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Modeling dislocation structure development and creep–swelling coupling in neutron irradiated stainless steel

A.A. Semenov [a,b], C.H. Woo [a,*]

[a] Department of Electronic and Information Engineering, The Hong Kong Polytechnic University, Kowloon, Hong Kong SAR, China
[b] On Leave from Institute for Nuclear Research, Russian Academy of Sciences, Moscow, Russia

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ABSTRACT

Anisotropic nucleation and growth of multi-classes of dislocation loops under the combined actions of fast-neutrons and an external applied stress are considered in modeling dislocation structure development in metals and alloys. The stochastic nature of the nucleation kinetics is formulated via the Fokker–Planck equation. The strain derived from the climb of the anisotropic dislocation structure is separable into volumetric and deviatoric components, corresponding respectively to swelling and creep. The creep contribution resulting from the development of the stress-induced dislocation anisotropy is found to be very significant and exhibits a strong correlation with swelling. For stainless steel, our model explains very well the complex deformation behavior observed in a wide variety of in-reactor experiments.

1. Introduction

Microstructure record left by an applied stress in stainless steels during irradiation is often found characterized by an anisotropic dislocation structure [1–5]. This is evident [5] of the operation of stress-induced preferred absorption (SIPA) [6–11], a mechanism that may produce irradiation deformation both directly and indirectly. Directly, deviatoric strain is produced by the differential climb speeds of dislocations with different orientations due to the stress-induced bias differential. The associated creep rate is directly calculable based on point-defect properties obtainable from atomistic methods [6], and has been the focus of most irradiation creep studies [7–11]. Indirectly, the stress-induced differential climb creates an anisotropic dislocation structure [4,5], which causes deformation via a mechanism called SIPA-induced growth (SIG) [12]. Theoretical estimates indicate that the associated strain rate is sensitive to the swelling rate, with magnitudes that may be very significant [12–14].

Experimentally, in-reactor deformation measurements in stainless steels [15–25] indeed exhibit two components, one independent of swelling and the other coupled to swelling and has a strain rate directly proportional to the swelling rate. In addition, irradiation creep is often observed to be accompanied by an anisotropic dislocation structure [5,20–25]. At the same time, the strain rate usually persists for a substantial period of time, even after the applied stress is removed [5]. These observations are strongly reminiscent of the operation of SIG.

Most theories on irradiation-induced deformation have focused on the direct component [7–11]. The indirect component is difficult to calculate, absent a good theory for interstitial loop nucleation under an applied stress. Any investigation in this respect has to be limited to qualitative studies based on simplifying assumptions [12–14].

Recent developments in the theory of nucleation kinetics [26,27] provide a good basis for treating the high sensitivity of nucleation events to the net point-defect flux. The successful modeling of nucleation and growth of dislocation loops in unstressed samples in [26,27] helps explain dislocation structure development with production bias [28] operating. In the present paper, this theory is extended to treat the nucleation and growth of multi-classes of differently oriented dislocation loops in the development of dislocation structure under an applied stress.

The objective of this paper is to holistically study irradiation deformation in stainless steels, particularly the coupling between creep and swelling associated with dislocation structure development under an applied stress. Comparing the calculated results with the experimental ones in the literature, we also hope to clarify the role of the stress-induced anisotropy of the dislocation structure in the complex deformation behavior of stainless steels under stress in a fast-neutron flux. Finally, the comparison may also test the predictive capability of our dislocation structure development model in the presence of an applied stress.

* Corresponding author. Tel.: +852 2766 6646.
E-mail address: chung.woo@polyu.edu.hk (C.H. Woo).

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2. Formulation

2.1. Preliminary considerations

Under cascade damage conditions of a fast-neutron flux, we have to face the complication that a significant fraction of primary interstitials produced are retained in clusters. Recognition of this fact has led to the introduction of the production bias concept [28]. This concept is based on the premise that point defects in clusters do not participate in the conventional segregation of interstitials and vacancies via preferential attraction of single interstitials to dislocations. However, within this concept, the commonly observed network formation via the nucleation and growth of sessile Frank interstitial loops does not seem plausible. Indeed, at elevated temperatures, vacancy clusters are thermally unstable, so that the supersaturation of single vacancies is higher than that of the single interstitials. The mean net vacancy flux received by the thermally stable primary interstitial clusters makes nucleation impossible without statistical variations. In reality, however, the net vacancy flux fluctuates because of the stochastic nature of migratory jumps and cascade initiation, so that interstitial loop nucleation and growth is not a deterministic, but a probabilistic event. In this connection, a stochastic treatment such as followed in [26,27] is necessary. To consider the action of external stress, this approach can be extended to take into account the loop orientation dependence of the nucleation rate. The details will be discussed in the following subsection.

In a related issue, the effects of one-dimensional transport of small interstitial clusters [29–31] observable in computer simulations in pure metals [32] on interstitial loop nucleation and growth should be considered. However, the invariable presence of compositional disorder in the crystal lattice due to alloying and various thermal–mechanical treatment may lead to the trapping or scattering of the clusters [6,33–35], drastically reducing the likelihood of long-range one-dimensional transport of interstitial defects. Moreover, recent investigations [36,37] showed that void lattice formation in "pure" metals cannot occur if more than ~1% of the interstitial atoms undergo one-dimensional diffusion. The development of large-scale heterogeneous void swelling found near grain boundaries and dislocation walls can also be understood without invoking the one-dimensional diffusion [38–40]. Most importantly, the majority of void swelling models that have stood the test of decades of experiments do not require the involvement of 1-D SIA kinetics. All these suggest that the inclusion of one-dimensional diffusion in irradiation-damage studies may not always be necessary. Accordingly, we neglect the effects of the 1-D diffusion SIA component in the present paper.

Small interstitial clusters coalesce with faulted loops during climb, and may also serve as a source of interstitials to their growth. This is clear from the in situ observations in dual-beam experiments of Jenkins [41]. Indeed, both numerical [42] and analytical [26,27] calculations show that sufficiently large interstitial loops may grow under the combined action of the dislocation bias and continuous loop coalescence, despite the net vacancy flux that they receive. The swelling produced by loop growth in this way is in quantitative agreement with experiments [26,42].

2.2. Evolution equations of the Frank loops

Different populations of Frank interstitial loops and network dislocations of different classes have different dislocation biases according to their orientations with respect to the applied stress [11]. The governing equation for evolution of the Frank loop population of each class is similar to that previously derived for the case of a single class of dislocations [26,42–43]. With the last two terms describing the creation and annihilation of loops in the population, the evolution of the kth loop class can be described by the Fokker–Planck equation:

$$\frac{\partial f_{ik}(n,t)}{\partial t} = -\frac{\partial}{\partial n}\left\{V_{ik}(n) - \frac{\partial}{\partial n}D_{ik}(n)\right\}f_{ik}(n,t) + \frac{\varepsilon_{ik}G}{n_{ig}}\delta(n-n_{ig}) - \left.\frac{\partial f_{ik}(n,t)}{\partial t}\right|_{\text{loss}} \quad (1)$$

Here $f_{ik}(n, t)$ is the distribution function of interstitial loops of the kth class in the space of loop sizes n at time t. Small immobile interstitial clusters continuously generated in collision cascades are considered as interstitial loop embryos. In the spirit of the production bias theory [28], the formation of loop embryos are assumed to be intra-cascade events, and the initial sizes, n_{ig}, of the loop embryos are the same for all loop classes, as reflected by the δ-function in Eq. (1). They are treated as small dislocation loops of radius $r_i = (n\Omega/\pi b)^{1/2}$, where n is the number of interstitials in the cluster, Ω is the atomic volume, b is the Burgers vector. The rate of generation of embryos in collision cascades is given by $\varepsilon_{ik}G/n_g$, where G is the *effective* generation rate of point defects both in cluster and free form [28], and ε_{ik} is the fraction of interstitials forming embryonic loops of the kth class.

The "diffusivity" $D_{ik}(n)$ in Eq. (1) describes the stochastic spread of the size distribution of interstitial loops in time due to random fluctuations in the point-defect fluxes [43,44],

$$D_{ik}(n) = D^s_{ik}(n) + D^c_{ik}(n), \quad (2)$$

with

$$D^s_{ik}(n) = \left(\frac{\pi n}{\Omega b}\right)^{1/2}(Z_{ik}D_iC_i + Z_{\nu k}D_\nu C_\nu), \quad (3)$$

$$D^c_{ik}(n) = \frac{N_d G n}{4b}\left[Z^2_{\nu k}\frac{\langle N^2_{d\nu}\rangle}{k_\nu N^2_d} + Z^2_{ik}\frac{\langle N^2_{di}\rangle}{k_i N^2_d}\right], \quad (4)$$

where Z_{jk} ($j = i, \nu$) is the reaction constant between the loop of the kth class and point defects, C_j and D_j are respectively the average concentration of point defects and their diffusion coefficient. N_d is the average number of point defects generated per cascade both in cluster and free form, $\langle N^2_{dj}\rangle$ is the average square of the number of vacancies and interstitials generated per cascade. We also denote the total sink strength for vacancies by $k_\nu{}^2$, and for mobile interstitials by $k_i{}^2$. The two terms on the right-hand side of (2) are, respectively, the contribution to D_{ik} due to the randomness of the point-defect jumps, and that of the cascade initiation [43,44].

The "drift velocity" $V_{ik}(n)$ consists of the two terms. The first one is given by the conventional expression for the growth rate of interstitial loops due to point-defect absorption:

$$V_{ik}(n)|_{pd} = \frac{2\pi r_i(n)}{\Omega}(Z_{ik}D_iC_i - Z_{\nu k}D_\nu C_\nu). \quad (5)$$

The second one represents the rate of change in the loop size due to the absorption of smaller loops by coalescence and has the following form [26,42]:

$$V_{ik}(n)|_{cls} = \frac{2\pi r_i(n)}{\Omega}\int_{n_{\min}}^{n} x f_{ik}(x,t)W_k(x,n)dx \quad (6)$$

Here $n_{\min}$ is the size of interstitial clusters at which they become mobile. According to Eq. (6), in the present approach the loop coalescence is restricted only to the coalescence of the loops with the same orientation.

The coalescence between loops of sizes n' and n ($n' < n$) is described by the reaction constant $W_k(n',n)$ [26,42],

$$W_k(n',n) = \frac{4r_i(n')}{b}\left[D_{lk}(n) + (D^2_{lk}(n) + V^2_{lk}(n)b^2/4)^{1/2}\right], \quad (7)$$