Computational Materials Science 148 (2018) 116–130

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Advanced atomistic models for radiation damage in Fe-based alloys: Contributions and future perspectives from artificial neural networks ☆

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ARTICLE INFO

Article history:
Received 26 October 2017
Received in revised form 16 January 2018
Accepted 9 February 2018
Available online 23 February 2018

Keywords:
Artificial neural networks
Kinetic Monte Carlo
Irradiation damage
Multiscale modelling

ABSTRACT

Machine learning, and more specifically artificial neural networks (ANN), are powerful and flexible numerical tools that can lead to significant improvements in many materials modelling techniques. This paper provides a review of the efforts made so far to describe the effects of irradiation in Fe-based and W-based alloys, in a multiscale modelling framework. ANN were successfully used as innovative parametrization tools in these models, thereby greatly enhancing their physical accuracy and capability to accomplish increasingly challenging goals. In the provided examples, the main goal of ANN is to predict how the chemical complexity of local atomic configurations, and/or specific strain fields, influence the activation energy of selected thermally-activated events. This is most often a more efficient approach with respect to previous computationally heavy methods. In a future perspective, similar schemes can be potentially used to calculate other quantities than activation energies. They can thus transfer atomic-scale properties to higher-scale simulations, providing a proper bridging across scales, and hence contributing to the achievement of accurate and reliable multiscale models.

1. Introduction

It all starts with an energetic particle, often a neutron, hitting an atom. This statement could be found at the inception of any manuscript, report, or presentation at a conference, undertaking a complete characterization of the effects of irradiation in structural materials. The devil thus hides from the smallest time- and length-scales, at the atomic level, and even below, at the electronic level. Irradiation with bombarding particles (provided they are energetic enough) results in a continuous creation of point-defects in the bulk of the studied material, i.e., vacancies (Vac) and self-interstitials atoms (SIA). The increased concentration of vacancies will then enhance the kinetics of diffusion-driven process (such as precipitation of insoluble species), but might also alter the thermodynamic equilibrium, as a consequence of the establishment of fluxes of them towards sinks. Moreover, SIA are produced. They are essentially absent in unirradiated materials. SIA exhibit a profoundly different behaviour from vacancies, potentially giving rise to processes not normally observed in materials. SIA migrate generally faster than vacancies and sometimes they follow one-dimensional diffusion paths, exhibiting in addition longer range elastic interactions of a highly anisotropic character. The changes induced in the material by the production and diffusion of these defects, as observable at the macroscopic scale, are thus not only irradiation-enhanced, but often irradiation-induced.

Because it all starts at the atomic level, thorough and non-empirical physical models capable of describing the effects of irradiation up to the macroscopic level must necessarily entail a largely multiscale strategy. Fig. 1 depicts an overview of a modelling approach based on kinetic Monte Carlo (KMC) methods, which is one of the possible choices to bridge the gap from the electronic to coarse-grained level. Other possible approaches are mean field models, rate theory, cluster dynamics, etc. Interested readers are directed to Ref. [1,2] for a general overview. Addressing the macroscopic level requires higher-scale models such as dislocation dynamics and continuum mechanics calculations with adequate plastic flow laws: these are not shown in Fig. 1. In the lowest left corner, two fundamental sources of input data are: (a) Calculations based on first principle physics to address the electronic structure, most often using the density functional theory (DFT);

☆ This article belongs to the special issue: Radiation Effects

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https://doi.org/10.1016/j.commatsci.2018.02.025
0927-0256/

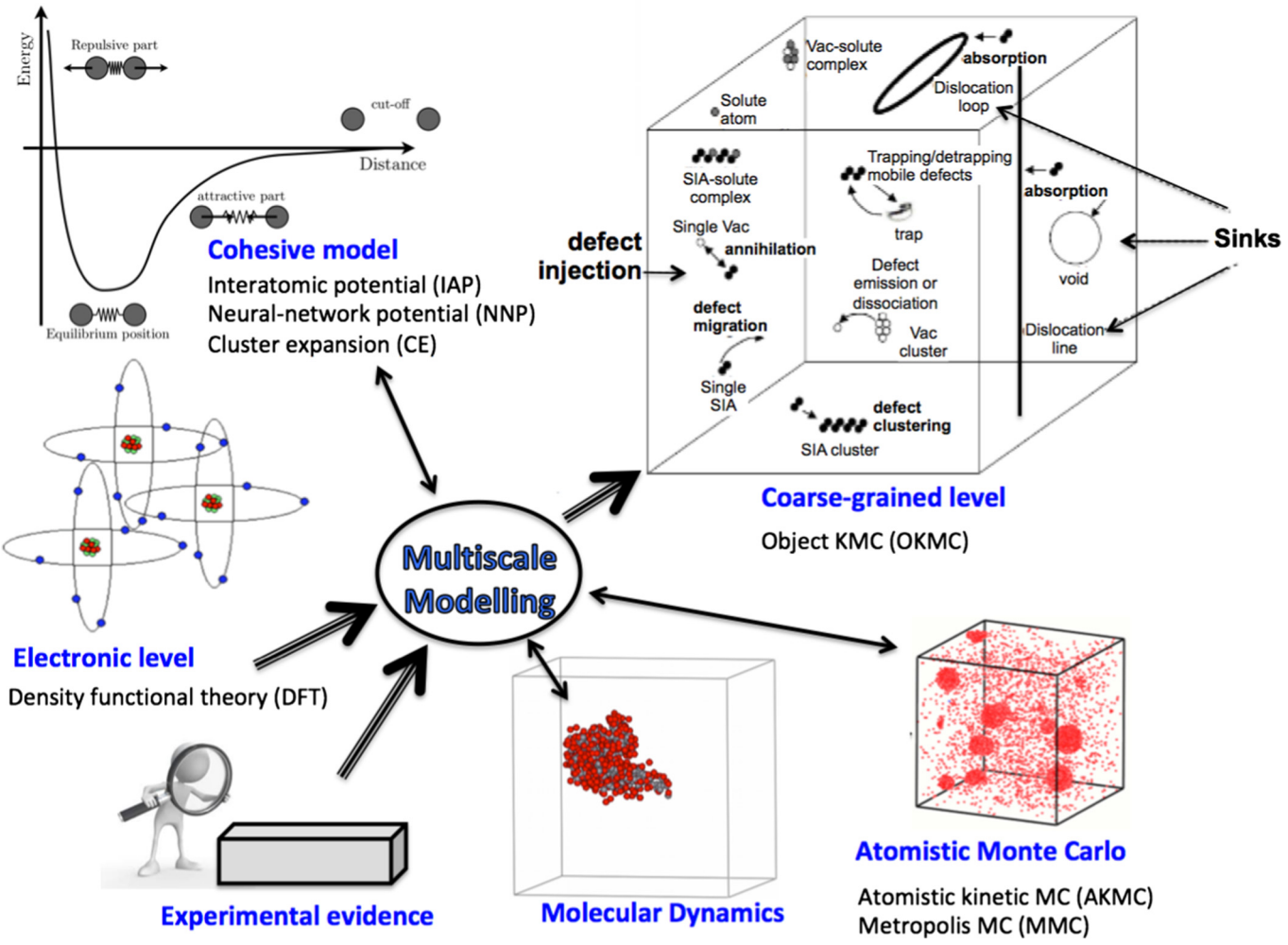

Fig. 1. Multiscale modelling approach for describing the effects of irradiation in structural materials.

(b) Any kind of experimental evidence, which can be of a wide variety, ranging from formation energies, diffusion coefficients, elastic constants, phase diagrams, etc. Unquestionably, experimental evidence remains the only true final judge on any model prediction. The story ends at the coarse-grained level, which is in this work implemented by the object kinetic Monte Carlo (OKMC) method. There, the processes undergone by the defects injected during irradiation are described as thermally-activated events that correspond, for the objects involved, generally clusters of point-defects, to specifically designed laws for mutual interactions, mobility and stability. All regular elements of the microstructure are also explicitly present in the model, for example grain boundaries, dislocations, solute or foreign interstitial impurities. A substantial number of reactions must be carefully parametrised in OKMC models, which is achieved summoning a variety of methods and models at lower scales, ranging from DFT, molecular dynamics, and atomistic kinetic Monte Carlo.

Playing the role of a reference metrics for the physical description of the studied material, vital pieces of this puzzle are, undoubtedly, cohesive models. Given a set of atoms described by their coordinates in space and their chemical species, their task is to provide a numerical value for the total energy of the system in any configuration, determining the driving forces for its evolution, including interatomic forces. In a quantum mechanism framework, *Ab initio* methods, e.g., DFT, are, for many good reasons, regarded as the most reliable choice to explore the energy landscape of the system. There are, however, limitations. Firstly, some degree of empiricism remains. Unfortunately, a blind use of DFT may, in some cases, provide imperfect predictions (see e.g. [3,4]). Secondly, even with state-of-the-art computing facilities, using DFT still implies a huge cost in CPU resources which is often unaffordable and, sometimes, unwarranted. For these reasons, alternative cohesive models are still extensively used, empirical interatomic potentials (IAP) being a very popular example. On the one hand, in addition to the largely reduced computing cost, the main advantage of these potentials is the possibility to achieve a tunable compromise between various target properties. It can mix DFT-originated with experimental-originated data, as conveniently as required. For example, the FeCu potential proposed by Pasianot et al. in Ref. [5] was fitted to faithfully reproduce the experimentally observed Cu solubility limit in Fe, whereas DFT is known to underestimate it (see discussions in Ref. [4]). The affordable computing time allows large and complex systems, containing up to several million atoms, to be studied. On the other hand, the simplicity proper to IAP also implies an intrinsic limitation in their capacities of making accurate prediction of various set of properties at the same time.

Suitable low-computing-cost cohesive models allow the gap between the basic atomic level and the realm of longer time-scale Monte Carlo (MC) models to be bridged. Many more gaps remain to bridge, however. Even using IAP, the precise calculation of the energy barriers the system has to overcome through thermal activation, which are at the core of MC methods, pose severe