around the ion/recoil as it moves forward, making it enough to have only a few hundred atoms in the simulations.

The MD-RIA was first developed by Karpuzov and Yurasova in 1971 [249], but the use of the method did not continue in that group. It was then later reinvented by Nordlund [178], whose group took it into wide use. Another implementation was made by Beardmore et al. [188]. The MD-RIA approach has proven to be useful especially for understanding channeling effects, both the reduction of electronic stopping in channels [179,183,189,250] and for systematic analysis of in which crystal directions channeling takes place, using so called 'channeling maps' [251].

MD-RIA is available in the open source MDRANGE code [252,253].

7. Binary collision approximation (BCA)

In the binary collision collision approximation, the motion of an ion or recoil in a material is treated as a sequence of independent binary collisions. For each collision, the classical scattering integral is solved to give the scattering angle and energy loss to sample atoms. This allows for a very efficient treatment of ion passage in materials (frame A in Fig. 1).

The BCA approach was first developed by Robinson and Oen in 1963 [254]. Even though they authors used, by current standards, fairly crude interatomic potentials, they obtained remarkably good agreement with experimental range profiles, see Fig. 10. Very soon after this initial study, the BCA approach was extended to be able to also deal with ions moving in a crystalline structure. These simulations discovered the ion channeling effect [255,256], which was soon afterwards confirmed experimentally [257,258]. This likely is one of the first cases ever where an atomistic computer simulation successfully predicted a physical effect.

The BCA simulations can be further categorised by how they treat the structure of the material in which the ion moves:

1. The by far most used approach is to select the position of the next colliding atom randomly, in a Monte Carlo approach [22,254,259]. This approach is set up to ensure the material has the correct density, but otherwise has no information on the structure of the material. Naturally, it treats ion passage in a fully amorphous material.

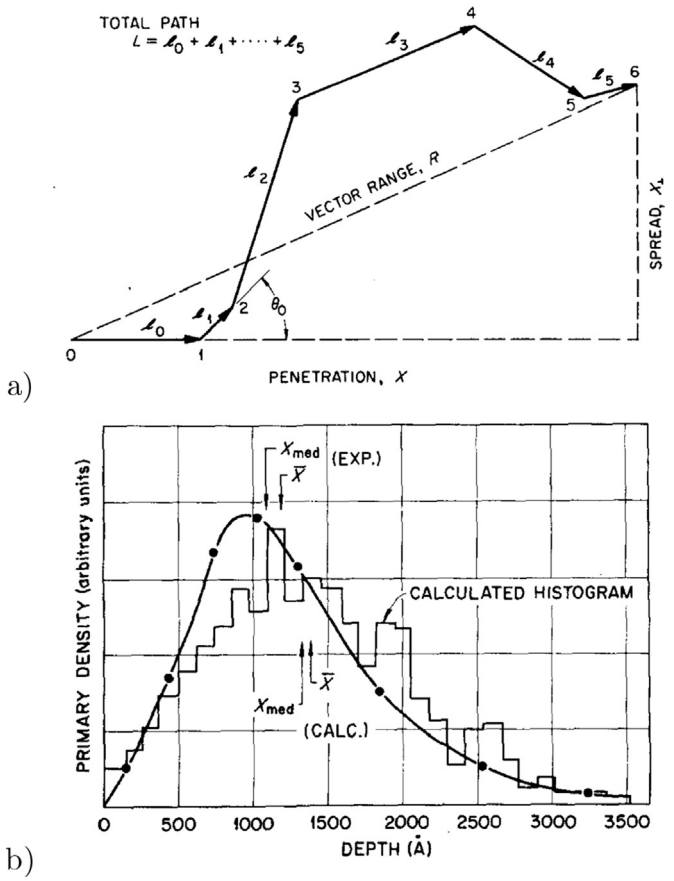

Fig. 10. Top (a): Original picture of a sequence of binary collision and the associated range concepts [254]. Bottom (b): Reasonable agreement with experimental range profiles obtained in the very first BCA simulations, for 60 keV Na ion in Al. [254]. Reprinted with permission from AIP publishing. Copyright (1963) the American Institute of Physics.

2. It is also possible to set up BCA for ions moving in a perfect crystal [255,256,260–262], possibly with thermal displacements obtained from the Debye model [263].
3. Very recently, an approach was introduced where BCA is run on arbitrary atoms positions read in from a file, existing for the entire penetration depth of the ion [264]. For typical ion ranges in the 10–100 nm range, doing this requires millions to hundreds of millions of atoms, which is entirely feasible to handle with modern computer memory capacity. This approach allows taking complex defective structures from MD and simulating either ion passage or backscattering from these positions [214,229].

Another important distinction in BCA methods is whether they are run for the ion only, or whether also the recoils are followed. The latter, so called 'full cascade' mode can describe linear collision cascades fully. Such a mode is implemented in two of the most used BCA codes, MARLOWE [260] and TRIM/SRIM [22,265,266].

In spite of the basic idea of binary collisions, there are actually varieties of BCA where several binary collisions are treated simultaneously [260,267]. This may be necessary to treat some channeling conditions correctly, but the way to implement "multiple binary collisions" is not unique, and different approaches do not give quite the same results [267,268].

After the start, the BCA approach became a very widely used method for simulating range profiles, sputtering, and energy deposition in materials, see e.g. Refs. [262,269–278]. Most recently, its use has been extended to nanostructures [279–281].

When the MD-RIA simulations became available, it also became possible to test the lower-energy limit of BCA. Roughly speaking, for heavy ions, BCA is valid down to energies of a few 100 eV, while for light ones it may be fairly accurate even down to energies of a few tens of eV's [282,283].

The original BCA code, MARLOWE [260], is still in active use [267,276,284,285], i n spite of being originally written in the 1960's in a very peculiar Fortran variety known as Mortran. However, BCA is by far most used in the Stopping and Range of Ions in Matter (SRIM) code, which has an executable that is freely available has a very easy to use graphical user interface for Windows systems [23,266]. SRIM is originally based on the TRIM code [22,265], which also has other derivatives: TRIDYN [259], SDTrimSP [286], Crystal-TRIM [261]. Other, independently developed BCA codes include SASAMAL [287] and CASWIN [288,289].

Some uses of the BCA method can be considered outdated by now. Even though BCA simulations can give some sort of numbers of vacancies, these numbers are not unique [290], and BCA cannot in any reliable way describe production of vacancy or interstitial clusters, as this is driven by thermodynamic processes. Hence for simulations of defect production, MD can be considered to have superseded BCA. A bit similarly, for simulating channeling under conditions where multiple collisions are significant, the MD-RIA approach is usually sufficiently fast, reducing the need for a BCA approach. However, BCA does remain a very efficient and accurate method for calculating ion ranges, energy deposition profiles, recoil spectra, and when properly calibrated, also sputtering. For this kind of uses, the approach is likely to remain important far into the future.

7.1. Kinetic Monte Carlo (KMC)

The KMC method is in the most general term a way to simulate the time evolution of any system with known rates, provided the subsequent transitions are not correlated with each other and are Poisson processes [291]. If all possible transitions and their rates are known, then the KMC algorithm always picks one transition to

happen randomly, however, with the selection probability being proportional to the rate. The time is then advanced after each transition with the simple equation

$$t = t - \frac{\ln u}{R} \quad (1)$$

where u is a random number between 0 and 1, and R is the sum over all rates. The KMC algorithm is very powerful in that in case all input rates are correct and the transitions are independent Poisson processes, it is actually an exact algorithm, i.e. it would simulate the real stochastic time evolution perfectly correctly [291].

The Kinetic Monte Carlo method has an interesting history, in that almost exactly the same algorithm appears to have been independently invented at least three times. The basic aim of the KMC approach is to simulate atomic jump or transition processes with a realistic time scale (note that the MMC method does not have a physical time). The first attempted development of such an approach was by Flinn and McManus in 1961 [292]. The crucial time advancement algorithm that takes into account the sum of all rates was developed by Young and Elcock in 1966 [293] for simulating vacancy migration in binary alloys (i.e. a radiation effect). Apparently independently of this, Bortz, Kalos and Lebowitz developed in 1975 an approach to simulate the time development of spin systems with the same time advancement scheme [294]. Finally, in 1976 Gillespie also reinvented essentially the same time advancement scheme for simulation of chemical reactions. Due to the varied origins of the KMC method, it has been used with many names: Kinetic Monte Carlo, Dynamic Monte Carlo, the n-fold way, the BKL algorithm [294] or the Gillespie algorithm. Recently it seems the naming convention is converging towards the KMC term, perhaps because the wikipedia page on the method uses that as the title.

The original KMC approach was one where each atom in a system was simulated [293], an approach now called Atomic KMC (AKMC) and often used to simulate vacancy migration in alloys and surface reactions [295,296]. Another approach is to simulate only 'objects' that are assumed to move in a 'background' of perfect crystal, an approach now called Object KMC or OKMC [297]. In the OKMC approaches, the background perfect crystal atoms are not explicitly included in the software arrays, saving a huge amount of memory.

The reason the KMC method is very interesting for radiation effects, is that radiation defect and impurity migration typically fulfils the KMC precondition of being uncorrelated Poisson processes [28]. Hence, OKMC can be used to simulate the defect or impurity mobility after a cascade, frame D in Fig. 1. Moreover, KMC has the major advantage compared to MD, that the time scale is not dependent on atom vibrations, but rather depends inversely on the jump rates. In other words, the slower the defect migration rates, the longer the time steps in KMC become.

The major weakness of KMC is that all possible jumps and reactions between defects have to be known in advance, and coded or parameterized into the KMC. This, however, is where the lower-level simulations can come in: either BCA or MD can be used to simulate the defect production, and MD or DFT the defect jump rates and reactions (if not known experimentally).

The OKMC method has been widely used to simulate radiation effects since the 1990's. Heinisch started in 1990 simulating damage production in BCA full cascade simulations, and then the defect migration by KMC [298,299]. This line of simulations has proven to be particularly useful for simulations of ion beam processing of Si, since there the post-implantation annealing crucially involves point defect and impurity migration [276,300,301]. Particularly noteworthy is the very advanced KMC simulator of the ion beam processing of Si, with inputs on hundreds of rates from other methods, that has been developed by Pelaz et al. [197,302–304]. This simulator can simulate the behaviour of defects and impurities in Si up to the final electrical activation that is crucial for the device functionality [305–307], see Fig. 11.

Another big thrust in OKMC use has been the study of defect migration including impurity effects in Fe. A quite good understanding of interstitial and di-interstitial mobility has been achieved with KMC simulations [308]. Related modelling has also shown that even low concentrations of carbon impurities have a major effect on defect structure growth in Fe [309,310]. KMC has also been used to examine the migration and bubble formation by He in W [311,312]. By extending the base KMC algorithms to surface roughening, this line of simulations has enabled providing a reasonable explanation to the mechanism and time and temperature dependence of bubble formation in W [313] and the so called fuzz growth in W by He irradiation [314,315].

In the 2000's, several interesting further developments of the basic AKMC and OKMC algorithms have emerged.

The AKMC approach has also been very important in studying ordering reactions in metal alloys [31,316]. For instance, Enrique and Bellon showed around 2000 how a balance of radiation disordering and chemical ordering effects can lead to compositional patterning in CuAg alloys [295,317]. In 2010 Clouet and Soisson used AKMC to determine the radii of Cu precipitates in FeCu alloys, finding very good agreement with experiments [318]. Even more recently, Messina et al. showed in studies of Mn and Ni solute atoms in steels that increasing the solute content has a stabilizing effect on that vacancy clusters [319].

AKMC on defect migration in alloys has the problem that for each different elemental composition around a defect leads to a different migration energy. The amount of different energies goes up to the millions even in a binary alloy. Two approaches have been taken into efficiently determining barrier energies without having to explicitly precalculate all of them. Djurabekova et al. introduced using artificial intelligence (neural networks), which as least for bulk binary alloys seems to work quite well [320,321]. A completely different approach is 'on the fly'-KMC, where barriers are determined as needed during an AKMC run [322,323].

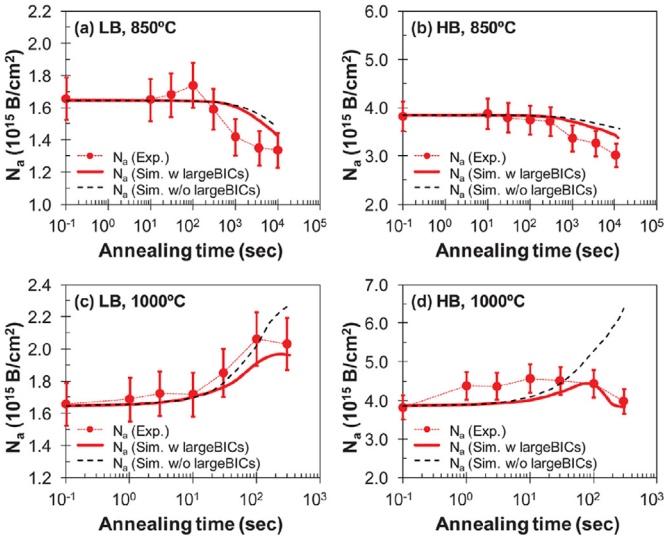

Fig. 11. KMC results on the fraction of electrically activated B defects in Si as a function of annealing time compared to experiments. The two different simulation curves are results on two model varieties, with and without large boron-interstitial clusters. From Ref. [307]. Reprinted with permission from AIP publishing. Copyright (2011) the American Institute of Physics.

A practical problem in OKMC simulations is often that most of the simulation time goes into simulating a few rapidly moving defects (typically interstitials) that very slowly proceed by random walk from one area to another. To overcame this computational limitation, two approaches have been developed. Event KMC aims at skipping the slow motion and model only the "events" i.e. defect reactions of interest [324]. The other approach for the same purpose, which appears to be more rigorously formulated, is First-passage KMC, FPKMC [325].

All the basic KMC approaches assume that a defect is moving by a random walk, except when it is reacting with another defect. However, in reality defects have a relaxation volume [326,327], which means that they also have a strain field and an elastic interaction energy associated with it [328]. Hence e.g. defects with relaxation volume of the same sign will repel each other, and pairs with opposite sign, attract. Recently, the first KMC code that incorporates such elastic interaction effects has been developed [329].

Since there are many KMC varieties, that from a programming point of view are not naturally compatible, there are not really any wide-use general-purpose KMC codes (such as LAMMPS is for MD). For OKMC, there is a new open source code MMonCa that is quite adaptable to different systems, and hence has potential to become a wide-use OKMC code [330], and for AKMC surface simulations the KiMOCS code is available open source [331].

8. Discrete Dislocation Dynamics (DDD)

Discrete dislocation dynamics is a much newer method than the ones cited above. In this method, dislocations [332] are treated as a connected set of lines or curve segments, which interact with each other via the elastic strain energy [333]. The energy gives an elastic force between the segments, and a molecular-dynamics like algorithm can then be used to simulate the motion of the dislocations.

DDD was first developed for two-dimensional systems by Lepinoux and Kubin as recently as 1987 [334]. The theoretical formulation for realistic dislocations was formulated and applied for 2D simulations by Amodeo and Ghoniem in 1990 [335,336]. The approach and extended to three dimensions in 1992 by Kubin and Canova [337].

Since the strain field around defects decays slowly, the method is rather computationally heavy, as it needs to in principle sum all interactions from all other dislocations.

The most common DDD approach solves the interaction between segments using the elastic equations for an isotropic medium [333]. However, since common metals are highly elastically anisotropic [338], this is not fully realistic. In 2010, Fitzgerald et al. implemented anisotropic elasticity in DDD [339,340].

The method has gained wide use in modelling mechanical deformation of materials, see e.g. Refs. [341–345]. The relevance for simulating radiation effects comes from the fact that after prolonged irradiation, damage in metals is dominated by dislocations (frames E, F in Fig. 1), and their behaviour will determine the final mechanical property change of the material. Hence for a complete simulation capability of radiation damage in metals, some variety of DDD will be crucial.

The first studies of irradiation effects by DDD were done around 2000 by Diaz de la Rubia et al. [346,347], and gave a reasonable-seeming explanation to plastic flow localization in materials. Another example of a similar study, including a comparison with experimental data [343], is shown in Fig. 12. However, it seems now clear that to simulate dislocations in realistic materials, one needs to include several effects that are not included in basic dislocation theory. This includes at least how dislocation motion is slowed down by low-concentration impurity atoms such as C and N (always present in real metals), how dislocations interact with precipitates, and with each other. Due to this, extensive efforts are underway to use classical MD to deduce how dislocations interact with other objects and each other, and then introduce this into the DDD codes, [63,348–356]. For instance, Terentyev et al. deduced from MD simulations of dislocation mobility in FeCr alloys that one of the reasons to the high radiation hardness of ferritic-martensitic steels is that Cr strongly slows down interstitial dislocation loop mobility [63]. In another recent advance, Lehtinen et al. deduced from MD how dislocations interact with spherical obstacles, and introduced this into the DDD code ParaDis [357,358].

All of these studies are at least indirectly relevant to irradiation, even though many of them do not actually explicitly mention the term "radiation". This is one reason why the publication statistics on DDD and radiation gives quite low values (Fig. 3). However, due to the crucial role of dislocations on both radiation effects and mechanical properties of metals, it seems clear that the use of DDD to study radiation effects will extend, as the method matures. For instance, very recently in 2018, Cui et al. used DDD to show that plastic flow localization can, depending on size scale, be either irradiation-controlled or dislocation source-controlled [359].

Implementing the long-range elastic displacement field is rather complicated, and hence there are not too many 3D DDD codes available. The perhaps most used code is ParaDis, developed at LLNL by Bulatov et al. [360,361]. Other codes include microMegas maintained at CNRS-ONERA [337,362], NumoDis/Tridis by Fivel et al. [363–365], as well as a code developed by Weygand et al. that does not apparently have a definite name, but is sometimes called the "Karlsruhe dislocation tool" [366,367].

9. Density functional theory (DFT)

The idea for DFT was originally developed in 1964 and 1965 by Hohenberg, Kohn and Sham [368,369], and has since then developed to be such a key method in physics, chemistry and materials science that Kohn got the Nobel prize in chemistry for it in 1998. To put it in a simplified way, DFT solves a Schrödinger-like equation for the electron densities (rather than the many-body wave functions) of non-interacting electrons, then uses a special "exchange-correlation" functional to correct for the error associated with the initial use of hypothetical non-interacting electrons. After 5 decades of development, the DFT algorithms have become quite accurate for a wide range of solid-state and molecular systems; although it is important to be aware that it has serious problems in describing e.g. some molecular transition barriers [370].

DFT is by definition an electronic ground state method [371–373] and hence not directly suitable for simulation of nonequilibrium radiation effects. Moreover, it is computationally very demanding, and hence most DFT simulations even today still only involve a few hundred atoms. However, DFT is also widely used related to radiation effects, as is evident from the publication statistics in Fig. 3. It can be used in many ways to benefit understanding of radiation effects.

1. DFT is the de facto standard method for studying the properties of point defects: their formation energy, relaxation volume, etc. etc. We do not attempt to review the vast literature on DFT studies of defect properties, as there are many other recent comprehensive reviews on the topic [370,374,375]. This usage are is, of course, not limited to radiation effects, but the results are valid regardless of how defect were produced. On the other hand, many kinds of defects, especially interstitial-like ones, are typically produced mainly by irradiation, and hence the DFT defect studies are often motivated by radiation effects. Such DFT defect results can be very useful for selection or constructing

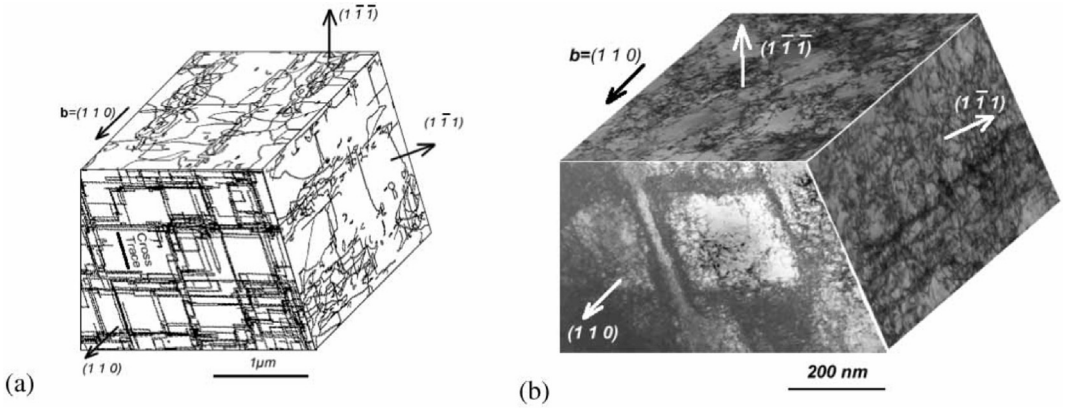

Fig. 12. Example of capabilities of DDD. a) DDD simulation model of steel after loading. b) experimental image of steep after thermal fatigue loading. From Ref. [343]. Copyright Taylor and Francis (2004).

analytical interatomic potentials, before these are used in classical MD studies of radiation effects.

2. The DFT defect calculations can also be extended to determine transition barriers between two different defect positions, i.e. the migration energy of the defect. [376,377]. This can be achieved with one of several transition calculation approaches [27,378]. This is a very important approach to get input for KMC or RE studies of the long-term defect migration [69,379].
3. Due to the limitation to a few hundred atoms, it is challenging to use DFT for studies of extended defects. However, by selecting a suitable cell symmetry, it can be used to study the core structure and energetics of dislocations and stacking faults [380–386].
4. As noted above in section 6, molecular dynamics can also be run with forces obtained from DFT (DFT-MD). So far, due to the small number of atoms involved, such simulations have been mainly limited to studies of the threshold displacement energy [126,216,387–389]. An example of a near-threshold defect formation process is shown in Fig. 13.

Also other, more approximate but efficient quantum mechanical methods such as tight-binding MD (TBMD) have been used to study threshold displacements [390,391]. TBMD has also been used to study surface impacts [392,393].

As computers became more efficient, and DFT methods further optimized, I foresee that soon DFTMD will be able to be used to simulate full collision cascades at least for keV energies. This should be very helpful in resolving some of the remaining uncertainties about choosing interatomic potentials in classical MD.

Since DFT is a very widely used method, there also is a wide range of different codes. In the field of radiation damage studies, some widely used codes are VASP [394], SIESTA [395] and QuantumEspresso [396,397].

10. Time-Dependent Density Functional Theory (TDDFT)

The TDDFT method aims to solve the time-dependent Schrödinger equation for a system of atoms and electrons. However, just like the time-independent DFT method, the equation solved is not the true Schrödinger-equation, but an approximation to it. Hence it is not guaranteed that the solution corresponds to reality.

TDDFT is based on a generalization of the DFT method by Runge and Cross from 1984 [398]. To simulate atom motion (TDDFT-MD), one can use the approach coupled to Ehrenfest dynamics [399–401], and the method has gotten wide use to simulate electronic excitations in materials and molecules. The method is very

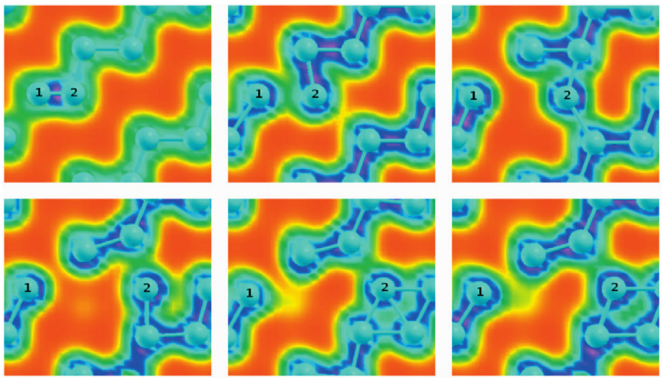

Fig. 13. DFTMD results of defect formation in Si. The image sequence shows the electron density in a 110 plane around a replacement collision sequence in Si that is observed for recoils in the 111 direction. Atom no. 1 is initially given a recoil in the 111 direction, which results in atom no. 2 falling into a tetrahedral interstitial position, leaving a vacancy behind at its original lattice site. Red indicates low electron density. From Ref. [387]. Reprinted figure with permission from [E. Holmström et al., Physical Review B 78, 045202 (2008)] Copyright (2008) by the American Physical Society. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

interesting for radiation effects because it could, at least in principle, describe electronic stopping and electron phonon coupling fully from first principles. Due to this, its use to study radiation effects has increased strongly since 1995, see Fig. 3 (although a large fraction of the papers deals with radiation effects from non-ionizing electromagnetic radiation).

TDDFT is a computationally extremely heavy method, and hence TDDFT simulations tend to be limited to 100 atoms or less. This naturally makes simulation of electronic stopping or electron-phonon coupling very challenging. The first calculations of electronic stopping by TDDFT were thus done on nanostructures with limited number of atoms. Kunert et al. studied projectiles impacting on fullerenes already in 2001 by TDDFT [402], and Nazarov et al. in 2005 the model system of a homogeneous electron gas [403].

Starting in 2007, Krasheninnikov and coworkers have systematically used TDDFT to examine electronic stopping in graphene, first for protons and more recently also for heavier ions [404,405]. These simulations seem to be give stopping powers that are on average consistent with experimental values. However, they can be extremely useful for explicitly deducing how electronic stopping varies in individual trajectories.

For bulk materials, several studies in the early 2000's considered

the issue of what the low-energy limit of electronic stopping is, in association with contemporary experimental studies. Both simulation [406,407] and experimental [408-411] works now give strong evidence that at energies below roughly 1 keV, electronic stopping is weaker than in the standard velocity-proportional Lindhard model.

Since around 2012, several studies have started to determine the electronic stopping in bulk materials [401,412–414]. These simulations can be very valuable in giving insight on how the electron density is modified by individual projectiles, see Fig. 14. Most recently, TDDFT simulations were also used to start to get insight into electron-phonon coupling [193], although the small number of atoms the simulations can handle, makes it challenging to model phonons. From such recent exciting and insight-providing developments, it is clear that the use of TDDFT methods will keep increasing in radiation effects simulations.

Since the TDDFT method is still under strong development, one cannot state that there would be widely used "standard codes" for it.

11. Finite element methods (FEM)

In FEM space is divided into a set of elements, typically triangular (2D) or prism-shaped (3D) all connected to each other in the corners, and a given equation system is solved in this grid. The solution can be either static or dynamic. The finite-element method developed from several approaches in structural mechanics in the 1930–1950's. A crucial step towards the modern FEM methods was done by Turner et al., who introduced the approach to divide space into triangular segments [415]. The term "finite element method" was first used in 1960 [416]. From the radiation damage point of view, the most relevant use of FEM is that where the equations solved are the elastoplastic ones describing the response of a material to external stress. Out of all the methods described in this review, FEM is by a far margin the most widely used in general, as it is the standard method for structural design in mechanical engineering. FEM is, because of this wide use, very reliable for describing stresses and deformation in standard engineering materials (steels, aluminum, etc.) under usual processing conditions.

The radiation condition is not a usual one, and due to all the physics effects described in this Article, after irradiation the elastoplastic response (constitutive equations) of a material will be significantly different from the initial one. Currently the radiation effects are introduced into FEM based on empirical inputs, see e.g. Refs. [417,418] and Fig. 15.

One of the key aims of radiation damage modelling is to be able to use all the lower-level methods to formulate physics-based input laws including all radiation effects for FEM. While this goal still is far away, a very promising step forward was obtained recently, when Dudarev et al. showed MD data of how radiation defects alter the elastic properties of metals, can be transferred directly to FEM [419].

FEM modelling is in practise to a very large extent done with commercial codes.

12. Comparative discussion

The breadth of the use of the methods reviewed in this article is naturally to a large extent determined by the available computer capacity. Rate theory (RE) analysis of defect diffusion can to some extent be done analytically or with traditional numerical integration without computers, and hence this method predates the use of computers. The other methods can only be of practical use with electronic computers, and hence emerged after the 1940's. The RE

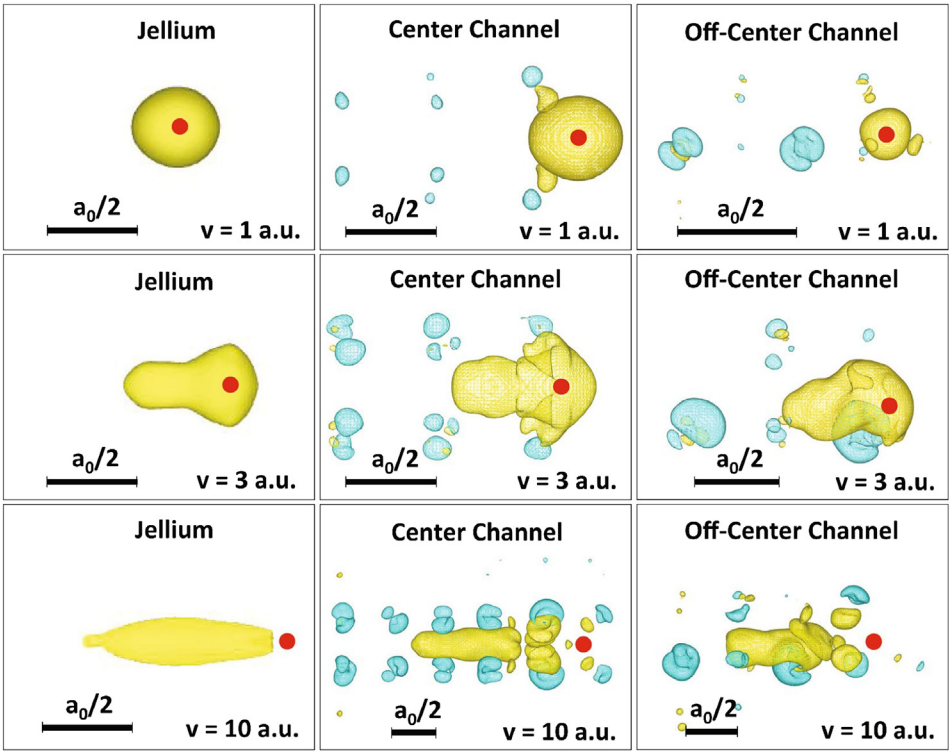

Fig. 14. Example of how TDDFT can be useful for understanding electronic excitations in specific ion trajectories. The images show Ni moving either in jellium (left side) or in different positions at different velocities in crystalline Ni. The surfaces are iso-electron densities. From Ref. [401]. Reprinted with open access permission. Copyright Springer Nature (2017).

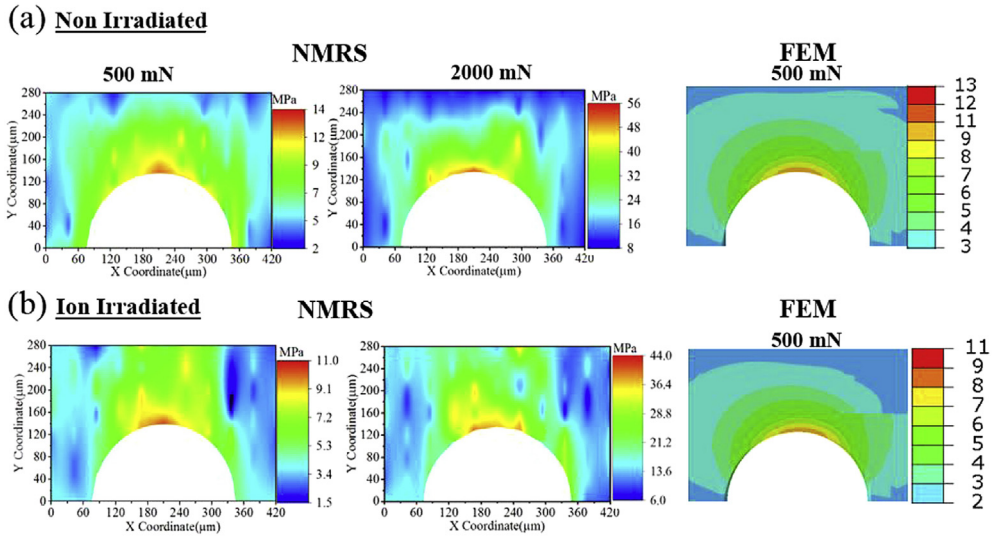

Fig. 15. Comparison of experimental 'NMRS' and FEM results on the stress distribution in non-irradiated and ion-irradiated SiC. From Ref. [418]. Reprinted with permission from publisher. Copyright Elsevier (2017).

and FEM methods are essentially continuum methods, while all the others treat discrete particles (or in case of DDD, dislocation segments). To be of relevance for radiation effects, one can roughly say that these methods need to be able to treat at least of the order of 100 particles (nuclei, atoms, electrons or dislocation segments). The MCN, MMC, MD, BCA and KMC approaches can be implemented for $\sim$ 100 particle systems even with quite limited computer capacity, and hence their use for radiation effects started already more than 60 years ago. On the other hand, the quantum mechanical DFT and TDDFT methods reached the stage of being able to treat 100-particle (atom core + valence electrons) systems only around the 1980's, and hence it is natural that their use for radiation effects is more recent. On the other hand, the DDD method was only invented around the 1980's.

Computers have become dramatically more efficient over the last 70 years, and the development is still going on at least via increasing the parallelization and alternative architectures [420]. This does not, however, mean that a newer, physically more accurate method is likely to completely replace an older one. This is well reflected in the statistics in Fig. 3: even though by now the analytical potential MD method (section 6) in principle can do practically all of the tasks of BCA (section 7), the use of BCA still keeps slowly increasing. The reason to this is simply that for some purposes (such as range distributions in amorphous materials), BCA is accurate enough, and hence there is no need to use the slower MD method. On the other hand, this kind of BCA calculations are rather routine, and for gaining new scientific insights, the MD method clearly is more important in contemporary use.

The comparison of DFT-based MD (section 10) with analytical potential MD (section 6) might at first glance suggest that DFT-MD would soon replace analytical potential MD for cutting-edge science. While this may indeed happen, the transition is likely to be much more gradual and slower, since the computer capacity requirement of most DFT methods scale as N^2 or N^3 with the number of particles, while analytical potentials scale as N or $N\log(N)$. Hence simulating large collision cascades, which requires handling millions of atoms, is likely to remain out of the reach of DFT-MD still for a long time to come. On the other hand, if an efficient and reliable parallellized linear-scaling DFT approach is developed, then DFT-MD may well replace classical MD on exascale, and beyond, supercomputers.

Somewhat similarly, the KMC approach in principle can do all that the RE can. However, for very large systems and ones where the time scales vary widely, it seems likely that also the RE approach will stay in use for a very long time.

The use of TDDFT methods for understanding electronic excitations during irradiation is clearly on the rise, as is the use of the CP and PFM approaches for modelling complex radiation-driven microstructure development issues.

Finally, I note that while this review has been focused on the basic research developments of the methods, some of the approaches are also in wide industrial use. The MCN approach is of course in wide use in the nuclear industry. The largest industrial use of radiation effects modelling is, however, likely in the semiconductor processing field. The SRIM BCA software is widely used also for modelling industrial semiconductor ion implantation. Since the software is free, this does not have direct commercial value. On the other hand, at least RE-like solution of differential equations, DFT, MD, BCA and KMC are included in commercial Si "Technology computer aided design (TCAD)" manufacturing codes [421,422]. The market for these codes is very significant (the revenue for the largest company in the field, Synopsys, was 3.1 billion USD in 2018 [423]), although the share of this relevant to radiation effects is of course only a fraction of the total. Nevertheless, this example shows that radiation effects modelling methods have developed from basic research into an industrially significant endeavour.

13. Conclusions

In conclusion, in this article I have reviewed the historic development of the use of nine different simulation methods in modelling radiation effects, and given a personal view on how they are likely to develop in the future (cf. Fig. 2 and section 12).

All of the methods reviewed will clearly remain in use for a long term to come. The relative importance of the BCA method for basic science is declining, as the more versatile classical MD simulations can now handle most of the cases originally studied by BCA. On the other hand, the quantum-mechanical DFT-MD and TDDFT-MD show great promise in resolving the uncertainties associated with the choice of interatomic potential and electronic excitation model, respectively, in classical MD simulations. Advanced KMC simulation approaches show great promise for being able to address

increasingly complicated microstructure development issues. Finally, the capabilities to use the atom-level DFT, MD and KMC methods to parameterize mesoscale DDD and macroscale FEM simulations are clearly advancing.

In semiconductors, a predictive capability of the multiscale modelling has already been achieved at least for the typical Si processing conditions. I am optimistic that also for metals, the combination of advancing simulation efforts will enable predictive simulations of the materials response to irradiation within a decade or two.

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