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A self-consistent plasticity theory for modeling the thermo-mechanical properties of irradiated FCC metallic polycrystals

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ABSTRACT

A self-consistent theoretical framework is developed to model the thermo-mechanical behaviors of irradiated face-centered cubic (FCC) polycrystalline metals at low to intermediate homologous temperatures. In this model, both irradiation and temperature effects are considered at the grain level with the assist of a tensorial plasticity crystal model, and the elastic-visocoplastic self-consistent method is applied for the scale transition from individual grains to macroscopic polycrystals. The proposed theory is applied to analyze the mechanical behaviors of irradiated FCC copper. It is found that: (1) the numerical results match well with experimental data, which includes the comparison of results for single crystals under the load in different directions, and for polycrystals with the influences of irradiation and temperature. Therefore, the feasibility and accuracy of the present model are well demonstrated. (2) The main irradiation effects including irradiation hardening, post-yield softening, strain-hardening coefficient (SHC) dropping and the non-zero stress offset are all captured by the proposed model. (3) The increase of temperature results in the decrease of yield strength and SHC. The former is attributed to the weakened dislocation–defect interaction, while the latter is due to the temperature-strengthened dynamic recovery of dislocations through the thermally activated mechanism. The present model may provide a theoretical guide to predict the thermo-mechanical behaviors of irradiated FCC metals for the selection of structural materials in nuclear equipment.

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1. Introduction

Due to the significant roles and important applications for next-generation nuclear reactors, metallic polycrystals used as structural materials in nuclear equipment are often exposed to severe irradiation and high temperature environment. The study of the nonlinear thermo-mechanical responses of irradiated polycrystalline metals at low to intermediate homologous temperature has been motivated in recent years (Odette and Lucas, 2001; Fabritsiev and Pokrovsky, 2011; Zinkel and Was, 2013).

Numerous experiments have been devoted to investigate the irradiation and temperature effects on metallic materials under mechanical loading (Singh et al., 1997, 2001; Victoria et al., 2000; Fabritsiev and Pokrovsky, 2011). Under irradiation, atoms in the material could be removed from their original lattice positions by the impact of high energy particles, such as neutrons and protons. Consequently, experimentally detectable defects including interstitials, vacancies, defect clusters (precipitates, dislocation loops (DLs) and stacking fault tetrahedrons (SFTs)) would be formed (Samaras and Victoria, 2008). At low displacements per atom (dpa < 0.1) and intermediate homologous temperature ($T \leq 0.3T_m$), the main defects are defect loops in irradiated BCC metals while SFTs in irradiated FCC metals (Singh et al., 1995; Satoh et al., 2004; Fabritsiev and Pokrovsky, 2009). These less movable defects usually act as obstacles and impede the movement of dislocations. Therefore, extra stresses are needed to force slip dislocations to get through the immobile defects, which results in irradiation hardening. Once the onset of yielding, the defects would be annihilated by the passage of dislocations and defect free channels could be formed, which may lead to the heterogeneous flow localization and yield dropping in most irradiated metals (de la Rubia et al., 2000). The main mechanical behaviors of irradiated metals include irradiation hardening, post-yield softening, strain-hardening coefficient (SHC) dropping and yield stress decreasing with the increase of temperature. To analyze the influences of irradiation dose and temperature on SHC and irradiation hardening, Fabritsiev and Pokrovsky (2007, 2009) performed a series of experiments on irradiated FCC materials. It was found that the increase of the irradiation dose will lead to the drop of SHC, while the increase of temperature will result in the decrease of yield stress. Therefore, the irradiation-induced defect–dislocation interaction and temperature both play very important roles in the mechanical behaviors of irradiated metals.

To reveal the fundamental mechanisms underlying the localization phenomena in irradiated materials, computational simulations such as molecular dynamics (MD) and dislocation dynamics (DD) simulations have been performed (de la Rubia et al., 2000; Martinez et al., 2008; Marian et al., 2009; Bai et al., 2010; Arsenlis et al., 2012; Song et al., 2014). For example, to get insight into the progress of hardening and embrittlement in irradiated BCC Fe, Arsenlis et al. (2012) used DD simulations with different concentrations of dislocations and found the highly localized inhomogenous interaction between defect loops and slip dislocations. For irradiated FCC materials, de la Rubia et al. (2000) revealed the plastic flow localization mechanisms in defect-free channels by applying three-dimensional multiscale simulations, which includes both MD and DD simulations. It should be noted that the interaction progress between SFTs and slip dislocations in irradiated FCC systems could be more complicated than the dislocation–loop interaction in irradiated BCC systems due to the complex three dimensional geometry of SFTs (Robach et al., 2006).

Because of the high cost of irradiation experiments as well as the time-scale and spatial-scale limitations of MD and DD simulations, theoretical modeling becomes an important approach in the study of fundamental mechanical behaviors of irradiated metals (Seeger, 1958; Blewitt et al., 1960; Singh et al., 1997). In fact, irradiation damage is in nature a multi-scale problem that the temperature dependent interaction between irradiation-induced defects and dislocations inside individual grains at microscale will determine the macroscopic properties of irradiated polycrystalline materials. Therefore, two key issues should be considered to model the thermo-mechanical behaviors of irradiated metallic polycrystals: (1) the appropriate depiction of the defect–dislocation interaction with temperature effect at the grain level, and (2) the effective scale transition from microscopic scale to macroscopic scale.

Recently, several crystal plasticity models have been proposed to consider the effects of irradiation and temperature on mechanical behaviors (Beyerlein and Tomé, 2008; Krishna et al., 2010; Patra and McDowell, 2013; Barton et al., 2013; Xiao et al., 2015). For instance, Beyerlein and Tomé (2008) incorporated the temperature effects into the evolution law of dislocation density, and proposed a crystal model for single phase HCP materials, which can study the temperature-dependent transition from the slip-dominated to twinning-dominated deformation. Patra and McDowell (2013) formulated a continuum constitutive crystal plasticity model to simulate the post-irradiation behaviors of BCC materials, and the localized deformation because of the formation of dislocation channels were studied. The first tensorial plasticity model for irradiated BCC Fe was proposed by Barton et al. (2013) to capture the plastic flow localization in defect free channels, and it was suggested that the interaction between the defect loops and the slip dislocations can hardly happen when the dislocation slip plane coincides with the defect habit plane. While for irradiated FCC metals, due to the three-dimensional geometry of defect SFTs, the spatial dependent SFT–dislocation interaction will be more complicated (Robach et al., 2006). Xiao et al. (2015) recently proposed an irradiated tensorial crystal model to consider the spatial dependent interaction between irradiation-induced SFTs and slip dislocations. It should be noted that in those models mentioned above, the effects of irradiation and temperature on the mechanical behaviors of materials are considered separately. Irradiation will induce irradiation hardening because of the impediment of slip dislocations by irradiation-induced defects, while, the increase of temperature could lead to the decrease of flow stress owing to the thermal activation progress of dislocations. In most cases, the effects of irradiation and temperature on the behaviors of polycrystalline metals may exist simultaneously. For example, as observed in the experiments for irradiated FCC metals at different temperatures (Fabritsiev and Pokrovsky, 2007, 2009), both the defect–dislocation interaction strength