Modeling Microstructure and Irradiation Effects

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This article gives an overview of the strategy followed nowadays to model the evolution of metallic alloy microstructures under irradiation. For this purpose, multiscale approaches are very often used, which rely on modeling techniques appropriate to each time and space scale. The main methods used are *ab-initio* calculations, classical molecular dynamics (MD), kinetic Monte Carlo (KMC), mean field rate theory (MFRT), and dislocation dynamics (DD). These methods are briefly presented along with some of their typical uses and main drawbacks. Some examples are provided of the typical information obtained with each of the techniques.

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I. INTRODUCTION

THE development of numerical tools capable of simulating the effects of neutron irradiation on mechanical properties of materials is becoming more and more widespread because of, on the one hand, the increasing costs of the experiments and, on the other hand, the increasing power of computers. Usually, these numerical tools are linked within a multiscale platform. This is the approach followed, for instance, by the European, and wider, international scientific community created around

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Each of these 4 year projects involves around 30 research organizations (industry and academic) and the European Commission contribution is between 6 and 7 million euros.

The outcome of the FP6 PERFECT (<https://fp6perfect.net/site/index.htmproject>) has been published in a special issue of *Journal of Nuclear Materials*: volume 206 (2010).

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the FP6 PERFECT and FP7 PERFORM60 projects* for in-service fission reactors,^[1] the cross-cutting FP7 GETMAT project,^[2] in the fusion materials project managed by EFDA,^[3] and by several international initiatives, which are ongoing for generation IV structural materials.

This article presents an overview of some of the techniques used in the multiscale modeling approach of radiation damage in structural materials. This scheme resorts to different simulation techniques as many length and time scales are involved, as indicated in Figure 1, which applies to the modeling of pressure vessel steels as was done in the PERFECT project. As a complete and thorough description of all the possible techniques applied to all the possible materials is out of reach and would require the writing of an entire book, the focus of this article is on the modeling of the microstructure of metals and metallic alloys and most examples provided pertain to the case of pressure vessel ferritic steels for fission reactors. The same techniques, however, can be applied to other structural materials (as well as other irradiation conditions^[4]), such as zirconium alloys, which hold the fuel; FeCr and oxide dispersion strengthened/nitride dispersion strengthened (ODS/NDS) alloys; austenitic alloys used for the internals; or tungsten, which is considered to coat the divertor in the International Thermonuclear Experimental Reactor (ITER).

In the first section, we present the different bricks of the multiscale modeling scheme necessary to predict the microstructure of the irradiated materials. This sequence of models is represented in Figure 2.

In the second section, we come back to three of the main techniques used, *i.e.*, molecular dynamics (MD),

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*The main objective of the European projects PERFECT (2005–2009) and PERFORM60 (2009–2013) is the development of multiscale numerical tools capable of simulating the effects of irradiation on microstructure, and the mechanical and corrosion properties of structural materials. These projects take advantage of the continuous progress in computer technologies and advanced experimental methods as well as the better understanding of radiation damage mechanisms.

The materials concerned are light water reactor pressure vessel ferritic steels (and, in particular, the irradiation-induced evolution of fracture toughness properties) and internal structure austenitic steels (and irradiation-assisted stress corrosion cracking).

The multiscale modeling methods developed are capitalized through integrated tools. In addition, a set of experiments (on model as well as industrial alloys) is also included in order to better understand the physical phenomena and validate or adjust the models at each possible characteristic time or length scale.

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Fig. 1—Multiscale modeling scheme applied within the PERFECT project to the pressure vessel steels.

kinetic Monte Carlo (KMC), and mean field rate theory (MFRT) methods. After a brief description of the methods, we give an overview of the area they were used in and point out their main accomplishments. We then underline the weaknesses of the models.

In the third section, we underscore the increasingly important contribution of *ab-initio* calculations in the overall picture.

II. MODELING THE IRRADIATED MICROSTRUCTURE

A. From Neutrons to Primary Knock-On Atoms Spectrum

The first event is the arrival of energetic particles, the predominant ones being neutrons, which interact with matter. The neutron transfer parts of their energy to a few atoms called the primary knock-on atoms (PKAs), which will be ejected from their lattice sites, collide with neighbor atoms and create displacement cascades. Several codes can be used to determine the PKA spectrum, which gives the number of PKAs created by time and volume units obtained from the neutron spectrum. In the case of the PERFECT project, the PKA spectrum is determined by SPECTER.^[5] SPECTER calculates spectral-averaged displacements, recoil

spectra, gas production, and total damage energy for around 40 pure elements using the ENDF/B-V database of nuclear data derived cross sections.^[6] The only input from the user is the neutron energy spectrum. As SPECTER does not handle compounds, displacement damage for alloys, insulators, and breeder materials needs to be handled by SPECOMP. Both softwares can be found on the NEA web site^[7] in a special database dedicated to software related to radiation damage. Another program, DART, based on the binary collision approximation (BCA) was developed^[8,9] recently to calculate primary recoil spectra, weighted recoil spectra, and displacement cross sections induced by electrons, ions, and neutrons in solids. It is based on recent nuclear evaluations (ENDFB6^[10] and JEFF3^[11]) containing accurate angular distributions of recoils for all neutron atom interactions. An example of the use of DART in SiC and ODS can be found in Reference 12. For these different codes, the accuracy of the neutron cross section database, as input, is crucial.

B. From PKA Spectrum to Displacement Cascades

In principle, one should simulate displacement cascades for every damage energy of the PKA spectrum. This task, of course, is not feasible. Furthermore, the PKAs induce displacement cascades, which may split

Fig. 2—Modeling the microstructure.

into subcascades if their energies are high enough. For instance, subcascade formation in Fe is observed at PKA energies of 20 keV and above.^[13] Simulations within the BCA with the TRIM code^[14] indicate^[15] that cascades produced by high energy PKAs split almost linearly into subcascades. Theoretical justification for this behavior was provided in Reference 16, which shows that for high PKA energies, where the BCA holds, the mean free path between two high energy collisions (which is proportional to the inverse cross section) is large compared to the cascade extension. To obtain a finite number of low energy PKAs, *i.e.*, PKAs that can be simulated using MD, one can use, for instance, INCAS,^[16] which is based on an analytical model of binary collisions. This code predicts the number of (sub)cascades produced, as well as the energy deposited in each subcascade by the PKAs. BCA codes such as Marlowe^[17] or TRIM can be used as well. Note that TRIM does not take into account the crystalline character of many solids, and thus simulates displacement cascades in amorphous solids. This can be a problem in materials where channeling takes place. In the virtual reactor RPV-2 of PERFECT, a special module was developed in order to convolute the PKA spectrum with the subcascade decomposition.^[18] The PKA spectrum can also be obtained with the code DART.^[8,9]

C. From (Sub)Cascades to the Primary Damage

Once the amount of energy transmitted from the neutron to the PKAs was determined, one needs to obtain the primary damage. The primary damage consists of a certain amount of self interstitial atoms (SIAs) and vacancies, isolated and in clusters. The amount of in-cascade clustering is important, since small defect clusters can be very mobile and provide easy nucleation sites for larger defects to grow.

For this purpose, one needs to predict the trajectories of the neighbor atoms of the PKAs. Two different approaches can be followed whether the equations of motion of the atoms are solved simultaneously or within the BCA. In the former approach, MD, a system is considered as a whole and the evolution of its solid state toward equilibrium is followed stepwise in time. The movement of each atom is governed by its global environment. In the latter, collision cascades are approximated by sequences of binary encounters that

are not influenced by the environment. This approximation is too strong for slow particles in condensed matter, and MD has proven to be more appropriate provided an appropriate cohesive model (the interatomic potential) is found. We will come back to this later on. MD was used for almost 50 years to simulate the displacement cascades since the pioneering work of Gibson and co-workers.^[19] The simulations are performed until the end of the in-cascade recombination phase, typically 10 to 15 ps.

D. From the Primary Damage to Experimentally Resolvable Defects

The evolution of the point defects created by the PKAs and their interactions with the solute atoms as well as with other elements lead to the evolution of the microstructure and, thus, to the property changes of the materials. To extend the study to the formation of experimentally resolvable damage features (point defect clusters, dislocation loops, solute precipitates, etc.), one turns to computational tools based on KMC or on MFRT.^[20] The mean field models were used so widely for so long that the use of the name “rate theory” is commonly thought to imply a mean field model. Following the suggestion of Reference 21, we use the term MFRT here. KMC methods can be applied to objects (OKMC^[22–24]), events (EKMC^[25,26]), or atoms (AKMC^[27–36]) in a specific volume. Both KMC and MFRT can be globally defined as coarse-grained models, because atoms are not explicitly treated in either except in the atomistic (or lattice) KMC, *i.e.*, the AKMC. These codes produce size distributions of experimentally resolvable defects (voids, loops, precipitates, etc.), including defects with sizes lower than the resolution achievable experimentally. Another interest of these methods is to provide the complete evolution of the microstructure with time, whereas most of the time, for practical reasons, only a few “snapshots” of the microstructure are obtainable during its evolution. In the worst case, one only has access to the final microstructure.

E. From the Experimentally Resolvable Defects to the Yield Stress

The interaction of defects with dislocations is a fundamental but not completely solved problem, which

should strictly be studied at the atomic level. It is most of the time tackled with the use of MD, which allows determination of the binding energies and pinning forces between dislocations and each type of hardening defect at the atomic scale. The forces can then be used as input data in a Foreman and Makin^[37] type model. The defects are introduced as a three-dimensional (3-D) array of obstacles to the motion of a dislocation within its glide plane. The dislocation line shape is defined by the equilibrium between the tension line, the applied stress, and the pinning forces. The applied stress makes the dislocation glide and bow between the pinning defects. The maximum stress applied gives the local yield stress increase due to the irradiation-induced defects.

Algorithms to simulate dislocation dynamics (DD) appeared in the 1990s (for instance, References 38 through 43). In these methods, the collective behavior of an ensemble of dislocations is modeled by determining the forces on each dislocation and taking into account all the possible reactions between dislocations as well as the other elements of the microstructure. The dislocation lines are described as flexible strings, sequences of short rigid segments. The segments can have one or more integration points for force calculations and they can be on a network or not. The dislocations are created, move, join, and change shape as a consequence of applied stress and mutual interactions described using elasticity theory.

This brief overview indicates that each step requires its own models and we describe them in Section III along with their main accomplishments and weaknesses.

III. SIMULATION TECHNIQUES USED IN THE MULTISCALE MODELING SCHEMES OF IRRADIATED MICROSTRUCTURES

A. Molecular Dynamics

1. MD and the primary damage

The most appropriate method to simulate the primary damage is MD. This technique, originally developed in the 1950s, is nowadays used by a great number of scientists, particularly in materials science. MD is based on Newton's mechanics: the properties of a group of atoms or particles are obtained by computing the trajectories of each particle in time. For that purpose, the atoms are considered as point masses and Newton's law $\vec{f}_i = m_i \vec{a}_i$ (where $\vec{f}_i$ is the sum of the forces felt by atom i , m_i its mass, and $\vec{a}_i$ its acceleration). Unlike *ab-initio* calculations, MD codes are easy to program and many groups use their in-house developed software. However, many all purpose MD codes are available to simulate molecules, for instance, or proteins. LAMMPS,^[44] XMD,^[45] and DYMOKA^[46] are more materials oriented. Codes such as DYMOKA, MOLDY,^[47,48] MDCASK,^[49] and DLPOLY^[50] provide the essential features to simulate the primary damage. Note that the BCA, which is widely used to determine the distribution of implanted species and the associated defects, can also be used to simulate displacement cascades, and we will come back to that point in Section 2. The simulation of

the primary damage formation is initiated by giving one atom, the PKA, a momentum corresponding to energies varying from 1 to a few hundred keV.

In general, the MD codes only take into account elastic collisions between atoms and do not account for energy loss mechanisms such as electronic excitation and ionization. It is thus necessary to first determine the electronic losses that can be estimated using Lindhard's energy partitioning theory^[51,52] in order to give the simulated PKAs the correct amount of initial kinetic energy E_{MD} . Typical energies encountered in fission neutron spectra can be found in Table I of Reference 53.

The choice of the simulation box size depends upon the energy of the PKAs. It must be large enough to avoid the displacement cascade to interfere with itself by periodic overlap. Before initiating the displacement cascade, the system of particles is allowed to equilibrate, for a few picoseconds, at the chosen temperature. The simulations can be done in the micro-canonical ensemble with PBCs as in, for instance, References 54 through 57 or at constant pressure.^[48,58] At the beginning of the collision phase, the time-step has to be carefully monitored in order to keep the total energy constant. It is usually taken to be of the order of 10^{-17} seconds and can be increased to 10^{-15} seconds during the cooling of the cascade. In metals, some common approximations are often made such as not taking into account the electron-phonon coupling (EPC)^[48,59] and not damping the boundary atoms to extract heat or attenuate the outgoing pressure wave. One usually agrees on the fact that the final simulation temperature rise scarcely influences the defect population generated in displacement cascades. Indeed, according to Phythian *et al.*,^[59] the drift temperature dependence of the residual defects and the defect clustering fraction is weak. This was confirmed by Gao *et al.*,^[60] who investigated the problem very thoroughly. Ion-electron energy exchange is important in insulators for defect production and in semiconductors for defect motion. In metals, it will probably affect energy transport and act as an energy sink, but its extent is far from settled.^[61] A coupling between the electrons and the lattice would result in a fast distribution of the heat from the hot cascade core to the cooler electronic gas; however, modeling these systems properly is hard, both because of the degree of electronic excitation and because the Born–Oppenheimer approximation may well fail. A simple scheme to implement EPC in MD can be found in Reference 62 based on the models proposed by References 63 and 64. An alternative method can be found in Reference 65. The electronic energy loss can be included in an MD calculation as a friction force proportional to the velocity of the moving atom according to the Ziegler–Biersack–Littmark formula,^[66] as done in References 67 through 69. Taking into account the electronic stopping and EPC during the simulations of ion beam mixing in bcc Fe, Björkas *et al.*^[67] found that no statistically significant difference in the fraction of clustered defects can be observed; however, the production of Frenkel pairs (FPs) differed by 50 pct. Their general conclusion is that with respect to the final damage, the EPC has very little effect in the case they investigated. The electronic stopping is more

important there, if applied already at low energy atoms (~1 eV).

Variability is introduced by changing the initial distribution of the velocities (which follows a Maxwell distribution) as well as PKA direction. The PKA directions are chosen to be representative of an average behavior. Stoller^[58] examined the influence of the PKA direction, and his results support the view that the $\langle 135 \rangle$ cascades should provide a reasonable representation of average behavior in bcc Fe. We have observed similar trends for $\langle 253 \rangle$ directions.^[54] Another way to investigate the effect of the PKA direction was proposed in Reference 70 following the original work of Reference 71. Those authors calculated the threshold displacement energy as a function of the PKA direction, which allowed them to determine an average threshold energy (used subsequently to determine the displacement per atom (dpa)).

The primary damage formation was investigated in many metals and alloys. Fe, because of its industrial role, is one of the most investigated materials, and displacement cascades were modeled in pure Fe for more than 45 years.^[13,48,58–60,71–74] Fe alloys, chosen both because of their industrial interest but mainly because of their interatomic potentials, have also been intensively investigated. Because of the predominant role of Cu in the embrittlement of the pressure vessel steels discovered more than 40 years ago,^[75–77] the first simulations of displacement cascades in dilute Fe alloys were done in Fe-Cu dilute alloys.^[78–80] Despite its notorious role in steels, the influence of C in solution was studied only recently by Calder *et al.*^[80,81] certainly because of the lack of reliable Fe-C potentials. Another interstitial species of great interest, especially in the case of materials for fusion application, is He, and its influence on the primary damage in Fe is now the subject of extensive work.^[82–87] Phosphorous is well known for its embrittlement properties, and Fe-P alloys were modeled by Hurchand *et al.*^[88] Finally, high-Cr ferritic/martensitic steels are candidate structural materials for key components in most future nuclear options due to their superior mechanical properties and good radiation resistance. Fe-Cr alloys, being representative of such steels, are now being extensively investigated (for instance, References 80, and 89 through 93). A brief review of the main results obtained in these alloys can be found in Reference 94. MD investigations of the primary damage formation have also been pursued in other elements such as Ni,^[74,95–99] Cu,^[95,96,100–105] Zr,^[105–108] and Zr alloys,^[109–111] W^[112–114] and WC,^[115] Va,^[116] Si,^[117,118] and SiC,^[119–125] Pu,^[126–128] UO₂,^[129–131] and other oxides,^[132,133] ordered alloys,^[96,100,134–137] spinels,^[138] and GaN.^[139] The influence of strain on the defect production by displacement cascades in Fe was studied by Gao *et al.*^[140] The main aim of these displacement cascade simulations, so far, was mostly to characterize the primary damage in perfect crystals. For metals, the effects investigated are the influence of the crystal structure, the point defect spatial distributions, and the formation of point defect clusters and subcascades, whereas in oxides or semiconductors, one of the main issues is the possible amorphization of the

crystal. Fewer works have addressed the effect of pre-existing defects or extended defects on primary damage: the interactions of the displacement cascades with voids,^[141] He bubbles,^[142] grain boundaries,^[131,143–146] interfaces,^[147,148] surfaces,^[149] or other cascades^[150] were also investigated. A review of the first MD simulations related to irradiation, with a special emphasis on the role of surfaces, can be found in Reference 151. A comparison of the primary damage state in fcc, bcc, and hcp metals can be found in Reference 152. Another review emphasizing the properties of extended defects as well as their interactions with dislocation is available in Reference 153. A review of the formation of the radiation damage production in ceramics was published recently in Reference 154.

As an example, Figure 3 depicts the primary damage produced by a 10 keV PKA (or, more precisely, a PKA with energy $E_{MD} = 10$ keV) in FeNi alloys of various concentrations. The presence of the Ni changes the morphology of the cascade as well as the number of residual defects, showing the possible significance of alloying on the primary damage formation.

A certain number of findings have risen from the almost 50 years of simulations of displacement cascades. The first significant result is that the number of surviving point defects is always found, at least for metals and metallic alloys, to be a fraction of the number predicted by the standard secondary displacement model by Norgett, Robinson, and Torrens (NRT).^[155] The “NRT” dpa is the damage measure used for engineering applications as recommended by the ASTM.^[156] In this model, the dpa** is given by

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**The dpa is a standard measure of the damage. It does not measure the amount of residual lattice defects actually created in a material, but rather the “damage energy” deposited in the material by the irradiating particles. This damage energy is evaluated in terms of how many atoms could possibly be permanently displaced from their lattice sites to stable interstitial sites. As the calculation in Eq. [1] does not take into account possible recombinations between vacancies and interstitials, the NRT dpa overestimates the number of permanently created point defects.

$$\text{displacement per subcascade} = 0.8 \frac{E_{MD}}{2E_D} \quad [1]$$

where E_{MD} is the damage energy, *i.e.*, the fraction of the energy of the particle transmitted to the PKA as kinetic energy, and E_D is the displacement threshold energy (*e.g.*, 40 eV for Fe^[157]). Another interesting result is that, again at least for metals, the evolution of the number of point defects, n_{FP} , as a function of PKA energy, E_{MD} , is given by a power law:

$$n_{FP} = A(E_{MD})^m \quad [2]$$

The terms A and m are constants that are weakly dependent on the material and temperature; A is on the order of 5 or 6, while m is around 0.7 to 0.8.^[155] For instance, for bcc Fe, for PKA energy ranging between 0.5 and 20 keV, it was found that the number of defects

Fig. 3—MD modeling of the primary damage. 10 keV displacement cascades in FeNi at 600 K (327 °C). Top figures: atoms replaced (*i.e.*, which have left their initial site); and bottom figures: residual defects. The red spheres are vacancies, the blue ones are self-interstitial atoms, and the green ones are dumbbells.

produced increases with an exponent of about 0.75.^[13] The number of defects produced at lower and higher energies is greater than that predicted by an extrapolation (Eq. [2]) as lower energy cascades are not true cascades anymore, while larger energy PKAs induce the formation of subcascades.^[13] Also, because of the splitting of the cascade into subcascades, it was found that the ratio of the number of FP created to the number of FP predicted by the NRT is constant^[58] for large energy cascades.

One caveat to add is that the crucial ingredient of MD simulations is the interatomic potential, and the primary damage, *i.e.*, the amount and structure of the defects produced, can be very sensitive to it, as shown for Fe in Reference 54. This was confirmed by other studies in Fe^[67,158–160] and in W.^[114] Unfortunately, the displacement (sub)cascades initiated by the PKA evolve too quickly, and their sizes are generally too small to be observed experimentally. The exception is the case of W, which was investigated with the help of a field ion microscope.^[161,162] Thus, it is almost impossible to compare the results obtained with experimental data. The current solution to this problem is to assess the validity of the results obtained by using different interatomic potentials, as described, for instance, in References 54, 97, 158 and 163 through 169.

2. An approximation to MD to model the primary damage: the BCA

BCA codes such as Marlowe^[17] or TRIM^[14] can also be used to simulate displacement cascades. In that case, collision cascades in bulk materials are described as sequences of binary encounters between which atoms move freely along their scattering asymptotes. Individual collisions are governed by pair potentials that may have an attractive component.^[170] The BCA is several orders of magnitude less time consuming than MD, and it therefore allows reasonably significant statistics in the case of widespread statistical distributions. However, they lack an appropriate description of the many-body effects, very important in particular for low energy collisions. BCA calculations, however, can be tuned on MD results, as proposed in Reference 73, so as to produce a statistically meaningful database. This is the approach followed in Fe to investigate the influence of various displacement cascade features on the long-term evolution of the primary damage^[171–173] or in Reference 174 to study the amorphization of Si.

Conversely, BCA has also been used to determine the angular and energy distributions of the PKA created by high energetic ion beam in Si, and the data were then used in MD simulations to follow the recoil cascades.^[175]

3. MD and the interactions of defects with dislocations

The other important contribution of MD to these multiscale models is the characterization of the interactions between the resolvable defects and the dislocations. The accumulation of point defects and small point defect clusters formed in the displacement cascades leads to the formation of vacancy clusters, *i.e.*, nanovoids, as well as interstitial clusters and dislocations. These features lead to some hardening of the materials due to their interaction with dislocations, and MD appears also to be one of the most appropriate tools to evaluate these interactions.

The simplest method is to introduce the dislocation in the box close to the defect and to minimize the total energy of the system to obtain binding energies. This is the approach followed in References 176 and 177 to determine the binding energies between a dislocation and a carbon atom in Fe or in Reference 178 to evaluate the interaction between the nanoscale defect cluster voids, dislocation loops, and irradiation-induced precipitates, produced in metals by irradiation in Fe or in FeCr.^[179] An alternative to this method is to use elasticity theory, which was shown in Reference 180 to work remarkably well even close to the dislocation core as the binding energy between a C atom and a screw dislocation obtained by anisotropic elasticity theory was in agreement with molecular statics calculations for distances larger than 1.5 Å from the dislocation line. This approach is also the one followed in Reference 181 to investigate the interaction and accumulation of glissile defect clusters near dislocations. The nudged elastic band (NEB) method^[182] can also be used in complex systems as in the study of the interaction of dislocation in Al^[183] or the investigation of the jog migration in screw dislocation in Cu.^[184]

The influence of temperature can be obtained by performing MD simulations as in Reference 185, where the authors looked at the interactions between SIAs and edge dislocation in bcc transition metals, or in References 186 and 187 for the interactions of Cu precipitates, vacancy clusters, SIA loops, and irradiation-produced defects in Fe. The literature regarding the interaction between dislocations and the possible strengthening elements of the microstructure is mostly dedicated to pure metals such as Fe, Ni, and Cu, and various obstacles were modeled. SIAs and edge dislocations in bcc transition metals were examined in Reference 185; voids, stacking fault tetrahedra (SFT), and point defects in Cu in Reference 188; dislocations in Ni in References 189 and 190; mobile dislocation loops in Cu and Fe in Reference 191; and Cu-rich precipitates and irradiation-produced defects in alpha-Fe in Reference 192. The formation of stable sessile interstitial complexes in reactions between glissile dislocation loops in bcc Fe was studied in Reference 193.

The binding energies or the forces thus obtained can then be introduced in larger scale models such as a Foreman and Making type model^[37] or DD models. Note that introducing MD or atomic scale results in larger scale models is not straightforward, and a step-by-step method analyzing, from the perspective of the

continuum scale, the results of MD simulations of dislocation-defect interactions can be found in Reference 194.

With the increase in computer power, dynamics simulations, where a dislocation is forced to glide and move toward a defect, can now be done^[195] and was used to study the interaction between an edge dislocation and a $\langle 100 \rangle$ interstitial dislocation loop^[196] or a void^[168] or the interaction between a screw dislocation and a Cu precipitate^[197] in Fe, as well as the interaction of SFT with edge and screw dislocations^[198,199] or the interactions between dislocations^[200] in Cu. Moving twin boundaries in hcp metals were investigated in Reference 201, the interaction among dislocations in Al was characterized in References 202 and 203, and screw dislocations interacting with Frank loops in Ni were investigated in Reference 204. The interactions of glide dislocations with weak interfaces in Cu-Nb alloys were also investigated using this technique.^[205] Dislocation gliding in Si crystals was also looked upon (for instance, References 206 and 207), and in the case of tungsten, the interaction of dislocations with dislocations and point defect clusters can be found in Reference 208. Note, however, that some uncertainties of this approach are still to be solved, *i.e.*, the boundary conditions, the applied stresses and strains, which are still much too high, and of course the validity of the interatomic potentials (especially in bcc structures).

Figure 4 presents the results of dynamical simulations of the interaction of a screw dislocation with a C atom in bcc Fe at 100 K (−173 °C). In the course of these simulations, three types of behavior were observed. The application of a constant shear strain to the simulation box makes the dislocation move on its gliding plane, a $\{110\}$ plane. When the dislocation arrives close to the carbon atom, it can in some cases, here referred to as type 1, just keep moving on its plane (Figure 4(a)). In a second scenario, the dislocation changes slip plane; this is a typical example of cross-slip (Figure 4(b)). In the third type of behavior, it is the carbon atom that moves when the dislocation is too close to it. It can jump to an adjacent octahedral site of the same plane (Figure 4(c)) or move onto another plane (Figure 4(d)). The kind of behavior observed depends on the local structure of the dislocation core in the vicinity of the C atom, the influence of which can be felt only for short interaction distances.

A review of the theory and computation of ideal strength, dislocation activation processes, and brittle fracture from the atomic perspective can be found in Reference 209; a review of a number of dislocation-obstacle interactions studied at the atomistic level in irradiated metals is available in Reference 210, whereas a more general review on dislocation in solids, which tackles this problem, was published very recently.^[211]

B. KMC and MFRT: Evolution of the Primary Damage

The accumulation of point defects and small point defect clusters formed in the displacement cascades leads to the formation of vacancy clusters, *i.e.*, nanovoids as

Fig. 4—Motion of a screw dislocation in the presence of a carbon atom (black circle) at (a) and (b) 100 K (173 °C) and (c) and (d) 300 K (27 °C) in bcc Fe. The dislocation core is underlined using Vitek's differential displacement method.^[345] In this scheme, the arrow length is proportional to the displacement difference. The longest arrow corresponds to $b/3$, and arrows shorter than $b/20$ are omitted for clarity. The trajectory of the dislocation core is represented by the gray dots. The different circle colors indicate on which $\{111\}$ plane the atoms lie: (a) type 1 behavior, (b) type 2 behavior, and (c) and (d) type 3 behavior. The text provides additional details.

well as interstitial clusters, dislocation loops, and in fcc metals SFT. Because the formation of these experimentally resolvable features involves diffusion, one cannot use MD, despite the increase in computer power. The techniques commonly used at the moment are based on the chemical reaction rate theory (alternatively, transition state theory) and typically employ either the KMC or MFRT. MFRT methods^[212–219] are analytical methods in which a set of N coupled differential equations of balance is solved. They are known as mean-field techniques as only defect concentrations are taken into account and spatial inhomogeneities are not treated. For the evolution of the concentration of single vacancy c_V , the equation is of the form

$$\frac{dc_V}{dt} = K_V - k_V^2 D_V c_V - \alpha c_I c_V \quad [3]$$

The first term on the right-hand side corresponds to the production rate of the monovacancies, the second term concerns the disappearance of the vacancies at sinks, and the third one characterizes the recombination of the vacancies with SIAs. K_V is the production rate of monovacancies, D_V is the diffusion coefficient of the monovacancy, k_V^2 is the sink strength, and c_I is the concentration of SIAs. Similar equations have to be solved for each cluster size and type. The advantage is that, without having to take the volume into account, the computing time is really short. A thorough description of MFRT can be found in Reference 52.

The KMC methods are MC methods, which can be classified as rejection free in contrast with the more classical MC methods based on the Metropolis algorithm.^[220] The KMC methods provide a solution to the Master equation, which describes a physical system whose evolution is governed by a known set of transition rates between possible states.^[221] The solution proceeds by choosing randomly among the various possible transitions and accepting them on the basis of probabilities that depend directly on the corresponding transition rates.^[221] KMC methods have the advantage of going beyond the mean field approximation by explicitly accounting for spatial correlations between the elements of the physical system and the overall geometry of the system. Spatial correlations are a significant feature of the primary damage, as demonstrated by the difference in damage between an electron irradiation and a neutron irradiation. In Reference 173, spatial correlations were shown to strongly influence the cluster size distributions in the long term. KMC methods can be applied to study the evolution of systems of mobile species, such as atoms in atomistic KMC^[27–31,33–36,222] or larger defects, formed, for instance, under irradiation in so-called coarser-grained KMC models.^[22–26,223] Many coarse-grained KMC models were formulated to describe the long-term evolution of the primary damage produced by irradiation. In OKMC models,^[23,24,224] defect migration jumps are explicitly treated and reactions occur when two defects (mobile objects) meet each other, or meet traps or sinks. EKMC models^[25,26] do not treat individual migration jumps explicitly, and only reactions (events) between objects drive the evolution of the system.

Contrarily to ab-initio or MD codes, no commercial or public codes are openly available, and each group develops the software needed for its own purpose. Many of the KMC techniques are based on the residence time algorithm (RTA) derived 50 years ago by Young and Elcock^[225] to model the diffusion of a vacancy in ordered alloys. Its basics are the following: for a system in a given state, instead of making a number of unsuccessful attempts to perform a transition to reach another state, as in the case of the Metropolis algorithm,^[220] one computes the average time the system remains in its state. One then performs one of the possible transitions according to its weight and determines the time it took for this transition to take place. According to standard transition state theory (see for instance Reference 226), the frequency Γ_x of a thermally activated event x such as a vacancy jump in an alloy (AKMC) or the jump of a void (OKMC) can be expressed as

$$\Gamma_x = \nu_x \exp\left(-\frac{E_a}{k_B T}\right) \quad [4]$$

where ν_x is the attempt frequency, k_B is Boltzmann's constant, T is the absolute temperature, and E_a is the activation energy of the jump. During the course of the simulation, the probabilities of all the possible transitions are calculated and one of them is chosen, at each time-step, by extracting a random number, according to its probability. The associated time-step length δt and average time-step length Δt is given by

$$\delta t = \frac{-\ln r}{\sum_n \Gamma_x} \quad \Delta t = \frac{1}{\sum_n \Gamma_x} \quad [5]$$

where r is a random number between 0 and 1.

The RTA is also known as the Bortz, Kalos, Lebowitz (BKL) algorithm.^[227] Other techniques are possible (for instance, Reference 228, where a thorough review can be found on the recent mathematical and algorithmic developments of AKMC with, in particular, some emphasis on the coupling with coarse-grained KMC). In the EKMC scheme, in contrast to the RTA, where all rates are lumped into one total rate to obtain the time increment, the time delays of all possible events are calculated separately and sorted by increasing order in a list. The event corresponding to the shortest delay, τ_s , is processed first, and the remaining list of delay times for other events is modified accordingly by eliminating the delay time associated with the particle that just disappeared, adding delay times for a new mobile object, *etc.*

The determination of the jump frequencies includes the physical input parameters of the models, and different strategies can be adopted to derive them. The different parameters can be obtained from experimental data; *i.e.*, the mobilities can be obtained from diffusion coefficients, or from lower scale simulations (*ab-initio* or MD simulations), or from theory: the attempt frequencies, for instance, can be calculated based on the Vineyard theory.^[229] They can also be adjusted so as to reproduce model experiments.

In KMC techniques, the simulation of an irradiation is treated as the occurrence of external events, which

depend upon the kind of irradiation that is simulated. All external events are characterized by occurrence probabilities $P_{\text{irrad.}}$, corresponding to the production rate: $P_{\text{irrad.}} = (\text{number of external events/cm}^3/\text{s}) \times (\text{simulation box volume})$. The production rate can be determined from the flux of impinging particles. In the case of neutron and ion irradiations, the impinging neutron flux is transformed into a production rate (number per unit time and volume) of randomly distributed displacement cascades of different energies (5, 10, 20, etc. keV), as well as residual FPs. New cascade debris are injected randomly in the simulation box, at the corresponding rate. In order to introduce more variability, the system of coordinates, to which the cascade debris is originally referred to, can be each time randomly permuted relative to the simulation box coordinates. In the case of electron irradiation simulations, FPs are introduced randomly in the simulation box according to a certain dose rate, assuming that each electron is responsible for the formation of only one FP, a valid approximation for electrons with energies close to 1 MeV (much lower energy electrons may not produce any FP, whereas higher energy ones may produce small displacement cascades with the formation of several vacancies and SIAs).

In MFRT, the irradiation is introduced in the source term, *i.e.*, the first item in the right-hand side of Eq. [1]. As no spatial correlation is explicitly considered in these techniques, the source term has to take into account intracascade agglomeration and recombination. The amount of agglomeration, and thus the source term for MFRT, can be obtained by annealing the cascade debris using, for instance, OKMC.

In addition, at the mesoscopic scale, phase-field methods start to be of use in radiation damage modeling to investigate the evolution of the nanoscale features formed under irradiation. Phase-field models were used for more than 50 years since the work of Cahn and Hilliard.^[230] An introduction to the method can be found in Reference 231, a review on microstructure modeling is available in Reference 232, a more general review about its use in materials science is published in Reference 233, but to our knowledge, this method was applied to radiation damage only very recently. A recent application of these methods to simulate void formation can be found in Reference 234.

1. AKMC

AKMC is a versatile method, which can be used to simulate the evolution of a complex microstructure at the atomic scale, dealing with elementary atomic mechanisms. It was developed to investigate diffusion events *via* the motion of a single vacancy^[225] and the introduction of heterointerstitials or self-interstitials in the models is yet under development. A very extensive description of the AKMC algorithm can be found in Reference 235, the theoretical basis for AKMC simulations in terms of the theory of Poisson processes in Reference 221, and another presentation of the “lattice kinetic descriptions” including KMC and mean-field approaches in Reference 236. We briefly review here the AKMC studies applied so far to the diffusion of point

defects on dilute alloys; a more precise description can be found in Reference 237. In the case of diffusion, the elementary mechanisms leading to possible state changes are the point defect jumps or the heterointerstitial jumps if any. Typically, vacancies and SIAs can jump from one lattice site to another lattice site (in general, first nearest neighbor sites). If foreign interstitial atoms such as C atoms or He atoms are included in the model as in References 238 and 239, they lie on an interstitial sublattice and jump on this sublattice.

AKMC was used extensively to study Cu precipitation in α -Fe under irradiation as well as under thermal aging,^[27–29,32–34,240] and a review article of AKMC simulations of aging in the FeCu system can be found in Reference 241. The Fe-Al system, typical example of superalloys, was studied by Athenes and co-workers,^[242–244] who reported the simultaneous occurrence of phase separation and ordering in a two-phase A2/B2 domain. Different phase separation or patterning conditions and regimes under irradiation were studied and modeled using the techniques by Bellon *et al.*^[245–248]

Fe-Cr alloys representative of high-Cr ferritic/martensitic steels are also extensively investigated.^[249–251] More complexity in the chemistry of Fe alloys was introduced by taking into account solute elements (Cu, Ni, Mn, and Si)^[35,252] to model dilute multicomponent Fe alloys more representative of the composition of the pressure vessel steels. The C was introduced in the models^[253] to study the hardening of high-strength steels by NbC precipitation and to investigate the heterogeneous precipitation of NbC on dislocations^[239] and grain boundaries.^[238] SIAs, which are introduced in a large amount during irradiation, have also been taken into account, first in a generic A-B alloy^[222,254] and then in dilute Fe-Cu-Mn-Ni alloys.^[255] Apart from the Fe alloys, some ternary alloys of industrial interest have also been modeled using this technique. Pareige and co-workers investigated ordering and phase separation in NiCrAl alloys, which are model systems of Ni-based superalloys used in the aerospace industry.^[30] In Al alloys, the introduction of transition elements such as Mn, Zr, or Sc leads to the formation of ordered precipitates, which increase the tensile strength and inhibit recrystallization, and Clouet *et al.* investigated the formation of L12 precipitates in Al-Zr-Sc alloys^[36,256,257] by means of a pair bond AKMC model. The behavior of He in Fe has also been investigated using this technique: the nucleation of He bubbles in bcc Fe was modeled by Deo *et al.*,^[258] and He-bubble migration in bcc Fe by Morishita *et al.*^[259]

Figure 5 represents the microstructure of an Fe alloy containing 1.12 pct at. Mn and 0.73 pct at. Ni at 9.3×10^{-3} dpa after being neutron irradiated at 573 K (300 °C) under a rate of 5.8×10^{-5} dpa·s⁻¹. The formation of Mn-rich precipitates decorated by Ni atoms is observed. A fair amount of point defect clusters is also observed.

AKMC can also be used to revisit and sometimes reinterpret experiments as presented in Reference 260, where we propose a different interpretation of isochronal experiments of dilute FeCu alloys. Despite the fact that the algorithm is fairly simple, the method is most of

Fig. 5—Microstructure of an Fe alloy containing 1.12 at. pct Mn and 0.73 at. pct Ni at 9.3×10^{-3} dpa after being neutron irradiated at 573 K (300 °C) under a rate of 5.8×10^{-5} dpa·s⁻¹. Only nonisolated point defects and solute atoms are shown. The gray, blue, and white spheres represent, respectively, Mn, Ni, and interstitial atoms.

the time nontrivial to implement in the case of realistic materials (as opposed to AB alloys, for instance). Most of the difficulties are related to:

- (1) The determination of the total energy of the system, *i.e.*, the construction of the cohesive model. Methods based on the cluster expansion method or interatomic potentials are often used for that purpose. As the validity of the AKMC results is strongly dependent on the quality of the energetic model used, the models have to be adjusted and checked on *ab-initio* data as well as on simple experiments performed on model alloys.
- (2) The knowledge of all the possible events and the rates at which they occur, *i.e.*, in the case of diffusion, the possible migration paths as well as their energies. Fast techniques to find saddle points on the fly such as the dimer method,^[261] the NEB method,^[182] or the eigen-vector following methods^[262] can be implemented as long as a reliable description of the cohesive energy of the system is available for all the possible configurations. Advanced methods were devised in the last 10 years where the possible transitions are found in some systematic way from the atomic forces rather than simply by assuming the transition mechanism *a priori*.^[263–267]

Another simulation method quite similar to AKMC, is called the self-consistent mean field (SCMF) method. It is mainly used to study radiation induced segregation (RIS) and flux coupling between point defects and solute species. SCMF can be considered as a one-dimensional (1-D) AKMC simulation and allows derivation of transport coefficients for dilute and concentrated alloys

by vacancies, and recently self-interstitials.^[268–270] It was applied to study RIS in austenitic alloys.^[271]

2. OKMC

The OKMC method, which is a coarse-grained KMC, is also based on the RTA, and the intrinsic difficulties are to introduce in the model all of the possible events of which can take place with their appropriate rates. In the case of the long-term evolution of radiation damage, the objects are the intrinsic defects (vacancies and self-interstitials) or impurities, and their clusters, which are located at known (and traced) positions in a simulation volume. The events are all the possible actions that these objects can perform and the reactions that they may undergo, such as (a) migration, (b) dissociation (emission of a smaller defect from a larger one), (c) aggregation of like defects or of defects and impurities, and (d) annihilation between opposite defects (self-interstitials and vacancies).

The probability for a migration event is given by the corresponding jump frequency, expressed as a thermally activated process, following the Arrhenius dependence, in a manner similar to Eq. [4]. The model also includes nonthermally activated events, such as the annihilation of a defect after encountering either a defect of opposite nature (*i.e.*, a SIA encountering a vacancy) or a sink, as well as aggregation, either by adding a point defect to a cluster or by forming a complex. These events occur only on the basis of geometrical considerations (overlap of reaction volumes) and do not participate in defining the progressing of time. Trapping and annihilation of defects with opposite defects or at sinks, as well as aggregation into larger clusters, take place spontaneously whenever the involved objects come to a mutual distance smaller than a reaction distance, which is equal to the sum of the capture radii associated to each of the two objects. Besides the fact that one has to try to introduce all the appropriate reactions in the model, the parameterization of these reactions is another very difficult task. To each possible motion corresponds a migration energy and an attempt frequency. One thus needs to know the migration energies (and attempt frequencies) of all the possible objects that the user believes can form and move in the course of the simulation. Because of the Arrhenius dependence of Eq. [4], efforts are usually concentrated on the determination of the migration energies, *i.e.*, the migration barrier the moving species have to go over, and the attempt frequencies are taken to be a constant of the order of the Debye frequency. The same reasoning is applied to the dissociation events, and efforts are then concentrated on the binding energies. The parameterization can be done with the help of *ab-initio* calculations^[272,273] for small object sizes, with MD for larger cluster sizes or the help of well-defined experiments such as isochronal annealing experiments following simple irradiations such as He implantation desorption^[274] or electron irradiation.^[275]

At the moment, the coarse-grained KMC methods have been mostly used to investigate the annealing of the primary damage, as in References 276 or 24, or the effect of temperature change in the damage accumulation,^[277]

Fig. 6—OKMC modeling of He desorption in W. 13 ppm of 400 eV He atoms were introduced either completely at random in the $399 \times 401 \times 1001$ (in lattice units) simulation box or according to the distribution profile determined using Marlowe. The experimental results are from Ref. 274.

but its strongest contribution in the field seems to be the study of parameters or assumptions such as the motion, 3-D vs 1-D motion, mobility of the SIA clusters,^[159,278–280] or to corroborate theoretical assumptions such as the analytical description of the sink strength.^[281] They were used also to model as well as re-examine simple experiments such as He desorption in W^[272] or in Fe^[273] as well as the influence of C in isochronal annealing experiments.

Figure 6 represents the evolution of the total number of defects in an OKMC simulation of below threshold energy He implantation in W performed by Soltan *et al.*^[274] The OKMC simulation, as the experiments, consists of two parts: the implantation sequence followed by isochronal annealing. 13 appm of 400 eV He were implanted at 5 K (−268 °C) in thin films of W of dimensions $399 \times 400 \times 1001$ in lattice units. Periodic boundary conditions (PBCs) were applied in two of the three directions, simulating a thin foil of tungsten, 63-nm thick. The experimental implantation rate was $10^{15} \text{ s}^{-1} \text{ m}^{-2}$,^[282] which corresponds to the introduction of 16 He per second in the simulation box. Two sets of implantations were done. One was obtained by introducing a spatially random flux of He atoms (curves labeled “random He” in Figure 6), while for the second set, the He distribution was done according to distribution provided by the BCA code, Marlowe (curves labeled “Marlowe cascades” in Figure 6). The parameterization was based on an extensive set of *ab-initio* calculations. The agreement between the experimental results and the OKMC data is very good, provided that the implantation is correctly modeled.^[283]

3. Mean field rate theory

The MFRT models were used for more than 40 years in the field of radiation damage,^[212–219,284,285] and all their accomplishments cannot be summarized in one paragraph. The MFRT was used to model irradiation-induced microstructures and, in particular, swelling of materials under irradiation (*e.g.*, the production bias model^[286,287]). Let's just underline that the MFRT

theory and coarse-grained (OKMC and EKMC) KMC methods ignore partially or totally the crystal lattice and rely on the same set of parameters: point defect diffusivity coefficients; binding energies of point defect with clusters and capture radii, which can be obtained from *ab-initio* calculations and MD simulations or specific experiments such as isochronal annealing following electron irradiation experiments as in Reference 288 or He desorption experiments.^[289,290] These techniques are thus complementary. They are also potential benchmarks of each others. This is the reason why a certain number of studies were published that compare the techniques on a specific (and generally simple) case. A direct comparison of MFRT and OKMC simulations was made in the domain of point defect cluster dynamics modeling, which is relevant to the evolution (both nucleation and growth) of radiation-induced defect structures and showed that the agreement between the two methods is best 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 dislocation.^[20] Resistivity recovery simulations of electron-irradiated Fe study done using both EKMC and MFRT can be found in Reference 291. EKMC, OKMC, and MFRT simulations of thin foil irradiation were compared in Reference 292. In addition, OKMC can be used to determine the value of the sink strength used in MFRT. In most cases, analytical expressions for sink strengths can be derived,^[293] but for complex objects or complex diffusion mechanisms such as 1-D or two-dimensional motion, such expressions are more difficult to obtain, whereas they are natural outputs of OKMC simulations.^[281,294,295]

One advantage of the MFRT approach is that there are essentially no limits to the density or size of the clusters when calculating their evolution, providing the opportunity to compare with a broad range of experimental observations. However, the spatial and temporal correlations in defect production are not accounted for, which may in some cases lead to a loss of specific information. Furthermore, to reach the typical size of dislocation loops or voids, which are observed experimentally, for instance, by transmission electron microscopy, the number of differential equations is very large. Grouping procedures or other approximate numerical schemes such as the Fokker–Planck formalism, which allows replacement of the N equations with a continuous variable x for large values of N ,^[296–301] thus have to be used. This becomes necessary when one wishes to take into account explicitly the chemistry of the materials, as is, for instance, the case for Cu atoms in ferritic steels, or if one wants to introduce a gas atom such as He for fusion or gamma heating modeling. In these cases, a much larger number of equations have to be integrated.^[18,285]

Many of the models described previously call for the knowledge of the mechanisms taking place at the atomistic level. In this context, *ab-initio* calculations appear now to be unavoidable, as underlined in the previous paragraphs. We thus now devote a small section to these techniques.

IV. STATUS/ROLE OF AB-INITIO CALCULATIONS IN THE MULTISCALE MODELING FRAMEWORK

Ab-initio calculations are techniques used to obtain atomic and molecular structures directly from the first principles of quantum mechanics, *i.e.*, without using quantities derived from experiment as parameters. They require a large amount of numerical computation as the amount of computing time increases rapidly as the size of the supercell, *i.e.*, the number of atoms or molecules, increases. The common objective of all the *ab-initio* techniques is to solve for the Hamiltonian of a system containing N_a atoms and N_e electrons. This is a many-body problem, which can only be solved with a certain number of approximations. In the field of materials science, *ab-initio* calculations are based on the density functional theory (DFT), which states that the ground state energy of a many-electron system can be expressed as a unique function of the electron density. The DFT has its conceptual roots in the Thomas–Fermi model, but it was put on a firm theoretical footing by Hohenberg and Kohn^[302] and Kohn and Sham^[303] in the mid 1960s. Many DFT codes are now available, which differ as follows:

- (1) The local basis sets, which are used to pave the space. In metals, plane waves, because of their simplicity, are very often used, but localized orbitals are also found in some codes.
- (2) The number of electrons that are explicitly taken into account. To simulate large systems, one usually considers that the core electrons are frozen. These kinds of simulations are less computationally demanding than the so-called “all electron” methods such as the linearized augmented plane wave method. In the former case, the inner core electrons are modeled using pseudo-potentials^[304–309] or more sophisticated techniques such as the projector augmented wave.^[310,311]
- (3) The method to reach the ground state.
- (4) The method to perform MD: one can use the classical Born–Oppenheimer approximation wherein the nuclear degrees of freedom are propagated using ionic forces, which are calculated at each iteration by approximately solving the electronic problem with conventional matrix diagonalization methods, or the Car–Parrinello^[312] approach, which explicitly introduces the electronic degrees of freedom as (fictitious) dynamical variables, writing an extended Lagrangian for the system, which leads to a system of coupled equations of motion for both ions and electrons. Because of the complexity of the problem, writing an *ab-initio* code is not a simple task, and most people turn to codes developed by groups, such as VASP,^[313] WIEN2k,^[314] CASTEP,^[315] SIESTA,^[316] PLATO,^[317] ELK,^[318] ABINIT,^[319] EXPRESSO,^[320] CPMD,^[321] and CRYSTAL.^[322]

Ab-initio calculations were used to determine, for instance, the properties of point defects and their clusters in Fe,^[323,324] which led to the construction of

improved interatomic potentials for this metal.^[325,326] It also has proven to be very useful to investigate the behavior of foreign interstitial atoms such as C, N, H, and He in Fe^[327–332] as well as He atoms in tungsten^[333,334] and other bcc metals.^[335] A key property of the dislocations, which plays a role in their mobility, is their core structure. Experimentally, the observation of the core structure even with high resolution microscopy is difficult except for materials where the dislocation core is dissociated, *i.e.*, low stacking fault energy materials. In this case also, *ab-initio* calculations are very relevant, as they indicate, for instance, that in the case of bcc materials, such as Fe, the core of the screw dislocation is compact^[336,337] rather than degenerate as predicted by most interatomic potentials. The behavior of solute atoms such as Cu,^[338] P,^[339–341] Ni, Mn, and Si^[342] has also been investigated, and the results obtained indicate, for instance, that Mn^[342] or Cr^[341] can bind to the SIAs and form mixed dumbbells, which implies that for these elements solute transport can take place *via* the motion of these mixed dumbbells. If this means of diffusion will not contribute to diffusion in structural materials most of the time, in the case of radiation damage, it can have a significant influence on the redistribution of the solute atoms in the matrix.

In the specific field of radiation damage, it is now possible to use *ab-initio* calculations and, more specifically, *ab-initio* MD simulations to determine threshold displacement energies. This was recently done in covalent materials SiC^[343] and Si,^[344] and good agreement was obtained between the experimental data available and the calculated ones.

Note that *ab-initio* calculations, as all numerical methods, have limitations and uncertainties, which must be kept in mind. Furthermore, they rely on some approximations. The first one is the Born–Oppenheimer approximation, which consists of decoupling the motion of the nuclei from that of the electrons. This approximation relies on the fact that the mass of the nuclei is more than three orders of magnitude larger than that of the electrons. As a result, the electrons are almost instantaneously in the ground state corresponding to the positions of the nuclei. Note that under some circumstances this approximation can be a little too crude for accurate calculations. For instance, the zero point motion of light nuclei such as hydrogen and lithium can have substantial effects on the ground state of some materials. Regarding the choice of a functional for exchange correlation, it must not be forgotten that the “A” in the acronyms GGA or LDA stands for approximation (GGA stands for generalized gradient approximation, and LDA stands for localized density approximation). The choice of the functional can lead to very different results as is well known for Fe for which the LDA predicts that its stable structure at low temperature is fcc and nonmagnetic in complete disagreement with the experimental facts. The reason behind this failing is that LDA underestimates the lattice constants, in general, which for Fe is a problem as there is a strong dependence of the magnetic moment on the lattice parameter. This issue can be solved by the use of GGA instead of LDA.

Fig. 7—*Ab-initio* insight into materials interactions: electronic density deformation map for two carbon atoms (gray spheres) close to one vacancy in bcc Fe (dark blue spheres). The “+” signs indicate regions where the electronic density has increased, while the “-” signs indicate regions where the electronic density has decreased. The units are electron volts per cubic angströms.

Figure 7 shows the electronic density deformation map for two carbon atoms (gray spheres) close to one vacancy obtained using the VASP code.^[328] The significant feature in this map is the occurrence of a covalent bond between the two carbon atoms. This covalent bonding is difficult to model with the typical many-body interatomic potentials, which most of the time do not take into account the angular contribution to the total energy and thus fail to correctly reproduce this interaction.

V. CONCLUSIONS

We have presented a rapid tour of the multiscale modeling schemes applied to understand and model metallic alloy microstructure evolution under irradiation. The task is immense and requires contributions from different techniques, as was shown here as well as from many different groups, as is proven by the collaborations promoted by the big international projects such as PERFECT, PERFORM-60, and GETMAT. The other mandatory ingredient in this task is the link with experiments and, in particular, the need for simple experiments that can help assess the validity of the models.

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