A void nucleation and growth based damage framework to model failure initiation ahead of a sharp notch in irradiated bcc materials

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Modeling the effect of irradiation-induced flow localization on failure initiation ahead of a sharp notch in bcc materials

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Abstract

A continuum damage framework is developed and coupled with an existing crystal plasticity framework, to model failure initiation in irradiated polycrystalline bcc materials at intermediate temperatures. Constitutive equations for vacancy generation due to inelastic deformation, void nucleation due to vacancy condensation, and diffusion-assisted void growth are developed. The framework is used to simulate failure initiation at dislocation channel interfaces and grain boundaries ahead of a sharp notch. Evolution of the microstructure is considered in terms of the evolution of inelastic deformation, vacancy concentration, and void number density and radius. Evolution of the damage, i.e., volume fraction of the voids, is studied as a function of applied deformation. Effects of strain rate and temperature on failure initiation are also studied. The framework is used to compute the fracture toughness of irradiated specimens for various loading histories and notch geometries. Crack growth resistance of the irradiated specimens are computed and compared to that of virgin specimens. Results are compared to available experimental data.

Keywords: damage, void, irradiation, dislocation channel, bcc.

1. Introduction

The mechanical behavior of irradiated metals loaded in tension is characterized by an increase in yield stress, decrease in ductility and lower strain to failure (Klueh and Vitek, 1989; Rowcliffe et al., 1998; Spätig et al., 1998). The deformed microstructure shows formation of narrow dislocation channels along which majority of the inelastic deformation is localized (Farrell et al., 2004; Hashimoto et al., 2001; Lупpo et al., 2000). The observed mechanical behavior may be correlated to the irradiated microstructure, which shows the formation of a large number of irradiation-induced defects, e.g., interstitial loops, complex dislocation networks, voids, precipitates, etc. Glide of dislocations through the field of these defects becomes difficult, thus contributing to irradiation hardening and an increase in the yield stress (Lucas, 1993). When the dislocations have achieved enough driving force, they glide along preferred crystallographic directions, sweeping out the radiation-induced defects (Arsenlis et al., 2012). This leads to the formation of defect-depleted dislocation channels, which provide paths for easy dislocation glide and flow localization in irradiated materials (Luft, 1991). The dislocation channels are typically 50-200 nm wide (Eyre, 1962; Lупpo et al., 2000; Rice and Zinkle, 1998). The spacing between channels is of the order of $\sim 10 \mu\text{m}$ in the uniformly deformed region. However, the channels have been found to be more dense near the fracture surfaces; the channel spacing decreases by more than an order of magnitude from that in the uniformly deformed region (Zinkle and Singh, 2006).

Flow localization along these dislocation channels correlates to failure in irradiated alloys. In terms of mechanical properties, the fracture toughness has been found to universally degrade with increasing radiation dose under quasi-static loading (Little, 1986; Lucas, 1993; Maloy et al., 2001; Rowcliffe et al., 1998). Fracture has been found, in many cases, to propagate along the ‘faceted’ interfaces of dislocation channels with the uniformly deformed bulk (Chaouadi, 2008; Fish and Hunter, 1976). Further, intergranular cracks have been found to initiate at the intersections of dislocation channels and grain boundaries (West et al., 2012). Inability of grain boundaries (GBs) to accommodate the highly localized strains from dislocation channels has been suggested as one of the dominant factors contributing to irradiation assisted intergranular stress corrosion cracking (McMurtrey et al., 2011).

These experimental observations motivate the present study of flow localization and failure initiation ahead of a sharp notch in irradiated bcc materials by coupling crystal plasticity models with nucleation and growth of damage. A void nucleation and growth-based continuum damage framework is developed and coupled to an existing defect density-based crystal plasticity framework for irradiated bcc materials (Patra and McDowell, 2013, 2012) to explore dislocation channel patterns, and void nucleation and growth in the regions of high stress triaxiality ahead of the notch. Effects of loading rate and temperature on failure initiation are studied. The framework is also used to predict the crack growth resistance and fracture toughness of irradiated specimens.

2. Background

2.1. Flow localization and ductile failure in irradiated metals

Failure in irradiated metals is triggered, in many cases, by plasticity mismatch at the interface of dislocation channels with the uniformly deformed bulk. The fracture surface of a ferritic/martensitic Eurofer-97 steel, irradiated at 300°C, shows evidence of ‘zigzag’ fracture, and the dimples associated with ductile failure become more shallow with increasing radiation dose, suggesting pathways of localized shear, in particular (Chaouadi, 2008). *This ‘zigzag’ fracture pattern suggests a faceted crack path along intertwined dislocation channels in the deformed material.* It was proposed (Chaouadi, 2008) that plasticity mismatch, at the interface of the ‘hard’ matrix and the ‘soft’ dislocation channel, promotes void nucleation, growth and coalescence, ultimately resulting in failure. It was also found (Chaouadi, 2008) that the crack growth resistance of the quasi-statically loaded irradiated material degrades significantly as compared to the unirradiated material. This was attributed to the occurrence of mixed mode (Mode I + II) fracture ahead of the crack tip. However, the crack resistance was found to increase under dynamic loading and was comparable to that of the virgin, unirradiated material.

Observation of ‘shallow’ ductile fracture was also reported for irradiated 9Cr-1Mo martensitic steel at both room temperature and at 250°C, along with evidence of secondary cracks, which were not present in the *virgin, unirradiated* specimens (Henry et al., 2003). Further, evidence of limited-ductility ‘channel’ fracture with separation of fracture surfaces along localized-shear dislocation channel paths has been found in 304 stainless steel (Fish and Hunter, 1976), 321 austenitic steel (Little, 1986), and 308 and 316 stainless steel (Michel and Gray, 1987) at elevated temperatures and high radiation doses. Fracture surfaces show relatively flat facets along dislocation

channels that intersect and are intertwined with other channels (Fish and Hunter, 1976), akin to the ‘zigzag’ fracture (Chaouadi, 2008) mentioned earlier, but without any dimples. This ‘channel’ fracture mechanism may be considered as a limiting case of transgranular ductile failure along dislocation channels in irradiated metals with little or no dimple formation.

Note that failure in irradiated materials does not always occur by ductile fracture. Although the quasi-static fracture toughness of metals has been found to universally degrade as a result of radiation, the failure mode is temperature dependent, with brittle cleavage fracture occurring at low test temperatures (Jia and Dai, 2006) and an increase in the apparent ductile-brittle transition temperature (DBTT) with increasing radiation (Dai et al., 2003; Wakai et al., 2005; Was, 2007). In a recent study (Byun et al., 2013), it has been shown that the irradiation temperature has a dominant effect on the fracture toughness, as opposed to irradiation dose, in the regime of moderate to high radiation doses (3-148 dpa). Brittle fracture was observed when the ferritic/martensitic HT9 steel was irradiated at temperatures below 400°C, while ductile fracture was observed when the irradiation temperature was higher (Byun et al., 2013).

2.2. Models for void nucleation and growth

Ductile failure occurs by nucleation, growth and coalescence of voids subsequent to significant plastic deformation in metals (Anderson, 2005). In unirradiated metals, nucleation of voids generally occurs at the interfaces of second phase particles and inclusions. Voids may nucleate by the condensation/clustering of vacancies in regions of heavy plastic deformation (Cuitiño and Ortiz, 1996). Under the influence of high plastic strain and hydrostatic stress (developed due to plastic instability during tensile loading, for example), these voids grow rapidly and coalesce, thus forming macroscopic flaws or cracks.

The physics of void nucleation has been studied using the classical theory of heterogeneous nucleation at interfaces (GBs, inclusions) (Chen and Argon, 1981a; Hirth and Nix, 1985; Raj and Ashby, 1975; Raj, 1978; Wang et al., 1985; Yoo and Trinkaus, 1983). In these studies, it is implicitly assumed that the driving force for void nucleation is derived from the condensation of supersaturated vacancies (cf. (Brager et al., 1977; Hirth and Nix, 1985)), while not explicitly tracking the vacancy concentration in the material. The energy barrier and critical radius for void nucleation was calculated given the applied normal stress and interfacial energy at GBs and second phase particles (Raj and Ashby, 1975; Raj, 1978), and also considering local internal stresses due to the presence of voids (Hirth and Nix, 1985). A major conclusion from all these calculations was that high local stress concentration, more specifically high tensile normal stresses, are necessary for voids to nucleate. Based on experimental observations of voids in 304 stainless steel under creep loading (Chen and Argon, 1981a), it was also concluded that many of the voids were formed in the material prior to mechanical loading, possibly during primary forming processes, thus bypassing the requirement for the presence of high stress concentration for voids to nucleate.

It should be noted that majority of the studies mentioned here concern intergranular fracture under quasi-static tensile or creep loading. In the context of the present problem, heterogeneous void nucleation is of interest because localization of deformation along dislocation channels in irradiated materials leads to the formation of interfacial regions with plasticity mismatch within the grains. In regions of high stress concentration (e.g., ahead of a sharp

notch or crack-tip), nucleation and growth of voids would presumably be promoted at such interfaces, ultimately leading to transgranular ‘zigzag’ fracture (Chaouadi, 2008) or ‘channel’ fracture (Fish and Hunter, 1976).

The problem of void growth has received much attention in the past, especially in the context of correlating void growth with macroscopic applied stress and plastic strain. The mechanics of void growth is generally studied using/extending models developed most notably some 30-40 year ago (Gurson, 1977; McClintock, 1968; Rice and Tracey, 1969; Tvergaard and Needleman, 1984; Tvergaard, 1982, 1981). The influence of stress triaxiality and plastic strain on the growth rate of an isolated cylindrical void was first studied by McClintock (1968). Analytical solutions of the growth of an isolated spherical void in a perfectly plastic material (Rice and Tracey, 1969) showed an exponential dependence of the growth rate on the stress triaxiality ratio. Gurson (1977) considered material softening as a result of void growth and developed a void porosity-dependent, and hydrostatic stress-dependent plastic potential function for a cell containing a void. This model was further extended to a periodic array of cells containing voids in a hardening material by Tvergaard (1982, 1981) and later modified by Tvergaard and Needleman (1984) to account for void coalescence once a critical porosity is reached. More recently, models for the micromechanics of void growth and coalescence have also been developed and compared to experiments by Benzerga and co-authors (Benzerga and Leblond, 2010; Benzerga, 2002; Benzerga et al., 2004). A review of the current advances in continuum modeling of void phenomena (growth and coalescence) and associated implications for fracture is given in Besson (2010).

However, these models are mostly phenomenological in nature and focus on strain-driven void growth. Void growth by vacancy diffusion mechanisms has also been studied (Chen and Argon, 1981b; Cocks and Ashby, 1982; Cuitiño and Ortiz, 1996; Fischer and Svoboda, 2008; Hull and Rimmer, 1959; Needleman and Rice, 1980; Raj and Ashby, 1975; Speight and Harris, 1967; Stoller and Odette, 1981; Weertman, 1974). It is generally agreed (Chen and Argon, 1981b; Cocks and Ashby, 1982; Cuitiño and Ortiz, 1996; Fischer and Svoboda, 2008; Stoller and Odette, 1981) that vacancy surface diffusion and GB diffusion (where present) are the dominant mechanisms contributing to void growth in a supersaturated field of vacancies, as may arise in the case of irradiated metals. Among these studies, the work of Cuitiño and Ortiz (1996) is of particular interest in that it employs a dislocation density-based crystal plasticity framework to model vacancy supersaturation and void growth in fcc metals subject to plastic deformation.

The present authors have previously developed a dislocation density-based continuum crystal plasticity framework (Patra and McDowell, 2012) to model the mechanical behavior of irradiated bcc materials under quasi-static and creep loading. A phenomenological material softening rule was constituted to account for the reduction in density of the irradiation-induced defects along favored crystallographic planes, leading to the formation of dislocation channels (Patra and McDowell, 2013). This framework was used to model localized deformation along dislocation channels in bcc materials. Based on finite element (FE) simulations of irradiated polycrystalline ensembles (Patra and McDowell, 2013), it was concluded that channel formation and associated flow localization is greatly influenced by intergranular heterogeneity combined with ‘constitutive’ material softening.

In the present work, a novel mechanistically-informed continuum damage framework is developed to model heterogeneous nucleation and growth of voids due to condensation of vacancies formed by excessive inelastic

deformation. The damage framework is coupled with the existing crystal plasticity framework to study flow localization and failure initiation ahead of a sharp notch in irradiated bcc metals.

3. Constitutive model framework

The constitutive model framework considers the following physical phenomena:

- a) inelastic deformation of bcc materials in the field of irradiation-induced defects (primarily interstitial loops) that evolve with inelastic strain,
- b) vacancy supersaturation in the regions of localized inelastic deformation along dislocation channels,
- c) void nucleation by condensation/clustering of supersaturated vacancies in the regions of stress concentration, further promoted along dislocation channel interfaces (via plasticity mismatch with the surrounding interior) and GBs,
- d) void growth via diffusional transport of vacancies from the bulk to the void surface under the influence of multi-axial stress.

These phenomena principally account for the decrease in ductility and eventual failure of irradiated metals. While flow localization associated with dislocation channel formation is modeled using the existing crystal plasticity framework (Patra and McDowell, 2013, 2012), constitutive equations for items (b)-(d) above are developed here, and coupled to the crystal plasticity model in terms of the field of vacancies in the material. Note that the ferritic/martensitic steels modeled in this work have high swelling resistance; voids/vacancy loops are not generally observed post-irradiation, even with transmission electron microscopy (Zinkle and Matsukawa, 2004). Accordingly, it is assumed here that voids are not formed directly due to irradiation; rather they are assumed to form by vacancy condensation subsequent to inelastic deformation.

3.1. Crystal plasticity framework

The finite deformation crystal plasticity model is based on the multiplicative deformation of the deformation gradient ($\mathbf{F}$) into elastic ($\mathbf{F}^e$) and inelastic ($\mathbf{F}^i$) parts (Asaro and Rice, 1977; Asaro, 1983). The inelastic velocity gradient ($\mathbf{L}^i$) given by $\mathbf{L}^i = \dot{\mathbf{F}}^i \cdot \mathbf{F}^{i-1}$, is the tensor sum of the crystallographic shearing rate, $\dot{\gamma}^\alpha$, over all slip systems, N_s , i.e.,

$$\mathbf{L}^i = \sum_{\alpha=1}^{N_s} \dot{\gamma}^\alpha \mathbf{m}_0^\alpha \otimes \mathbf{n}_0^\alpha \quad (1)$$

where $\mathbf{m}_0^\alpha$ and $\mathbf{n}_0^\alpha$ are unit vectors corresponding to the slip and slip plane normal directions in the reference (or intermediate) configuration. The crystallographic shearing rate, $\dot{\gamma}^\alpha$, is a function of the resolved shear stress, τ^α , and the internal state variables (ISVs) on each slip system α .

The constitutive framework models the evolution of the following physically-based ISVs: interstitial loops (number density, N_i^α , and size, d_i^α), density of mobile dislocations, ρ_M^α , and immobile dislocations, ρ_I^α , for each slip system α , and the local concentration of interstitials, c_i , and vacancies, c_v , present in the material as a result of irradiation and inelastic deformation processes. Note that interstitial loops are the primary irradiation-induced defects observed in bcc metals (Zinkle and Matsukawa, 2004). In addition, the number density of voids, N_v , and the respective mean radius, r_v , is also modeled using a continuum damage framework.

Details of the crystal plasticity relations that comprise item (a) above are given in Patra and McDowell (2013, 2012). The complete set of constitutive equations is summarized in Table 1.

The total crystallographic shearing rate in Eq. (T1.3) is the sum of the shearing rate due to dislocation glide (Eq. (T1.1)) and the shearing rate enhancement due to dislocation climb (Eq. (T1.2)). Dislocation glide is modeled using Kocks-type activation enthalpy driven rate kinetics (Kocks et al., 1975), and dislocation climb is assumed to occur by virtue of the net flux of point defects (interstitials and vacancies) absorbed by mobile dislocations (Was, 2007). In particular, climb of mobile dislocations occurs via stress-induced preferential absorption (SIPA) of point defects (Bullough and Willis, 1975; Heald and Speight, 1974) prevalent under irradiation. While dislocation glide is dominant during quasi-static deformation, dislocation climb dominates during irradiation creep deformation at elevated temperatures.

The athermal slip resistance to dislocation glide in Eq. (T1.4) is comprised of barriers in the form of mobile and immobile dislocations, interstitial loops generated due to irradiation, and voids generated prior to failure. This is modeled using a dispersed barrier hardening model (Lucas, 1993; Odette and Frey, 1979) that assumes a square root dependence of the slip resistance on the defect densities. Note that the constitutive equations for athermal slip resistance and mobile dislocation density evolution given in Eq. (T1.4) and (T1.5), respectively, have been modified from their original form to incorporate consideration of voids. The thermal slip resistance is assumed to comprise of the intrinsically high Peierls stress, τ_p , in bcc metals.

Mechanisms for the evolution of mobile dislocations in Eq. (T1.5) include dislocation multiplication (Essmann and Mughrabi, 1979), migration of mobile dislocations by climb and cross-slip (Patra and McDowell, 2012), mutual annihilation of dislocation dipoles with opposite Burgers vectors, and immobilization of mobile dislocations by trapping at barriers. The mobile dislocations trapped at barriers ‘transform’ to immobile dislocations (first term in Eq. (T1.6)). The last term in Eq. (T1.6) represents the dynamic recovery of dislocation density.

Point defects, namely interstitials (Eq. (T1.7)) and vacancies (Eq. (T1.8)), evolve by the following mechanisms: point defect generation under irradiation, mutual recombination of interstitials and vacancies to form regular lattice atoms, and absorption of point defects by dislocations, both mobile and immobile. In addition, we also account for the generation of vacancies due to inelastic deformation processes of dislocation cross-slip and dipole annihilation (cf. Section 3.1.1). The rate-theory equations employed here to model these phenomena are commonly used for point defect evolution under irradiation (Brailsford and Bullough, 1972; Sizmann, 1978).

As for the interstitial loops (primary irradiation-induced defect structures), we assume that mobile dislocations climb by absorbing irradiation-induced point defects and ‘transform’ to interstitial loops (in Eq. (T1.9)). Accordingly, the size of interstitial loops in Eq. (T1.10) is governed by the number of interstitials absorbed per interstitial loop.

Physical mechanisms for the annihilation of interstitial loops that lead to flow localization and dislocation channel formation in bcc metals are still a matter of ongoing research. However, it is understood that the irradiation-induced defects are ‘cleared’ by the glide dislocations (Robach et al., 2006, 2003) once they have sufficient flow stress. As a result, subsequent glide of mobile dislocations through these defect-depleted regions becomes easier, thus facilitating flow localization, manifesting in the form of dislocation channels (Zinkle and Singh, 2006). We have earlier developed a phenomenological relation (last term in Eq. (T1.9)) in which the rate of annihilation of interstitial loops depends on interstitial loops and mobile dislocations interacting within a critical capture radius. See Patra and McDowell (2013) for a detailed description of the interstitial loop annihilation model. Other forms of flow localization models for irradiated fcc and bcc metals are given in (Arsenlis et al., 2004; Barton et al., 2013; Krishna et al., 2010).

These equations represent the dominant deformation mechanisms under combined mechanical loading and irradiation in bcc metals. As has been shown elsewhere (Patra, 2013), this crystal plasticity framework is able to model the mechanical behavior and deformed microstructure of irradiated bcc metals, specifically irradiation hardening and subsequent flow localization due to dislocation channel formation under quasi-static loading, and accelerated deformation rates under irradiation creep loading. Model predictions concur with relevant experimental trends/observations.

Table 1. Constitutive equations in the defect density based crystal plasticity framework.

Constitutive equation	Notes
Crystallographic shearing rate due to dislocation glide:	ΔF_g : zero-stress activation barrier, l_g : average dislocation glide distance between barriers, b : Burgers vector magnitude, ν : cooperative attempt frequency, k : Boltzmann's constant, T : absolute temperature, s_a^α : athermal slip resistance due to long-range stress field of barriers, s_t^α : thermal slip resistance due to local short-range barriers.
$\dot{\gamma}_g^\alpha = \begin{cases} \rho_M^\alpha b l_g \nu \exp\left(-\frac{\Delta F_g}{kT} \left(1 - \left(\frac{ \tau^\alpha - s_a^\alpha}{s_t^\alpha}\right)^p\right)^q\right) \text{sgn}(\tau^\alpha); & \tau^\alpha > s_a^\alpha \\ 0; & \tau^\alpha \leq s_a^\alpha \end{cases}$	(T1.1)
Crystallographic shearing rate enhancement due to dislocation climb:	Climb-governed migration rate of mobile dislocations that depends on the rate of absorption of point defects by mobile dislocations.
$\dot{\gamma}_c^\alpha = \frac{\rho_M^\alpha b l_g}{l_c} \frac{\Omega}{b} (z_i^\alpha D_i c_i - z_v^\alpha D_v c_v)$	(T1.2)
Total shearing rate due to dislocation glide and glide enhancement via dislocation climb:	z_i^α : interstitial capture efficiency, z_v^α : vacancy capture efficiency of mobile dislocations on slip system α , D_i : interstitial diffusivity, D_v : vacancy diffusivity.
$\dot{\gamma}^\alpha = \dot{\gamma}_g^\alpha + \dot{\gamma}_c^\alpha$	(T1.3)
Athermal slip resistance:	Stress-induced preferential absorption: $z_i^\alpha = z_i^0 \left(\frac{\sigma_c^\alpha}{E}\right), z_v^\alpha = z_v^0 \left(\frac{\sigma_c^\alpha}{E}\right), z_i^0, z_v^0$: material constants, and E : Young's modulus. Dispersed barrier hardening model for irradiated materials.
$s_a^\alpha = Gb \sqrt{\sum_{\xi=1}^{N_s} q_\rho A^{\alpha\xi} \rho^\xi + q_i N_i^\alpha d_i^\alpha + q_v N_v r_v}$	(T1.4)
Mobile dislocation density evolution:	G : shear modulus, q_ρ : dislocation barrier strength, q_i : interstitial loop strength, q_v : void barrier strength, $A^{\alpha\xi}$: slip system dislocation interaction coefficient (between α^{th} and ξ^{th} slip systems), and $\rho^\xi = \rho_M^\xi + \rho_I^\xi$.
$\dot{\rho}_M^\alpha = \frac{k_{mul}}{b} \sqrt{\sum_\xi \rho_M^\xi} \dot{\gamma}^\alpha - \frac{ \dot{\gamma}_c^\alpha }{b l_g} - k_{cs} \exp\left(-\frac{(\tau^* - \tau^\alpha) V_a}{kT}\right) \rho_M^\alpha \dot{\gamma}^\alpha - \frac{2R_c}{b} \rho_M^\alpha \dot{\gamma}^\alpha - \frac{1}{b \lambda^\alpha} \dot{\gamma}^\alpha $	(T1.5)
Immobile dislocation density evolution:	1 st term: Rate of formation of new mobile dislocations by multiplication at existing dislocation segments, 2 nd term: rate of migration of mobile dislocations by climb, 3 rd term: rate of migration of mobile dislocations by cross-slip, 4 th term: rate of mutual annihilation of mobile dislocation segments, 5 th term: rate of trapping of mobile dislocations at barriers. k_{mul} : dislocation multiplication constant, k_{cs} : cross-slip constant, R_c : critical capture radius for mutual annihilation, $\frac{1}{\lambda^\alpha} = \beta_\rho \sqrt{\rho^\alpha} + \beta_i \sqrt{N_i^\alpha d_i^\alpha} + \beta_v \sqrt{N_v r_v}$: effective mean free path of dislocation trapping on slip system α , as function of the square root of dislocation and interstitial loop densities. β_ρ , β_i , and β_v are constants. 1 st term: rate of addition of immobile dislocations

$$\dot{\rho}_I^\alpha = \frac{1}{b\lambda^\alpha} |\dot{\gamma}^\alpha| - k_{dyn} \rho_I^\alpha |\dot{\gamma}^\alpha|$$

(T1.6) by trapping of mobile dislocations, 2nd term: rate of annihilation of immobile dislocations by dynamic recovery.

k_{dyn} : dynamic recovery constant.

Interstitial evolution:

$$\dot{c}_i = K_0 - K_{iv} c_i c_v - \sum_{\alpha} K_{is}^\alpha (\rho_M^\alpha + \rho_I^\alpha) c_i$$

(T1.7) 1st term: point defect generation rate, 2nd term: recombination rate of interstitials and vacancies, 3rd term: absorption rate of defects by dislocations.

K_0 : defect pair creation rate, K_{iv} : interstitial-vacancy recombination rate coefficient,

$K_{is}^\alpha = |z_i^\alpha| D_i^l$: interstitial-dislocation reaction rate coefficient.

Vacancy evolution:

$$\dot{c}_v = K_0 - K_{iv} c_i c_v - \sum_{\alpha} K_{vs}^\alpha (\rho_M^\alpha + \rho_I^\alpha) c_v + \dot{c}_v|_{in}$$

(T1.8) 1st, 2nd, and 3rd terms same as above, except

$K_{vs}^\alpha = |z_v^\alpha| D_v^l$: vacancy-dislocation reaction rate

coefficient, 4th term: vacancy generation rate due to inelastic deformation (cf. Section 3.1.1).

Interstitial loop density evolution:

$$\dot{N}_i^\alpha = \frac{1}{\pi d_i^\alpha} \frac{|\dot{\gamma}^\alpha|}{b l_g} - \frac{1}{d_i^\alpha} \frac{R_{ann}}{b} (N_i^\alpha d_i^\alpha)^c (\rho_M^\alpha)^{1-c} |\dot{\gamma}^\alpha|$$

(T1.9) 1st term: rate of creation of new interstitial loops due to climb of mobile dislocations by absorbing interstitials (SIPA), 2nd term: rate of reduction of interstitial loops due to interaction (sweeping out) with mobile dislocations.

R_{ann} : critical capture radius of interstitial loops on interaction with mobile dislocations, c : areal loop density exponent.

Interstitial loop size evolution:

$$\dot{d}_i^\alpha = \frac{2}{\pi} \frac{\pi (d_i^0)^2}{4i^0} \frac{K_{is}^\alpha \rho_M^\alpha c_i}{N_i^\alpha d_i^\alpha}$$

(T1.10) Growth rate of interstitial loop size, assuming all interstitials absorbed by mobile dislocations during climb contribute to the growth of loops.

d_i^0 : threshold size of interstitial loops, i^0 : number of interstitials in loop of threshold size d_i^0 .

3.1.1. Vacancy supersaturation due to inelastic deformation

The crystal plasticity framework developed earlier (Patra and McDowell, 2012) did not consider vacancy formation due to inelastic deformation. The vacancy concentration may be expected to be significant, especially in the regions of excessive inelastic deformation and at high deformation rates (Cuitiño and Ortiz, 1996; Essmann et al., 1981; Kiritani, 2003; Repetto and Ortiz, 1997). In irradiated microstructures undergoing deformation, such regions may occur in the vicinity of localized dislocation channels and crack tips. It is therefore essential to track the vacancy population that contributes to nucleation and growth of voids along these dislocation channels.

Cuitiño and Ortiz (1996) developed a model for vacancy formation due to inelastic deformation in a dislocation density based crystal plasticity framework for fcc materials. They assumed that intersection jogs, formed during dislocation glide and cross-slip, leave behind a trail of vacancies during their subsequent motion. The formation of vacancies by edge dislocation dipole annihilation during cyclic deformation of fcc metals was also modeled by Repetto and Ortiz (1997) to predict fatigue crack initiation. Neglecting remnant vacancy population, if any, due to prior irradiation, we assume that vacancies are primarily formed by the following inelastic deformation processes: cross-slip of dislocations, and mutual annihilation of dipoles within a critical capture radius of the associated glide dislocations. The constitutive equation for cross-slip is represented by the 3rd term, and that for mutual annihilation of mobile dislocation dipoles is represented by the 4th term in Eq. (T1.5) in Table 1.

The cross-slip model (Patra and McDowell, 2012) assumes that mobile screw dislocations from slip system α migrate to slip plane χ , which has the lowest stress-biased activation energy barrier, $(\tau^* - |\tau^\chi|)V_a$, amongst all possible slip systems $\alpha \in \Theta$, such that all slip systems of subset Θ have the same Burgers vector direction. Here, τ^* is the critical activation stress for double-kink nucleation, τ^χ is the resolved shear stress on slip system χ and V_a is the activation volume for cross-slip. Accordingly, the rate of migration of mobile screw dislocations from slip system α is given as

$$\dot{\rho}_{cs}^\alpha = -k_{cs} \exp\left(-\frac{(\tau^* - |\tau^\chi|)V_a}{kT}\right) \rho_M^\alpha |\dot{\gamma}^\alpha| \quad (2)$$

where k_{cs} is a material constant, k is Boltzmann's constant, T is absolute temperature, and $\dot{\gamma}^\alpha$ is the crystallographic shearing rate on slip system α . The corresponding rate of accumulation of mobile screw dislocations on slip system χ with the lowest activation barrier for cross-slip is given as

$$\dot{\rho}_{cs}^\chi = - \sum_{\alpha \in \Theta, \alpha \neq \chi} \dot{\rho}_{cs}^\alpha = \sum_{\alpha \in \Theta, \alpha \neq \chi} k_{cs} \exp\left(-\frac{(\tau^* - |\tau^\chi|)V_a}{kT}\right) \rho_M^\alpha |\dot{\gamma}^\alpha| \quad (3)$$

This migration rate, when multiplied by the Burgers vector magnitude, b , and the average line length of mobile dislocations, $l_M^\alpha \approx 1/\sqrt{\rho_M^\alpha}$, gives the number of migration events per unit time. The corresponding rate of vacancy

generation due to cross-slip is obtained as the product of the migration events per unit time with the atomic density $N_0 = 1/\Omega$, i.e.,

$$\dot{c}_v^\alpha|_{cs} = N_0 b l_M^\alpha |\dot{\rho}_{cs}^\alpha| = \frac{b l_M^\alpha}{\Omega} k_{cs} \exp\left(-\frac{(\tau^* - |\tau^z|)V_a}{kT}\right) \rho_M^\alpha |\dot{\gamma}^\alpha| \quad (4)$$

where Ω is the atomic volume.

Mutual annihilation of mobile dislocation dipoles within a critical capture radius, R_c , of the gliding mobile dislocations is accounted for by the relation (Arsenlis and Parks, 2002; Essmann and Mughrabi, 1979; Repetto and Ortiz, 1997)

$$\dot{\rho}_{mutual}^\alpha = -\frac{2R_c}{b} \rho_M^\alpha |\dot{\gamma}^\alpha| \quad (5)$$

where the factor of two accounts for the fact that two mobile dislocations with opposite Burgers vectors are annihilated via this mechanism. The total number of mutual annihilation events per unit time is obtained as half the product of the mutual dislocation annihilation rate with the Burgers vector and the capture radius, i.e., $bR_c |\dot{\rho}_{mutual}^\alpha|/2$ (Essmann and Mughrabi, 1979; Repetto and Ortiz, 1997). Following a similar procedure as in Eq. (4), the corresponding vacancy generation rate is given as

$$\dot{c}_v^\alpha|_{mutual} = N_0 \frac{bR_c}{2} |\dot{\rho}_{mutual}^\alpha| = \frac{R_c^2}{\Omega} \rho_M^\alpha |\dot{\gamma}^\alpha| \quad (6)$$

The factor of two here avoids double counting of the dislocation annihilation events. The total vacancy generation rate due inelastic deformation on all slip systems is thus given as

$$\dot{c}_v|_{in} = \sum_{\alpha, \alpha \neq \chi} \dot{c}_v^\alpha|_{cs} + \sum_{\alpha} \dot{c}_v^\alpha|_{mutual} \quad (7)$$

Having determined the rate of vacancy generation in the material, we now describe the constitutive equations for void nucleation and growth in the damage framework.

3.2. Damage framework

A continuum damage approach is used to model the evolution of an isotropic damage variable, ϕ , in the material. Using the concept of effective stress, i.e., $\tilde{\sigma} = \sigma/(1-\phi)$, and the strain equivalence principle (cf. (Lemaitre, 1992)), the elastic stiffness of the damaged material is given as

$$\tilde{C} = (1-\phi)C \quad (8)$$

where C is the elastic stiffness of the undamaged material and $\tilde{\sigma}$ is the effective stress in the damaged material. The damage variable, ϕ , is the volume fraction of voids, **considering both the density and size of voids at any material point**. In what follows, the voids are assumed to be spherical in shape, and their volume number density, N_v , and mean radius, r_v , are used as ISVs here.

3.2.1. Void nucleation model

Based on the classical theory of void nucleation due to vacancy condensation, the steady state nucleation rate of voids that are each composed of j vacancies is given as (Brager et al., 1977; Was, 2007)

$$\dot{N}_v^j = Z\beta_j N_v^p \exp\left(-\frac{\Delta G_j}{kT}\right) \quad (9)$$

where Z is the dimensionless Zeldovich factor, β_j , is the rate of impingement of vacancies on a void nucleus having j vacancies, N_v^p is the number of potential nucleation sites, and ΔG_j is the Gibbs free energy change associated with the formation of a void nucleus having j vacancies. A relation between the radius, r_v , of the void and the number of vacancies, j , in the void can be obtained by equating their respective volumes, i.e.,

$$\frac{4\pi}{3} r_v^3 = j\Omega \Leftrightarrow r_v = \left(\frac{3j\Omega}{4\pi}\right)^{1/3} \quad (10)$$

where Ω is the volume of a single vacancy. An implicit assumption, of course, is that the voids are composed only of vacancies; there are no gas atoms present within the voids. Accordingly, the free energy change associated with the formation of a spherical void composed of j vacancies under the influence of local tensile hydrostatic stress, σ_H , is given as

$$\Delta G_j = -j\sigma_H\Omega + (4\pi)^{1/3} (3j\Omega)^{2/3} \Delta\Upsilon = -\left(\frac{4\pi}{3} r_v^3\right) \sigma_H + (4\pi r_v^2) \Delta\Upsilon \quad (11)$$

where $\Delta\Upsilon$ is the associated interfacial energy change, and is given as the difference between the surface energy of new void surfaces created and the surface energy of interfaces annihilated as a result of void formation. The present framework considers both heterogeneous void nucleation at the dislocation channel-induced plasticity mismatch interfaces and homogeneous void nucleation in the homogeneously deformed grain interiors; $\Delta\Upsilon$ would vary accordingly depending on whether the nucleation site is at a dislocation channel interface or a GB ($\Delta\Upsilon = \Delta\Upsilon_{het}$), or in the homogeneous interior ($\Delta\Upsilon = \Delta\Upsilon_{hom}$). The critical number of vacancies, j^* , required to form a void nucleus of radius, r_v^* , is obtained from the stationary point of ΔG_j , i.e.,

$$\frac{\partial \Delta G_j}{\partial j} = 0 \Rightarrow j^* = \frac{32\pi}{3\Omega} \left(\frac{\Delta\Upsilon}{\sigma_H}\right)^3 \Leftrightarrow r_v^* = \frac{2\Delta\Upsilon}{\sigma_H} \quad (12)$$

and the associated critical free energy change is

$$\Delta G^* = \frac{16\pi}{3} \frac{\Delta \gamma^3}{\sigma_H^2} \quad (13)$$

The non-equilibrium Zeldovich correction factor, Z , accounts for fluctuations between the subcritical and supercritical nuclei (Yoo and Trinkaus, 1983), and is given as (Brager et al., 1977; Was, 2007)

$$Z = \left(-\frac{1}{2\pi kT} \left[\frac{\partial^2 \Delta G_j}{\partial j^2} \right]_{j^*} \right)^{1/2} \quad (14)$$

The impingement rate of vacancies on the void nucleus, β_j , depends on the probability of finding vacancies within an atomic layer, $\Omega^{1/3}$, of the void surface, i.e., $(4\pi r_v^2)\Omega^{1/3}/\Omega$, and the jump frequency of vacancies, given by $D_v/\Omega^{2/3}$ (Yoo and Trinkaus, 1983). Here, D_v is the vacancy diffusivity. Accordingly, the impingement rate is given as

$$\beta_j = \frac{4\pi r_v^2}{\Omega^{2/3}} \frac{D_v}{\Omega^{2/3}} \quad (15)$$

From Raj and Ashby (1975), the number of potential nucleation sites per unit volume, N_v^p , is related to the available volume for void nucleation. Hence, it depends on the damage parameter, ϕ , and the current volume, $j\Omega$, of the void nucleus, i.e.,

$$N_v^p = \frac{1-\phi}{j\Omega} \quad (16)$$

As a result of nucleation of voids due to vacancy condensation, the vacancy concentration in the material is depleted. Based on the steady state void nucleation rate given in Eq. (9) and the critical number of vacancies required to nucleate the voids given in Eq. (12), the corresponding mean field vacancy absorption rate is given by

$$\dot{c}_v|_v^n = j^* \dot{N}_v^{j^*} \quad (17)$$

This framework tracks the number density and radii of voids at each material point. However, as a result of simultaneous nucleation and growth events, there would exist a distribution of void sizes at any instant of time. Keeping track of such a void size distribution for each material point in a crystal plasticity framework is computationally expensive, given that the slip system-ISVs must be tracked as well. Hence, we track only the average void radius at each material point, which is calculated by conserving the volume of the pre-existing and newly nucleated voids, i.e.,

$$\langle r_v \rangle_t = \frac{\left(\left(\dot{N}_v|_t \Delta t \right) r_v|_t^3 + N_v|_{t-1} \langle r_v \rangle_{t-1}^3 \right)^{1/3}}{\dot{N}_v|_t \Delta t + N_v|_{t-1}} \quad (18)$$

where subscripts t and $t-1$ in the above equation refer to values of the variable at the respective time steps, Δt is the time interval between these time steps, and values within $\langle \rangle$ represent mean values of the respective variables. For brevity, the average void radius at the current time step will be simply referred to as r_v in the following sections, unless mentioned otherwise.

Note that effect of the presence of interstitials on void nucleation and growth is neglected in the present work. This is reasonable given the fact that interstitials, though present due to prior irradiation, may be neglected in comparison to the significantly larger number of vacancies generated during inelastic deformation.

3.2.2. Void growth model

As mentioned earlier, surface diffusion is one of the dominant mechanisms contributing to void growth (in the absence of GB diffusion). Void growth may also be reaction rate controlled (cf. Was (2007)). Reaction rate controlled processes are those in which no macroscopic concentration gradients of the reactants exist; rather, these processes are governed by the ‘sink strengths’ of the respective reactants. In the initial stages ($r_v \leq 1$ nm), void growth may be reaction rate limited (Was, 2007). As the voids increase in size, the growth rate is controlled by the diffusive flux of vacancies from the surrounding material. As outlined in Was (2007), a mixed void growth rate equation may be used to reflect contributions from each of these mechanisms. However, for simplicity, we focus on modeling just diffusion controlled void growth. This is reasonable given the fact that initial reaction rate controlled void growth in the field of supersaturated vacancies will be swift, and diffusion controlled growth is the rate limiting step (a similar assumption has also been made in (Cuitiño and Ortiz, 1996; Fischer and Svoboda, 2008; Mansur, 1994)). Note that void growth is further accelerated in the regions of heavy inelastic deformation due to vacancy pipe diffusion along dislocations (Balluffi and Granato, 1979; Cuitiño and Ortiz, 1996; Repetto and Ortiz, 1997).

From Was (2007), assuming steady state diffusion in an infinite field of vacancies, the absorption rate of vacancies for void growth is calculated using a standard rate theory approach, i.e.,

$$\dot{c}_v|_v^s = 4\pi r_v D_v N_v (c_v - c_v^V) ; c_v > c_v^V \quad (19)$$

where c_v^V is the vacancy concentration at the void surface. This expression is obtained by solving the steady state diffusion of vacancies to a spherical void lying within a larger spherical shell, which is an infinite vacancy source. Applying conservation to the vacancy change rate within voids, the equivalent expression for uniform growth rate of voids is given by (Was, 2007)

$$N_v \dot{V}_v = N_v (4\pi r_v^2 \dot{r}_v) = \dot{c}_v|_v^s \Omega \Rightarrow \dot{r}_v = \frac{\Omega}{r_v} D_v (c_v - c_v^V) ; c_v > c_v^V \quad (20)$$

The vacancy concentration at the void surface, c_v^V , is a function of the force balance between the external tensile hydrostatic stress, σ_H (promoting growth), and the inward pressure due to surface tension, $2\gamma_v/r_v$ (resisting

growth). Following a similar procedure as in Was (2007), c_v^V as a function of the net resultant force due to surface tension and hydrostatic stress, is given by

$$c_v^V = c_v^0 \exp\left(\frac{\Omega}{kT}\left(\frac{2\gamma_v}{r_v} - \sigma_H\right)\right) = \frac{1}{\Omega} \exp\left(-\frac{E_v^f - TS_v^f}{kT}\right) \exp\left(\frac{\Omega}{kT}\left(\frac{2\gamma_v}{r_v} - \sigma_H\right)\right) \quad (21)$$

where c_v^0 is the equilibrium vacancy concentration, E_v^f is the vacancy formation energy, S_v^f is the vacancy formation entropy, and γ_v is the interfacial energy associated with creation of a new void surface. Note that this expression also gives the dependence of the void growth rate, $\dot{r}_v$, on σ_H . A higher value of σ_H would lower c_v^V , thus increasing $\dot{r}_v$ (from Eq. (20)), and vice-versa.

As mentioned earlier, vacancy diffusion is accelerated along dislocations (pipe diffusion) in the regions of excessive inelastic deformation. Based on the pipe diffusion model, the vacancy diffusion coefficient in the grain interior is a function of the dislocation density in the material, and is given as (Balluffi and Granato, 1979)

$$D_v = D_v^l + b^2 \left(\sum_{\alpha} \rho^{\alpha} \right) D_v^{\rho} \quad (22)$$

where D_v^l is the vacancy lattice diffusion coefficient, and D_v^{ρ} is the vacancy pipe diffusion coefficient.

Note that the present framework models only the initial stages of failure due to diffusion-driven void growth. It is expected that strain-driven void growth and coalescence will dominate in the later stages. Strain-driven void growth may be modeled using the Rice and Tracey (1969) model, for example. Further, our model assumes that the voids are spherical in shape. Ellipsoidal void growth is generally expected at high stress triaxialities (cf. Besson (2010)), and has been studied in Gologanu et al. (1993), for example. Future work may address these issues.

3.2.3. Modeling simultaneous void nucleation and growth

In the preceding sections, we have described constitutive equations for a variety of deformation phenomena. However, coupling them together is not entirely intuitive. A caveat regarding the void models described in Section 2.2 lies in the fact that they implicitly assume that vacancies are present in material, i.e., they do not generally track the vacancy population. During the initial stages of inelastic deformation, the vacancy concentration may not be sufficient to promote competitive void nucleation and growth. For example, nucleation of voids is subject to the availability of sufficient vacancies for a given stress state and temperature. Similarly, diffusional void growth depends on whether the vacancy concentration at the void surface, c_v^V , is lower than that of the surrounding exterior. There also exists a possibility that the vacancy concentration at a material point may not be sufficient for void nucleation but will still allow void growth. Further, modeling simultaneous void nucleation and growth presents another challenge, especially during the initial stages when the voids are vacancy-starved. An algorithm for void nucleation and growth is developed here considering these issues.

Void nucleation and growth are competitive processes. Initially, when there is little or no damage, void nucleation would obviously occur preferentially over void growth. However, with increasing damage, void growth takes preference over nucleation as potential nucleation sites decay in number (modeled using Eq. (16)). A simple strategy is implemented here to model void nucleation and growth, decomposing it into a two-step process. It is assumed that following inelastic deformation, void nucleation occurs if possible. Criteria for critical void nucleation are outlined in the algorithm given in Fig. 1. Subsequent to nucleation, void growth is allowed to occur according to Eq. (20). Though this is a deterministic treatment of the problem of simultaneous void nucleation and growth, the nucleation rate is slowed down at higher damage values due to the lack of potential nucleation sites according to Eq. (16). Figure 1 presents the detailed algorithm for modeling void nucleation and growth and coupling it to the crystal plasticity framework.

Figure 1. Algorithm for integration of void nucleation and growth-based damage model. Dashed black lines indicate operations performed by calling FE code.

4. Model Implementation

4.1. Loading and boundary conditions

The 3D constitutive model is implemented in the FE program ABAQUS (2007) as a User MATerial (UMAT) subroutine. Generalized plane strain elements are used along with fully 3D crystallography and the described constitutive model. The elements employ linear interpolation and reduced integration.

A single deep edge notch with semi-circular tip is created at mid-height on the side of a 800 X 800 μm simulation cell. A schematic of the loading and boundary conditions is shown in Fig. 2(a). Regions in the immediate vicinity of the notch are modeled using the coupled (incremental) crystal plasticity-damage material behavior described in Section 3. The microstructure is generated using an approximate Dirichlet (weighted Voronoi) tessellation achieved by packing of (randomly oriented) polygonal grains with Gaussian size distribution (25 μm mean size), through random sequential addition. Deformation plasticity model with Ramberg-Osgood hardening behavior is assigned to the outer region (shaded in green) in Fig. 2(a). Based on the dimensions of the respective regions indicated in Fig. 2(a), a representative simulation cell has ~ 45 grains in the crystal plasticity domain enveloping the notch root. Different notch depths and radii are used in the simulations; these values are specified where needed.

The bottom edge of the 2D simulation cell is constrained along the loading direction, and the far right node of the bottom edge is constrained in both x and y degrees of freedom (to prevent rigid body rotation). Displacement-controlled tensile loading is applied on the top edge in the y direction (remote applied straining), and the side edges of the simulation cell are traction-free. The simulation cell is loaded at quasi-static strain rate (10^{-4} s^{-1}), unless mentioned otherwise.

The simulation cell is freely meshed in ABAQUS using quadrilateral and triangular elements. A mesh size of 200 nm is used in the crystal plasticity zone in regions in the immediate vicinity and up to 5 μm away from the notch, with radially increasing mesh size up to 4 μm in the crystal plasticity zone, and up to 15 μm in the Ramberg-Osgood zone. A typical simulation cell has $\approx 15,000$ elements in the crystal plasticity zone, $\approx 5,000$ elements in the Ramberg-Osgood zone. A representative mesh ahead of a deep notch with radius, $\rho = 2 \mu\text{m}$, is shown in Fig. 2(b). This sharp notch effectively represents a crack.

Following Bennett and McDowell (2003) and Castelluccio and McDowell (2012), the crack tip displacement (CTD) is computed as the net displacement between nodes 1 and 2 labeled in Fig. 2(b), is used to characterize the driving force for fracture. The CTD relates to the J -integral for stationary crack growth (cf. (Anderson, 2005; Shih, 1981)), and is often used to quantify fracture; it is defined by $CTD = \sqrt{CTOD^2 + CTSD^2}$. Thus, CTD is able to characterize failure under mixed mode (Mode I and Mode II) loading, where $CTOD$ is the crack tip opening displacement, and $CTSD$ is the crack tip shear displacement.

Figure 2. (a): Schematic of loading and boundary conditions. (b): Representative mesh ahead of a notch of radius, $\rho = 2 \mu\text{m}$, with a minimum mesh size of 200 nm.

4.2. Algorithm for identifying dislocation channel interface and GB elements

An essential step in modeling void nucleation and growth in the present framework is identifying whether a material point is in the homogeneously deformed bulk, dislocation channel interface, or at a GB. This is implemented in our FE simulations in the following fashion:

- A list of nearest neighbor elements is stored that lie within a cutoff radius, $1.5d$ (d is the characteristic length of the material point, defined as the square root of the area of the respective element), of the centroid of the element in question.
- At each time step, the difference in effective inelastic strain, ϵ_{eff}^i , between the neighboring elements is computed. If the difference is greater than 0.05, and ϵ_{eff}^i is lower in the present FE than its neighbor, then the material point is at a dislocation channel interface.
- If the neighboring element belongs to a different grain, the material point is at a GB.
- If none of the above conditions are satisfied, the material point lies within the uniformly deformed bulk.

4.3. Non-local vacancy concentration at interface elements

This simple framework identifies interface elements along dislocation channels and GBs in the material. Heterogeneous void nucleation and growth processes are expected to be more prolific at these interface elements. Physically, the vacancy population at material points contiguous to the ‘interface’ should also contribute to the nucleation and growth of voids. This is implemented in our framework by taking a non-local estimate of the vacancy concentration at the interface elements. Using the nearest neighbor list computed in Section 4.2, the non-local vacancy concentration, $c_v|_{nl}^i$, at the interface element is calculated as the element area-weighted sum of vacancy

concentration over all nearest neighbors, including the vacancy concentration at the interface element. If void nucleation and/or growth occurs at the interface element, vacancy concentration in the neighboring elements is depleted proportional to their contribution to $c_v|_{nt}^i$.

4.4. Damage estimation

The crystal plasticity and damage framework outlined here employs 3D crystallography and 3D constitutive equations. However, as explained in Section 4.1, the polycrystalline simulations are performed using generalized plane strain FEs, effectively treating polyhedral grains as columnar (polygonal cross-section in the plane). We employ a commonly used microstructure scaling relation, which relates the mean areal density, $\langle x^A \rangle$, of convex-shaped particles to the volume density, x^V , according to the relation

$$\langle x^A \rangle = \langle D \rangle x^V \quad (23)$$

where $\langle D \rangle$ is the mean caliper diameter of the particle, to find the areal density (N_v^A) of voids across the material cross-section. Further, using Cavalieri's principle, the volume fraction of voids, V_v , is equal to the average area fraction of voids, A_A (cf. Underwood (1971)). Thus, the damage variable, ϕ , measuring the volume fraction of voids in the material, is given as

$$\phi = V_v = A_A = \frac{N_v^A \pi r_v^2}{A_0} = \frac{(2r_v N_v) \pi r_v^2}{A_0} \quad (24)$$

where A_0 is the cross-sectional area of the initially undeformed material.

4.5. Model parameters

The framework is used to simulate the deformation behavior of Mod 9Cr-1Mo steel loaded in quasi-static tension. This steel has good radiation resistance and high temperature properties. The microstructure of Mod 9Cr-1Mo steel is mainly comprised of ferrite and martensite phases. It is assumed that the crystal structure of the subsequently tempered martensite phase is body-centered cubic (cf. Schastlivtsev et al. (1999)). Accordingly, the material is assigned a uniform bcc crystal structure with 24 slip systems (12 {110}-type and 12 {112}-type). To save computational costs, deformation along the 24 {123} bcc slip systems is neglected for the example applications presented here.

The crystal plasticity model was calibrated earlier to match the experimental engineering stress-strain data of Mod 9Cr-1Mo steel (Maloy et al., 2001) for different radiation and temperature histories. **Without going into the details of parameter estimation for the crystal plasticity model, we point out that a significant number of the material parameters are based on physical constants for bcc-Fe. Parameters in the dislocation evolution and hardening (athermal slip resistance) models were calibrated to fit to the experimental hardening response. Parameters in the point defect evolution and interstitial loop evolution models are generally based on lower scale simulations of dislocation-defect interactions. See Patra and McDowell (2012) for details of the parameter estimation process. The**

parameters of the phenomenological flow localization model (last term in Eq. (T1.9)) were estimated such that the simulated engineering stress just beyond the point of material softening and up to $\approx 4\%$ applied strain matches the experimental values (cf. Patra and McDowell (2013)). It is of course noted that this may not be the only unique set of parameters for the crystal plasticity model. These parameters, along with the damage model parameters, are listed in Table 2.

The damage model adds only four new parameters to the framework: E_v^f , S_v^f , D_v^ρ , and $\Delta\Upsilon$. The vacancy formation energy, E_v^f , and entropy, S_v^f , are taken from Mendelev and Mishin (2009). Studies have shown (Mehrer and Lübbhusen, 1991; Shima et al., 2002) that the pipe diffusion coefficient, D_v^ρ , is ~ 3 -4 orders of magnitude higher than the lattice diffusion coefficient in bcc-Fe at elevated temperatures, and even higher at low and intermediate temperatures. Accordingly, we assume that $D_v^\rho = 10^4 D_v^l$. The interfacial energy change associated with homogeneous void nucleation is $\Delta\Upsilon_{hom} = \gamma_v = 1.95 \text{ Jm}^{-2}$ (Hirth and Lothe, 1982), where γ_v is the surface energy of the material. The exact value of $\Delta\Upsilon_{het}$ is not entirely known. From Hirth and Lothe (1982), the grain boundary interfacial energy of Fe, $\gamma_{GB} \approx 0.78 \text{ Jm}^{-2}$. Assuming that the energy of a dislocation channel interface is the same, the interfacial energy change associated with heterogeneous nucleation of a spherical void at an interface (in Eq. (11)) is ideally given by $\Delta\Upsilon_{het} = \gamma_v - \gamma_{GB}/4$. This expression accounts for the fact that a void of surface area, $4\pi r_v^2$, with interfacial energy, γ_v , is created by destroying a dislocation channel interface (or GB) of area, πr_v^2 , with interfacial energy, γ_{GB} ($4\pi r_v^2$ is already factored out in the corresponding term in Eq. (11)). Substituting values of the respective parameters into the above expression, $\Delta\Upsilon_{het} \approx 1.75 \text{ Jm}^{-2}$. This value of $\Delta\Upsilon_{het}$ is too high to allow spherical void nucleation even at peak stress for stress triaxialities on the order of 3-3.5. Note that an assumption of spherical voids is used here just to simplify the constitutive equations; the voids are seldom spherical in nature. This is because a spherical shape has the highest contact angle (90°) at the void-GB interface (cf. Raj and Ashby (1975)), and is the least energetically favorable. Contact angle-based shape factors of voids of various shapes and their effect on void nucleation and growth at different temperatures has been studied in detail by Raj and Ashby (1975). Based on their analysis of void nucleation at grain interfaces, plausible void-interface contact angles lie in the range 0° - 37° for Cu, meaning that the nucleated voids are essentially prolate spheroids with a high degree of eccentricity. The surface and interfacial energies of Fe are in the same range as Cu, allowing us to extrapolate these results to the present case. Using the shape factors given in Raj and Ashby (1975) and the contact angles mentioned above, $\Delta\Upsilon_{het} \leq 0.33 \text{ Jm}^{-2}$ for Fe. Note that the surface and interfacial energy values reported above are generally measured at $T > 1000 \text{ K}$. These values increase with decrease in temperature; at intermediate temperatures of 400-600 K, the calculated value of $\Delta\Upsilon_{het}$ would be higher. Accordingly, we have used a value of $\Delta\Upsilon_{het}$ in the range $0.32 - 0.38 \text{ Jm}^{-2}$ in our simulations. Effects of this parameter on damage initiation and the computed CTD are studied in Section 5.3.

An empirical relation given by Deo et al. (2008), for a similar 9Cr-1Mo steel, is used to correlate the interstitial loop density and size to the radiation dpa dose history (over a limited range), i.e.,

$$N_i = X \cdot \text{dpa}^{1/2} \text{mm}^{-3} \quad (25)$$

$$d_i = Y \cdot \text{dpa}^{1/2} \text{mm} \quad (26)$$

where $X = 1.0 \times 10^{15}$, $Y = 8.0 \times 10^{-6}$ for radiation dose < 1 dpa, and $X = 5.0 \times 10^{13}$, $Y = 3.7 \times 10^{-6}$ for higher radiation doses up to 10 dpa. Further, the interstitial loops are assumed to be uniformly distributed. Effects of irradiation temperature, material depth from irradiated surface, etc. are neglected here as beyond the scope of the present work.

Table 2. Material parameters for Mod 9Cr-1Mo steel.

<i>Parameter</i>	<i>Value</i>	<i>Meaning</i>
E, ν	$207300 - 64.58(T[\text{K}] - 273) \text{ MPa}, 0.3$	Young's modulus, Poisson's ratio
b	0.248 nm	Burgers vector
ΔF_g	$0.35Gb^3$	Activation barrier for dislocation glide
p, q	0.28, 1.34	Shape parameters for dislocation glide enthalpy curve
ν	10^{10} s^{-1}	Cooperative attempt frequency for dislocation glide
$A^{\alpha\alpha}, A^{\alpha\xi} (\alpha \neq \xi)$	1.0, 0.2	Dislocation self and latent interaction coefficients
q_ρ, q_i, q_v	0.3, 0.4, 1.0	Defect barrier strengths: dislocations, interstitial loops, and voids, respectively
τ_p	390 MPa	Peierls barrier stress
l_g	1.5 nm	Average dislocation glide distance
l_c	$3b$	Average dislocation climb distance
z_i^0, z_v^0	$1.2 \times 10^{-4}, 1.0 \times 10^{-4}$	Dislocation capture efficiency constants: interstitials and vacancies, respectively
D_i^l, D_v^l	$6.0 \times 10^{-2} \exp(-0.34 \text{ eV}/kT) \text{ mm}^2 \text{ s}^{-1},$ $6.0 \times 10^{-2} \exp(-0.67 \text{ eV}/kT) \text{ mm}^2 \text{ s}^{-1}$	Interstitial and vacancy lattice diffusion coefficients, respectively
D_v^ρ	$10^4 D_v^l$	Vacancy pipe diffusion coefficient
E_v^f	$1.724 + 2.79 \times 10^{-8} T^2 + 1.186 \times 10^{-10} T^3 \text{ eV}$	Vacancy formation energy
S_v^f	$1.2 \times 10^{-4} + 5.58 \times 10^{-8} T + 1.78 \times 10^{-10} T^2 \text{ eV}$	Vacancy formation entropy
Ω	b^3	Atomic volume
K_0	0	Point defect generation rate. No concurrent radiation during tensile loading
K_{iv}	0	Interstitial-vacancy recombination rate coefficient. Recombination rate negligible compared to absorption at dislocations
d_i^0, i^0	4 nm, 91	Threshold size of interstitial loops, number of interstitials in loop of threshold size
k_{mul}	0.143	Dislocation multiplication constant
τ^*, V_a, k_{cs}	$0.004G, 20b^3, 2.0 \times 10^4$	Activation barrier, activation volume, and material constant for cross-slip
R_c	1 nm	Capture radius for mutual annihilation of mobile dislocations
R_{ann}, c	3.0, 0.8	Critical capture radius for sweeping out of interstitial loops, areal loop density exponent
$\beta_\rho, \beta_i, \beta_v$	0.36, 0.3, 0.3	Immobilization constants for dislocations, interstitial loops, and voids, respectively
k_{dyn}	329.5	Dynamic recovery constant for immobile dislocations
ΔY_{hom}	1.95 Jm^{-2}	Interfacial energy change associated with homogeneous void nucleation
ΔY_{het}	$0.32 - 0.38 \text{ Jm}^{-2}$	Interfacial energy change associated with heterogeneous void nucleation (see Section 5.3)

As mentioned in Section 4.1, Ramberg-Osgood hardening behavior is assumed for the material far away from the notch in the context of a deformation plasticity model. Separate sets of Ramberg-Osgood model parameters, for different loading (temperature, strain rate and radiation dose) histories, were generated by fitting to the stress-strain response from the respective crystal plasticity simulations of smooth specimens with 125, randomly oriented cubic grains (30 μm size), deformed uniaxially up to 1.5% engineering strain.

5. Results and discussion

Post-irradiation tension test simulations are performed on the notched specimens at different test temperatures and loading rates. The following sections will first consider inelastic deformation and vacancy generation in the vicinity of the notch, and then describe the damage behavior. **Model predictions of the stress-strain response fit to the experimental data of irradiated and virgin smooth specimens for different loading and temperature histories are not presented here to avoid repetition with** Patra and McDowell (2013).

5.1. Channel formation and vacancy supersaturation

Figure 3 shows the distribution of inelastic strain and the corresponding vacancy concentration ahead of a circular notch of radius, $\rho = 2 \mu\text{m}$, with notch depth, $a = 250 \mu\text{m}$, in the material irradiated to 2.9 dpa and then strained normal to the notch to 0.7% remote applied engineering strain at 550 K. $\Delta Y_{het} = 0.38 \text{ Jm}^{-2}$ in these simulations. Figure 3(a) shows that the deformation is primarily localized in a single grain ahead of the notch. As mentioned earlier, localization of deformation occurs via sweeping out/reduction in density of the irradiation-induced defects along these channels, thus reducing the flow stress. This has been modeled phenomenologically in the 2nd term of Eq. (T1.9) as a function of the interacting defect density and mobile dislocation density (see Patra and McDowell (2013) for detailed description of the localization mechanism). Recent dislocation dynamics studies of irradiated Fe (Arsenlis et al., 2012) have suggested that reduction in flow stress may simply be due to transformation of these loops into ordinary network dislocations (without any annihilation of the loops), thus reducing their resistance to dislocation glide and promoting localization. With more physical insights, appropriate modification to the phenomenological rule given in Eq. (T1.9) may be made to account for this mechanism in the future. Nevertheless, the constitutive equation (T1.9) in its present form accounts for the reduction in loop density, and consequent reduction in flow stress, thus enabling us to study localization as a function of other mesoscopic factors, such as crystallographic orientations, loop density, etc. Multiple, intertwined channels are formed in the regions of stress concentration in the immediate vicinity of the notch. Reorientation and bifurcation of channels at GBs is also observed. The spacing between channels here is much lower than computed previously for the case of localization in smooth specimens (Patra and McDowell, 2013). **This is in agreement with experimental observation of higher density of dislocation channels (by up to an order of magnitude) near the fracture surface as compared to uniformly deformed regions** (Zinkle and Singh, 2006). We have also found earlier (Patra and McDowell, 2013) that the dislocation channel spatial patterns are strongly dependent on the crystallography of the material. **The driving force for flow localization is derived from the resolved shear stress on a given slip system. This is the reason dislocation**

channeling is observed only in certain grains that have favorable crystallographic orientations. The width of modeled dislocation channels is limited by the minimum mesh size at 200 nm, and is larger than the experimentally observed channel width of 50-200 nm (Eyre, 1962; Lупpo et al., 2000; Rice and Zinkle, 1998; Zinkle and Singh, 2006). Further, the localized inelastic strain in channels (~ 0.6 - 1.4) is lower than that seen in experiments (~ 1.0 - 5.0) (Sharp, 1967; Tucker et al., 1969). However, we have verified earlier that the simulated net localization of shear strain in the stress-strain response of polycrystalline, smooth specimen ensembles is comparable to experiments, and the product of the channel width with the localized strain within channels is more or less invariant (cf. Patra and McDowell (2013)). A finer mesh may be used to achieve the experimentally observed channel widths and localized strains, albeit at the cost of significantly increased computational times. For the present qualitative study of dislocation channel patterns and failure initiation ahead of the notch root, a mesh resolution of 200 nm is deemed sufficient.

Figure 3(b) shows that the vacancy concentration increases by ~ 3 -4 orders of magnitude in the regions of localized deformation, thus facilitating void nucleation and growth. The vacancy generation due to inelastic deformation has contributions from both dislocation cross-slip and annihilation of dislocation dipoles. We have verified that the vacancy contribution from these respective mechanisms is of the same order of magnitude using the model parameters specified in Table 2. As will be shown later, this vacancy concentration is, in general, sufficiently high to promote void nucleation even at GBs ahead of the notch root, where localized deformation is not that prevalent. While there is no direct experimental data for comparison with the model predictions, the work of Cuitiño and Ortiz (1996) also showed that the vacancy concentration increases by more than 3 orders of magnitude ahead of the sharp crack.

Figure 3. Distribution of (a): effective inelastic strain, and (b): vacancy concentration ahead of the notch after 0.7% applied strain. Grain boundaries are rendered. The material was irradiated to 2.9 dpa prior to tensile loading at 550 K.

5.2. Damage evolution

Figure 4 shows the distribution of voids (Fig. 4(a): number density, 4(b): radius) corresponding to the inelastic strain distribution shown in Fig. 3(a). Void nucleation and growth is observed at multiple regions along the dislocation channel interfaces. In some cases, voids nucleate on both sides of a dislocation channel, for example in the regions A and B marked in Fig. 4(a). The nature of void activity within the grain is consistent with the experimentally observed ‘zigzag’ fracture (Chaouadi, 2008) or ‘channel’ fracture (Fish and Hunter, 1976). In other words, failure path is found to propagate along faceted interfaces of the crisscrossing dislocation channels. Possible failure paths are highlighted using dotted white lines in Fig. 4(b). As mentioned earlier, similar faceted failure surfaces have been observed in other irradiated metals as well (Little, 1986; Michel and Gray, 1987). Strain-driven void growth and coalescence, not modeled here, would ultimately lead to transgranular fracture along these failure routes. Further, void activity is also prevalent at the intersection of dislocation channels with GBs ahead of the notch root. As mentioned earlier, incompatibility of the localized strains along dislocation channels at their intersection with GBs is known to contribute to intergranular stress corrosion cracking in irradiated materials (McMurtrey et al., 2011). Note that the interfacial energy change associated with heterogeneous void nucleation was assigned to be the same ($\Delta\gamma_{het} = 0.38 \text{ Jm}^{-2}$) for nucleation at both dislocation channel interfaces and GBs.

Figure 4. Distribution of (a): void number density, and (b): void radius corresponding to the effective inelastic strain in Fig. 3(a). See text for discussion of regions A and B. Dotted white lines in Fig. 4(b) show the failure paths along faceted interfaces of dislocation channels and GBs.

Figure 4(a) shows that the density of voids goes up to 10^7 mm^{-3} , and the void radius up to 1 μm in Fig. 4(b). It is emphasized that void number density, N_v , and radius, r_v , are two separate indicators that help us delineate the individual contributions to void nucleation and growth. The driving force for void nucleation is derived from the

tensile hydrostatic stress, σ_H , while that for diffusive void growth (as modeled here) is based on the vacancy concentration in the material. As seen in Fig. 4, although a fair number of voids have nucleated near the GBs, their growth (in size) is relatively inhibited due to the absence of vacancies along these GBs. In contrast, voids nucleated along the dislocation channel interfaces have grown relatively larger in size (by up to 2 orders of magnitude) due to the availability of vacancies in these regions.

Figure 5. (a): Evolution of total area-weighted damage (in a semi-circular region of radius $25 \mu\text{m}$ ahead of the notch) with applied strain. (b), (c), (d): Distribution of damage in the material after (b) 0.45%, (c) 0.55%, and (d) 0.70% applied strain, respectively. See text for discussion of regions C, D, E and F.

The evolution of damage (volume fraction of voids) for the same microstructure is shown in Fig. 5. Figure 5(a) shows the evolution of total damage with applied strain. This is calculated as the total area-weighted damage over all elements in a semi-circular region of $25 \mu\text{m}$ radius ahead of the notch root, i.e.,

$$(\phi)_t = \frac{\sum_i \phi_i A_i}{\sum_i A_i} \quad (27)$$

where A_i is the area of the i^{th} FE. The corresponding damage distribution at 0.45%, 0.55%, and 0.70% strain is shown in Figs. 5(b), 5(c), and 5(d), respectively.

As seen in Fig. 5(a), damage initiates first at $\approx 0.32\%$ applied remote strain in the present case. The evolution of damage is however not uniform; change in damage rate with applied strain is observed. This is associated with damage propagation along new regions(s), and can be correlated to the corresponding damage distribution plots. Initially failure propagates mainly along the region C marked in Fig. 5(b). At 0.55% strain, damage is also found to propagate along the new regions D and E marked in Fig. 5(c). With further applied deformation, failure is again initiated along region F marked in Fig. 5(d). Decrease in the damage rate, for example in the range 0.4-0.5% applied strain in Fig. 5(a), is due to relative saturation of damage in region C, and consequently its inability to accommodate the applied deformation, promoting failure elsewhere.

Note that a maximum damage of 0.65 is allowed in each element. Excessive element distortion beyond this damage level leads to convergence issues in our simulations. A higher order FE may be used to address this problem, but with increased computation costs. Even if damage were allowed to occur up to the maximum possible value of 1.0, a similar damage pattern may be expected.

5.3. Parametric study of $\Delta\gamma_{het}$

Figure 6(a) shows the evolution of $(\phi)_t$ with applied strain for three different values of $\Delta\gamma_{het}$. The material was irradiated to 2.9 dpa and then loaded at 550 K. $\rho = 0.5 \mu\text{m}$ and $a = 300 \mu\text{m}$ in all these simulations. Further, the same initial microstructure was used for all cases. Note that the simulation for $\Delta\gamma_{het} = 0.32 \text{ Jm}^{-2}$ failed to converge beyond 0.2% applied strain.

As expected, damage initiates earlier with a lower value of $\Delta\gamma_{het}$. Inspection of the deformed microstructure (not shown here) suggests that the damage initiation patterns are similar in all three cases, albeit delayed in time with increasing $\Delta\gamma_{het}$. A lower value of $\Delta\gamma_{het}$ allows failure to initiate prematurely at GBs (provided the hydrostatic stress is sufficient for void nucleation). This is because strain localization within a dislocation channel needs to be high enough such that the difference in ε_{eff}^i with the neighboring element exceeds 0.05, for an ‘interface’ to be created in our simulations (cf. Section 4.2). In the early stages of localization this might not be the case, allowing (aphysical) premature void nucleation at GBs.

$\Delta\gamma_{het}$ may be used as a parameter to calibrate our simulations to experiments. For example, if the critical value of damage were to be pre-defined as $(\phi)_t|_c = 1.0 \times 10^{-4}$ (say), the *CTD* (or fracture toughness) corresponding to $(\phi)_t|_c$ can be computed for different values of $\Delta\gamma_{het}$ and compared to experiments. Figure 6(b) shows the computed *CTD*

for different $\Delta\gamma_{het}$ at $(\phi)_{t_c} = 1.0 \times 10^{-4}$. As $\Delta\gamma_{het}$ increases, $(\phi)_{t_c}$ is found to occur at higher CTD . The CTD corresponding to $\Delta\gamma_{het} = 0.38 \text{ Jm}^{-2}$ is found to occur closest to the point of intersection of the 5% secant line (from the origin with linear elastic loading slope) with the load-displacement curve. Experimentally, intersection point of the 5% secant line with the load-displacement curve is generally used to estimate the critical fracture toughness (cf. (Anderson, 2005)). Using $\Delta\gamma_{het} = 0.32 \text{ Jm}^{-2}$ or 0.35 Jm^{-2} , the computed CTD was found to be much lower. Hence, a value of $\Delta\gamma_{het} = 0.38 \text{ Jm}^{-2}$ is used for the rest of our simulations.

It can be seen from the damage evolution plots in Figs. 5(a) and 6(a) that $(\phi)_{t_c} = 1.0 \times 10^{-4}$ roughly indicates the point at which ‘stable’ damage propagation begins. As will be shown in Section 5.7, this value is in agreement with the critical damage corresponding to the computed fracture toughness.

Figure 6. (a): Evolution of total area-weighted damage with applied strain for different values of $\Delta\gamma_{het}$. (b): Computed CTD as a function of $\Delta\gamma_{het}$ at $(\phi)_{t_c} = 1.0 \times 10^{-4}$.

5.4. Crack growth resistance

The framework developed here is used to estimate the crack growth resistance (R curve) in terms of the CTD of a stationary crack (sharp notch) of increasing crack length for monotonic remote loading. A circular notch of $\rho = 0.5 \mu\text{m}$ was placed at increasing depths in the range 50-400 μm within the material. The dimensions of the crystal plasticity zone, loading and boundary conditions remain the same as shown in Fig. 2(a). The material was loaded to 0.5% remote applied engineering strain at a quasi-static strain rate of 10^{-4} s^{-1} at 550 K. The material response was

found to be just at or beyond the point of intersection of the 5% secant line with the load-displacement curve at 0.5% engineering strain, in all cases. Further, damage initiation was observed in all the irradiated microstructures.

Figure 7. Crack growth resistance of irradiated material compared to that of the virgin material, computed in terms of the *CTD* of stationary cracks of increasing lengths.

Figure 7 shows the computed *CTD* of the 2.9 dpa irradiated specimens with increasing crack length, compared to the simulations of the corresponding *CTD* for virgin (no irradiation) specimens. As expected, a monotonic, R curve behavior is seen for both the irradiated and virgin specimens. Further, the crack growth resistance of the irradiated material is lower than that of the corresponding virgin material in all cases. This is in qualitative agreement with experimental observations of the degradation in crack growth resistance for another ferritic/martensitic steel under quasi-static loading (Chaouadi, 2008).

Figure 8. Distribution of effective inelastic strain for (a): irradiated (to 2.9 dpa), and (c): virgin specimens loaded to 0.5% strain at 550 K. (b), (d): Distribution of damage corresponding to the microstructures in (a), and (c), respectively.

A comparison of the deformed microstructures (loaded to 0.5% remote applied engineering strain) for the 2.9 dpa irradiated and virgin specimens for $a = 200 \mu\text{m}$ is shown in Fig. 8. Figures 8(a) and (c) show the distribution of inelastic strain for the irradiated and the virgin material, respectively. The corresponding damage distribution is shown in Figs. 8(b) and (d), respectively. The same grain distribution and initial crystallography was used in both cases. As expected, no dislocation channels are observed in the virgin specimen; the inelastic strain localization is typical of a plane strain, small-scale yielding (cf. (Anderson, 2005; McClintock, 1971)). Further, no damage is observed in the virgin specimens. Physically, failure may initiate in the regions of stress concentration at second phase particles and inclusions (microstructural features not considered here) in the unirradiated specimens. This may lead to even higher *CTDs* than computed for the virgin specimens in our simulations. In the context of the present

constitutive equations, a lower value of $\Delta\gamma_{het}$ may be used to initiate failure at GB interfaces in the virgin specimens.

The irradiated microstructure, in contrast, shows failure initiation along interfaces, both dislocation channels and GBs, in the vicinity of the notch. These heterogeneous interfaces provide paths for ‘easy’ crack propagation in the irradiated material, thus degrading the crack growth resistance. Though not supported by explicit experimental results, Chaouadi (2008) suggested a similar mechanism to be responsible for degradation in the crack growth resistance of irradiated materials. FE simulations of void growth at bi-material interfaces (Li and Guo, 2002) have shown that void growth is more prolific at the interfaces as compared to that in a homogeneous material. This further asserts that the experimentally observed degradation in crack growth resistance of irradiated specimens is due to ‘accelerated’ void nucleation and growth processes at the dislocation channel interfaces, as modeled in our simulations. Note that the stress levels ahead of the notch are higher in the irradiated material (higher flow stress due to irradiation hardening) than the corresponding virgin material. Higher stress facilitates void nucleation according to the constitutive relations given in Eqs. (9)-(13), all other conditions remaining the same.

As mentioned earlier, we have assumed a uniform initial microstructure in our simulations, and have not modeled second phase particles or inclusions. Void nucleation at these particle interfaces may be expected to be prolific (Raj, 1978) and lead to even lower *CTDs* in irradiated experiments. Future work may study the effect of competitive void nucleation at these second phase particles as compared to dislocation channel interfaces.

It should be also noted that dislocation channeling is not always observed in tensile deformation of irradiated metals. Based on dislocation dynamics simulations, Arsenlis et al. (2012) showed that there is a threshold radiation dose below which the formation of dislocation channels and flow localization is not obvious. In previous work (Patra and McDowell, 2013), we have shown that the amount of localized strain within the ‘apparent’ channels increases with radiation dose. This has also been observed in experiments (Jiao and Was, 2010; Sharp, 1967). As a result of lower density of dislocation channels and/or lower localized strains at low radiation doses, presumably fewer interfaces would be available for void nucleation and growth. This is expected to lead to relatively higher *CTDs* (and higher fracture toughness) with decreasing radiation doses. Future work will study these effects.

5.5. Strain rate effects

Figure 9(a) shows the inelastic strain distribution ahead of a 300 μm deep notch loaded at a strain rate of 1.0 s^{-1} . The same microstructure loaded at a strain rate of 10^{-4} s^{-1} is shown in Figure 9(b). The material was irradiated to 2.9 dpa and then deformed to 0.49% strain at 550 K in both cases. It can be seen that the level of localization is lower at higher strain rate and the dislocation channels are not fully developed. In contrast, parts of the quasi-statically loaded microstructure are already in the post-localization, softening regime. Note that the material is modeled using a viscoplastic flow rule (cf. Eq. (T1.1)). Rate effects in limiting ‘viscous’ inelastic dissipation may lower the extent of localization in the material loaded at 1.0 s^{-1} . We have also verified from the stress-strain curves that the material loaded at higher strain rate has a higher hardening rate (with respect to plastic strain). It has been shown earlier (Becker, 1998) that localization is accommodated less readily at higher hardening rates. As a result,

formation of dislocation channel ‘interfaces’ and subsequent failure initiation is delayed at higher strain rates. Further, void nucleation and growth, as modeled here, are diffusion-controlled processes. Diffusion time scales are much lower than the time scales of inelastic deformation, especially for the material loaded at 1.0 s^{-1} ; fewer voids would nucleate and grow (i.e., less damage) over the time scale of inelastic deformation at this loading rate. From simulations, ϕ_t was found to be 1.54×10^{-6} for the material loaded at 1.0 s^{-1} , and 1.02×10^{-4} for the quasi-statically loaded material, after 0.49% applied strain. **These model predictions are in qualitative agreement with experiments (Chaouadi, 2008) that report an increase in crack growth resistance, i.e., relatively lower degradation of fracture toughness, for another ferritic/martensic steel under dynamic loading as compared to that under quasi-static loading. Since the material loaded at higher strain rate has lower relative damage, its tearing resistance would be higher.**

Figure 9. Comparison of inelastic strain distribution for irradiated (2.9 dpa) specimen loaded at a strain rate of (a): 1.0 s^{-1} , and (b): 10^{-4} s^{-1} , to 0.49% strain at 550 K.

5.6. Temperature effects

Figure 10(a) shows the evolution of total area-weighted void number density, $(N_v)_t$, for three different test temperatures. The corresponding evolution of total area-weighted void radius, $(r_v)_t$, is shown in Fig. 10(b). $\rho = 2 \text{ μm}$ and $a = 250 \text{ μm}$ in all these simulations. The same initial microstructure as in Figs. 3 and 4 was used for all three cases. The material was loaded to 0.5% strain, after irradiation to 2.9 dpa. $(N_v)_t$ and $(r_v)_t$ were computed using a similar procedure described for $(\phi)_t$ in Section 5.2. Note that the simulation failed to converge beyond 0.5% strain for the 600 K case.

As can be seen in Fig. 10(a), voids nucleate earlier in the material loaded at higher temperatures. However, the evolution of $(N_v)_t$ is not intuitive beyond the point of failure initiation. The rate of evolution of void number

density is higher at elevated temperatures due to higher thermal ‘activation’ of void nucleation, as modeled in Eq. (9). Inspection of the deformed microstructure (not shown here) revealed roughly the same failure patterns in all three cases, albeit at lower applied strains for the materials loaded at higher temperatures. It can also be seen that $(N_v)_t$ for the material loaded at 437 K is initially lower, but exceeds that for material loaded at 550 K after $\approx 0.55\%$ applied strain. This is because the material at lower temperature has relatively higher flow stress, resulting in lower activation energy for void nucleation (cf. Eq. (13)). Another reason for this is also due to the fact that the void radius of the material loaded at 437 K is much lower than that at 550 K (Fig. 10(b)), meaning less overall damage. In order to accommodate the incompatible deformation, failure initiation takes place via higher void nucleation rate at 437 K.

Figure 10 (b) shows that the evolution of void radius is near-monotonic at all temperatures; the rate of change of void radius is higher at higher temperatures. This is because void growth, as modeled here, is governed solely by thermally-activated diffusion kinetics. Void nucleation, on the other hand, is dependent both on the material stress levels and the loading temperature. The void radius is much lower at 437 K than the higher loading temperatures, indicating a change in failure mechanism from ductile ‘zigzag’ fracture (Chaouadi, 2008) to limited ductility ‘channel’ fracture (Fish and Hunter, 1976) in the temperature range 437-550 K. Note that $\Delta\gamma_{het}$ was assumed to be temperature invariant in these simulations. However, $\Delta\gamma_{het}$ may be expected to increase with decrease in temperature, further lowering the rate of void nucleation and growth.

Figure 10. Evolution of (a): total area-weighted void number density, and (b): total area-weighted void radius as a function of temperature.

5.7. Fracture toughness calculations

In the limit of small-scale yielding, the stress intensity factor, K , in terms of the CTD , is given as (Anderson, 2005)

$$K = \sqrt{m\sigma_{ys}(CTD)E'} \quad (28)$$

where m is a dimensionless constant dependent on the stress state ($m = 2$ for plane strain), σ_{ys} is the yield stress, and $E' = E/(1-\nu^2)$ for plane strain. As mentioned earlier, the intersection of the 5% secant line with the load-displacement curve is generally used to assess the critical fracture toughness, K_c , in experiments. We adopt a similar procedure in the present work, computing the CTD at the point of intersection of the 5% secant line with the load-displacement curve, and calculating K_c using Eq. (28). Based on the true stress-true strain curve of Mod 9Cr-1Mo steel irradiated to 2.9 dpa (not presented here), $\sigma_{ys}|_{550\text{ K}} \approx 725\text{ MPa}$ at $T = 550\text{ K}$. Further, $\sigma_{ys}|_{437\text{ K}} \approx 750\text{ MPa}$, and $\sigma_{ys}|_{600\text{ K}} \approx 710\text{ MPa}$.

The values of K_c calculated for different notch depths and radii are listed in Table 3. There is a large discrepancy in the measured value of K_c between simulations and experiments. However, note that the experiments used a much larger notch radius, ρ . In general, the measured K_c is known to decrease with decreasing ρ for both metals (Akourri et al., 2000; Ritchie and Horn, 1978; Yoda, 1987) and ceramics (Damani et al., 1996; Fett, 2005; Nishida et al., 1994). The same was observed in our simulations, when ρ was decreased from 2 μm to 0.5 μm . It has also been suggested that K_c scales linearly with $\rho^{1/2}$, beyond a threshold notch root radius (Fett, 2005; Ritchie and Horn, 1978). See (Ritchie et al., 1976; Wilshaw et al., 1968) for analytical model to explain this effect. As shown in Fig. 11, if we were to extrapolate the simulated K_c as a function of $\rho^{1/2}$ for $a/W = 0.5$, the predicted K_c at $\rho = 60 - 80\text{ }\mu\text{m}$ is consistent with the experimental values. Possible reasons of slightly lower values of K_c reported in experiments may be due to higher radiation doses and lower test temperatures (reflecting in lower ductility). Also note that the experimental notch root radii are larger than the grain size ($\approx 25\text{ }\mu\text{m}$). At these notch root radii, intergranular interactions may homogenize and mitigate the effect of grain level heterogeneity on the fracture toughness that are observed for sub-grain size notch root radii, for example in the present simulations. Further, fracture toughness has also been found to vary with irradiation temperature (Byun et al., 2013). These effects are beyond the scope of the present work and not considered here.

It can be seen from Table 3 that the value of $(\phi)_t$ at critical fracture toughness is in the range $10^{-5} - 10^{-4}$ at 550 K. We have shown earlier in Section 5.3 that this value roughly corresponds to the stable damage propagation regime. In terms of classical fracture mechanics, the driving force for fracture, K , overcomes the material resistance, K_c , at this critical $(\phi)_t$ to allow stable crack propagation. Further, $(\phi)_t$ decreases with decrease in temperature, indicating

a decrease in ductility. $(\phi)_t$ may thus be used as an indicator of the material's fracture behavior in the present framework.

Figure 11. K_c , as a function of $\rho^{1/2}$, extrapolated to the experimental notch radii.

Table 3. Fracture toughness calculations for different notch radii, ρ , and depths, a . $W = 800 \mu\text{m}$ is the width of the specimens.

Radiation dose (dpa)	T (K)	ρ (μm)	a/W	$(\phi)_t$	CTD (μm)	K_c ($\text{MPa}\sqrt{\text{m}}$)
2.9	550	0.5	0.3125	2.44×10^{-5}	2.35	26.61
2.9	550	0.5	0.375	2.11×10^{-5}	2.21	25.84
2.9	550	0.5	0.4375	1.03×10^{-4}	2.00	24.58
2.9	550	0.5	0.5	3.29×10^{-5}	2.01	24.60
2.9	550	1.0	0.5	1.05×10^{-5}	3.01	30.15
2.9	550	2.0	0.5	1.86×10^{-5}	4.83	38.18
2.9	550	1.0	0.3125	1.97×10^{-4}	3.27	31.41
2.9	550	2.0	0.3125	1.48×10^{-4}	5.41	40.40
2.9	437	2.0	0.3125	1.10×10^{-9}	5.12	40.74
2.9	600	2.0	0.3125	4.18×10^{-4}	5.50	39.97
3.0	323-433	~65	0.5	-	-	100-140 ¹
4.3	523	~80	0.5	-	-	≈ 150 ²

¹ (Maloy et al., 2001), ² (Jia and Dai, 2006)

6. Conclusions

A void nucleation and growth based continuum damage framework has been developed and coupled with an existing crystal plasticity framework, to model failure initiation in irradiated bcc materials. Constitutive equations for vacancy generation via cross-slip and dislocation dipole mechanisms (during inelastic deformation) have been developed. Void nucleation has been modeled using a classical nucleation theory, while void growth is modeled using a diffusion-controlled mechanism. The framework has been used to model vacancy supersaturation along dislocation channels, and void nucleation and growth along these dislocation channels and GBs at high stress triaxialities.

Our simulations have been able to capture the microstructural evolution characteristics of transgranular faceted fracture along intertwined dislocation channel interfaces at intermediate temperatures. Further, the crack growth resistance of irradiated notched specimens has been found to be lower than that of the corresponding virgin specimens. The extent of localization and damage (in the irradiated microstructures) was found to decrease with increase in the loading rate. The effect of temperature on the evolution of void number density and radius has also been studied. There is a discrepancy between the irradiated specimen fracture toughness measured from simulations and from experiments. However, when the simulated fracture toughness values are extrapolated to the experimental notch root radii, they are consistent with the values measured from experiments.

The simulated failure initiation is strongly sensitive to the value of the interfacial energy change, $\Delta\gamma_{het}$, for heterogeneous void nucleation at dislocation channel interfaces and GBs. As has been demonstrated, this parameter may be used to calibrate the simulations to experimental results, in terms of the measured crack tip displacement and/or critical fracture toughness. Insights from atomistic simulations of the interfacial phenomena may also be used to refine the estimation of this parameter, for example its temperature dependence. Further, the value of $\Delta\gamma_{het}$ adopted here is used to study failure initiation ahead of sharp notches having radii in the range 0.5-2.0 μm . At lower stress triaxialities (larger notch root radii), this value of $\Delta\gamma_{het}$ may be too high to allow any void nucleation. Future work can address these issues by performing detailed parametric studies of the effect of notch geometry on failure initiation. **Detailed parametric study of the effect of radiation dose and strain rate on the fracture toughness would be informative.** Future work can also incorporate strain-driven void growth mechanisms in this framework.

The damage framework developed here combined with the crystal plasticity framework developed earlier (Patra and McDowell, 2013, 2012) represents a physically-based approach to model the mechanical behavior and deformed microstructure of irradiated bcc metals from initial irradiation hardening to flow localization along dislocation channels and subsequent failure along these dislocation channel interfaces. Due to the lack of systematic experimental data, it is not possible to quantitatively verify the various model predictions in terms of evolution of microstructure. However, the model predictions are in qualitative agreement with experimental observations of ductile fracture in another irradiated ferritic/martensitic steel (Chaouadi, 2008).

Defect-tolerant design of structures used in nuclear applications often relies on the fracture toughness master curve of the material used (cf. Odette et al. (2003)). This framework (calibrated to experiments) may be used to construct

such master curves for various loading histories. Further, the framework developed here is pretty general and may be applied to simulate void nucleation and growth-mediated failure for other deformation histories (no irradiation) as well, for example, at slip band interfaces during cyclic loading, or at second phase interfaces, etc. in different material systems.

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Figure 1

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