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Multiscale modeling of irradiation hardening: Application to important nuclear materials

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ABSTRACT

The recent progress in investigation techniques and the accumulation of relevant simulation results across the scales allow the development of a multiscale modeling framework for the rationalization, analysis and physical assessment of the flow stress of many industrial materials, with almost no fitting parameters. Although the construction of this framework is not yet complete, it has reached a maturity level enabling the investigation of some complex properties such as irradiation hardening. In this paper, modeling and experimental results are reviewed in order to derive the constitutive equations of the yield stress and of its fundamental components accounting for the microstructure features, such as dislocation network, precipitates, dislocation loops and voids. This approach is challenged in the case of reactor pressure vessel, high-Cr ferritic-martensitic and austenitic stainless steels. Predictions are discussed in connection with the well-known experimental trends reported in the literature.

Contents

1. Introduction

With the widespread use of nuclear energy around the world and the need to guarantee safety to continue its exploitation, including the option of extending the lifetime of existing plants, the prediction of the evolution of materials properties under irradiation has acquired a large economic impact. On the other hand, radiation effects involve many fundamental mechanisms in materials science, which has aroused the interest and the curiosity of the

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scientific community [1]. Although, radiation-induced embrittlement has been revealed longtime ago [2,3], the very nature and effect of the radiation-induced defects are still controversial in spite of the large investigation efforts made during decades. This can be attributed to many specific difficulties [4,5]. The radiation microstructure is highly sensitive to many parameters, such as the chemical composition, the fabrication process, irradiation temperature, fluence and flux. On the other hand, the nanometric size of the radiations defects significantly hampers experimental characterization and challenges the ability of the elastic theory to determine the nature, strength and outcome of the interaction of radiation defects with dislocations. A glaring example is the case of Solute Clusters (SCs) found in almost all irradiated industrial materials. Even using recent and sophisticated investigation techniques, it is not clear whether they are solute atoms atmosphere as shown in Atom Probe Tomography (APT) [6] or simply coherent precipitates as deduced from Small Angle Neutron Scattering (SANS) and other techniques [7]. Their association with point-defect clusters is equally debated. The ambiguity in determining the nature of SCs has strong impact on the interpretation of the experimental results. In classical metallurgy, coherent precipitates are known to cause substantial strengthening [8], while one can hardly conceive how a small diffuse clusters can efficiently impede dislocation mobility [9]. The determination of the nature and configuration of radiation defects is necessary to rationalize the evolution of the mechanical properties observed in experiment.

Even if the radiation microstructure was known with sufficient precision, its impact on the mechanical properties at all the relevant scales remains difficult to assess. At the atomic scale, radiation affects the matrix composition [10], creates cascade damage [11], enhances solute diffusion, etc. On the largest scale, the transition temperature of RPV steels is found to increase, while fracture toughness significantly drops at high irradiation dose [12,13]. Although the prediction of the macroscopic behavior induced by a specific radiation microstructure is complex too, it is often minimized in the efforts relating dose to damage, compared with the efforts dedicated to the prediction of the irradiation microstructure.

Combining the difficulties in predicting the evolution of the microstructure with those pertaining to the determination of the corresponding mechanical properties, it is difficult to physically assess radiation embrittlement. This is why most of the available correlations are more or less empirical [2], which keeps open the perspective of rationalization and prediction of radiation effects on physical basis.

A possible simplification of the problem is to separate the question of the evolution of the microstructure from that of the impact of a given microstructure on the mechanical properties. In this paper, the first feature will not be discussed. As illustrated in Fig. 1, the review focuses on the impact of the microstructure on the yield stress.

Given the nanometric size of radiation defects, the characterization of their interactions with moving dislocations by the current experimental techniques is not straightforward. In this context, numerical simulations can provide deep insights into the physical mechanisms involved in defect formation and interaction with dislocations [14]. The most investigated scale in nuclear science, which is also the most mature, is the atomic scale, including Density Functional Theory (DFT) [15], Molecular Statics and Dynamics, referred to as Atomistic Simulations (ASs) [16] and all variants of probabilistic methods [17,18]. ASs were of great help in identifying features of primary importance, such as the defect-dislocation interaction strengths and outcomes. Simulations at the larger scale (mesoscopic dislocation scale), such as line tension-based simulations [19], quasistatic dislocation dynamics [20], discrete Dislocation Dynamics (DD) [21], field dislocation mechanics [22], etc., have surprisingly received much less attention from the irradiation community. Most of these techniques are relatively recent and dedicated to the prediction of the collective behavior of dislocations, that is, the mechanical response at the grain scale. Simulations at the polycrystal scale [23] (homogenization, finite elements, etc.) are even less popular. In the absence of studies pertaining to the dislocation scale and to the appropriate scale transitions, it is almost impossible to inject more physical knowledge in the mechanical part of the current dose-damage

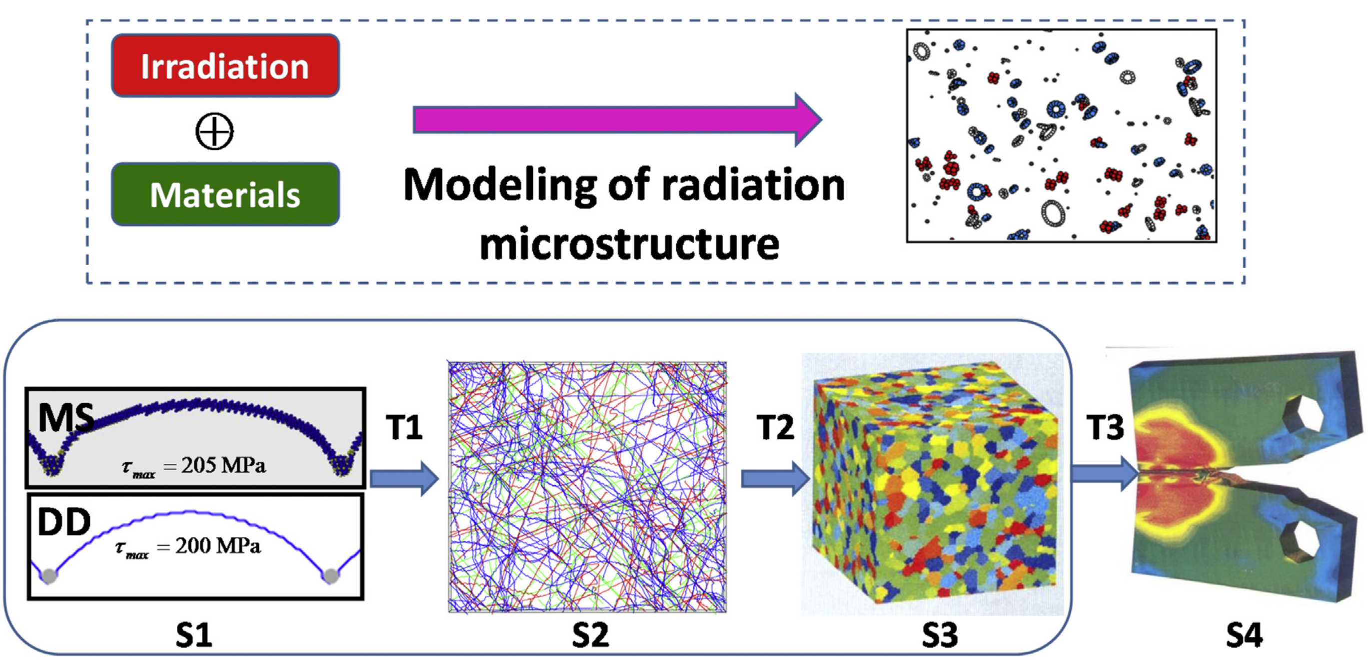

Fig. 1. Modeling efforts in radiation materials science. The upper part represents modeling of the microstructure evolution under irradiation. The lower part sketches the modeling of mechanical properties at the relevant scales (S1, S2 …) and using scale transitions (T1, T2 …). The scope of the review is delineated by the lower rectangle.

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