Probabilistic and constitutive models for ductile-to-brittle transition in steels: A competition between cleavage and ductile fracture

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\textbf{A R T I C L E   I N F O}

\textbf{Article history:}
Received 21 February 2019
Revised 25 November 2019
Accepted 27 November 2019
Available online 30 November 2019

\textbf{Keywords:}
Cleavage fracture
Void nucleation
Ductile-to-brittle transition
Temperature dependence
Irradiation hardening and embrittlement

\textbf{A B S T R A C T}

We propose a probabilistic model coupling with the temperature dependent constitutive relationship to describe the competition between the cleavage and ductile void failure of ferritic/martensitic steels with irradiation effects. It is found that both the material deformation and failure modes exhibit significant temperature dependence. Regarding the material deformation, two regimes have been found for the ductile-to-brittle transition (DBT). At low temperature, the flow stress is controlled by the mobility of screw dislocations. The failure modes depend on the carbide precipitate and temperature. Cleavage micro-cracks initiate at the carbide sites at low temperature giving rise to brittle behaviors. At high temperature, void nucleation evolving from the carbide precipitate suppresses the cleavage nucleation and propagation, and leads to good ductility. It is demonstrated that the competition between the cleavage fracture and ductile void failure is the major mechanism for the DBT. Our probabilistic model successfully predicts the temperature-dependent fracture toughness and ductile-to-brittle transition (DBTT). Besides temperature, irradiation has a significant effect on the DBT of steels. Upon irradiation, the steels exhibit both irradiation hardening and irradiation embrittlement, i.e., rise in yield and flow stresses, and increase on DBTT. The main reason for these irradiation effects is that the irradiation-induced hardening increases the flow stress, and the plasticity localization weakens the overall hindering effect from ductile void growth on the cleavage nucleation and propagation, promoting the development of cleavage. Our probabilistic model takes into account the cleavage nucleation-propagation process and the influence of ductile void growth simultaneously, and it gives a sound explanation for the fundamental relation between the DBTT and mechanical properties of metallic materials.

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1. Introduction

Metallic materials are commonly used as structural materials in the engineering and manufacturing industry. However, their applications are restricted by the brittleness or ductility, which is closely related to the DBT. For pure metals, the physical mechanism of the DBT is believed to be governed by the cleavage crack propagation or dislocation emission at the crack tip (Needleman and Tvergaard, 1995; Tvergaard and Needleman, 1986). Compared to pure metals, the DBT mechanism of steels becomes more sophisticated due to the solid solution and second phase strengthening associated with alloying elements as well as the carbide-induced precipitation strengthening. The study of the failure mechanisms of these metallic materials is essential for the development of the materials and the assessment of the mechanical integrity (Pineau, 2008). For ferritic/martensitic steels, their fracture properties show a large variation with temperature. At low temperature, small fracture toughness values are attributed to the transgranular cleavage fracture with minor plasticity. As the temperature increases, the ductile failure mode based on the void nucleation-growth-coalescence becomes the main fracture mechanism, which gives rise to a remarkable improvement in the macroscopic fracture toughness (Chakraborty and Biner, 2015). At medium temperature, a relatively small increase in temperature could lead to a large improvement in the fracture toughness, and this phenomenon is called the DBT phenomenon (Ruggieri and Dodds, 2015; Tiwari et al., 2018). Understanding the fundamental mechanism of DBT is of great significance for the improvement of mechanical properties and the development of advanced materials, and requires thorough researches on the transgranular cleavage fracture, ductile void failure and their inherent relations. So far, the mechanism of the competition between the cleavage and ductile failure remains veiled.

Cleavage fracture of steels is believed to have a connection to the carbide precipitate of the materials and temperature. For example, brittle second-phase particles such as carbides in ferritic/martensitic steels serve as the potential nucleation sources of cleavage fracture (Qian et al., 2018). During the loading process, the brittle particles within the region of high stress might break, and micro-cracks nucleate consequently. These micro-cracks could propagate even to neighbouring grains, though the crack propagation can be arrested by grain boundaries. As the propagation process further develops, unstable cleavage fracture takes place and leads to catastrophic structural failures. Existing experimental data on the fracture toughness of ferritic/martensitic steels exhibit large scatter owing to the complicated and stochastic distribution of the potential cleavage initiators in terms of their spatial locations, orientations, shapes and sizes (Chakraborty and Biner, 2015; Qian et al., 2018).

Over the past few decades, several approaches have been developed to analyze the cleavage fracture of ferritic/martensitic steels. (a) Master Curve Approach defining a characteristic transition temperature based on the impact toughness testing is introduced to evaluate the failure mode of materials (Wallin, 1984; 2011). It is assumed that the probability of ductile fracture can be neglected below the transition temperature and the transgranular cleavage fracture fully dominates the failure process. Note that the Master Curve Approach can only provide an empirical minimum tolerance, regardless of the microstructures of materials. Therefore, it offers a necessary but not sufficient assessment for cleavage fracture. (b) Conventional fracture mechanics can be adopted to calculate a single global parameter characterizing the fracture properties (e.g., the stress intensity factor $K$, $J$-integral and crack tip opening displacement) based on the applied stress, crack information and structure geometry (Shih, 1981). However, it cannot explain the inherent scatter of fracture toughness in cleavage fracture due to its essential deterministic assessment. (c) Fracture physics approach focuses on the micromechanism of cleavage fracture including the micro-crack nucleation and propagation processes, and contains a microstructure-dependent intrinsic cleavage strength to bridge the gap between the macroscopic fracture toughness and microstructures (Bordet et al., 2005). However, the influence of dislocation slipping and twinning on the cleavage nucleation and propagation is ignored, meaning that the relationship between the cleavage fracture and plasticity is not unveiled. (d) A nonlocal approach has been developed by Needleman and Tvergaard, 2000 to depict the cleavage fracture of metallic materials, and it was assumed that cleavage occurs as the average maximum principal stress in a subregion around where exceeds a critical value. (e) The statistical approach introduces a Weibull distribution of the fracture toughness to describe the intrinsic randomness of brittle fracture (Beremin, 1983). It is suggested that the global cleavage fracture toughness is controlled by the lowest toughness of a region in the specimen. A combination of the Weibull statistics and the weakest link theory can explain the scatter in fracture toughness measurements. However, this model is of phenomenological data fitting and lacks of the correlation with underlying physical mechanisms. In short, a physics-based modeling of cleavage fracture concerning the carbide precipitate and the dislocation behavior is called for describing the scatter of fracture toughness measurements and the overall mechanical behaviors of ferritic/martensitic steels.

In addition to the cleavage fracture, ductile void nucleation is another main mechanism involved in the DBT (Tvergaard and Needleman, 1993; Xia and Shih, 1996). It is known that unstable cleavage fracture can be impeded by ductile fracture based on the void nucleation-growth-coalescence (Chakraborty and Biner, 2015). The DBT is associated with a change in the fracture mechanism from cleavage initiation to ductile void nucleation (Needleman and Tvergaard, 2000; Wei and Anand, 2008). Since the latter one is usually accompanied by large plastic deformation (Lyu et al., 2016; Ren and Li, 2012), it is believed that a high fracture resistance is associated with the ductile mechanism and low fracture resistance with cleavage (Needleman and Tvergaard, 2000). As a matter of fact, the breaking of brittle carbides upon loading can lead to the nucleation of micro-cracks which then evolve into micro-voids (Xia and Shih, 1996). The continuing plastic deformation not only leads to void nucleation and growth but also blunts the crack tip. Therefore, the intrinsic mechanism for the DBT can be regarded as the competition between the cleavage initiation and ductile void nucleation. Void nucleation-growth-coalescence has an impact on the evolution of porosity in steels, and the porosity can soften the matrix and affect the material constitut-
tive relation. Gurson-Tvergaard-Needleman model has been widely used to describe the void nucleation-growth-coalescence of metallic materials (Gurson, 1977; Needleman and Tvergaard, 1984; Tvergaard and Needleman, 1984). At the grain level, an analytical expression has been obtained to determine the effective resolved shear stress on certain slip systems (Faleskog et al., 1998; Han, 2013; Ponte Castaneda and Zaidman, 1996; Tvergaard and Needleman, 1984). This offers a way to build a relationship between the void growth and the dislocation behaviors. In short words, the carbide precipitate and temperature affect the cleavage initiation and void nucleation, and their competition is the inherent mechanism of DBT.

Recently, many molecular dynamics (MD) simulations have been carried out to reveal the mechanism for the DBT at atomic level, which is found to be attributed with the cleavage micro-crack propagation or dislocation emission induced crack blunting (Andric and Curtin, 2017; El-Awady et al., 2009; El Nabi et al., 2015; Huang et al., 2009; Rajan and Curtin, 2016; Thaulow et al., 2011; Wu and Curtin, 2015; Zhou and Guo, 2015). From the theoretical point of view, Beltz et al. (1999) and Fischer and Beltz, 2001 calculated the critical energy release rate for the cleavage propagation and dislocation emission to determine the intrinsic brittleness or ductility of materials. Both MD simulations and theoretical analysis consider simplified slip systems and loading conditions. Consequently, they cannot be used to calculate the macroscopic mechanical behaviors of materials. Dislocation emission around the crack tip leads to good ductility and micro-void growth. Therefore, the essence of cleavage and dislocation emission can be regarded as the competition between the micro-crack propagation and void growth.

As mentioned above, the carbide precipitate and temperature are two important factors for the DBT region of steels. In addition, the irradiation can affect both the flow stress and plastic behavior of materials, and a coupling effect between the temperature and the irradiation makes the DBT more intricate. Ferritic/martensitic steels are good candidates of structural materials in fusion reactors due to their excellent anti-irradiation properties (Terentyev et al., 2013). Irradiation damage formed in service can give rise to the formation of irradiation defects in materials, i.e., stacking fault tetrahedrons in face-centred cubic (FCC) crystals (Chen et al., 2018; Xiao et al., 2015) and dislocation loops in body-centred cubic (BCC) crystals (Chakraborty and Biner, 2015). The irradiation defects can hinder the motion of slipping dislocations and increase the yield stress and flow stress, and this mechanism is called irradiation hardening (Patra and McDowell, 2013; Singh et al., 1995). However, the sliding dislocations under severe loading subsequently sweep and absorb the dislocation loops to create defect-free dislocation channels (Luft, 1991). These channels are the main reason for the reduction in the strain hardening capacity, softening and plasticity localization. Besides the irradiation hardening, the irradiation embrittlement is another factor regulating the DBT increase after irradiation (Yamamoto et al., 2006; Zinkle and Ghoniem, 2011), which seriously reduces the life span of structural metallic materials. It is regarded that the higher flow stress due to the existence of irradiation defects can accelerate the cleavage nucleation and propagation which deteriorate the fracture toughness of materials. Besides, the irradiation embrittlement induced increase in DBT is usually characterized by numerous costly and time-consuming experiments. Related theoretical framework is still not well developed. Therefore, a physics-based constitutive model is needed to explore the relationship between the mechanical behaviors and the irradiation-induced embrittlement, and it can provide important guidelines for the improvement of irradiation mechanical properties of metallic materials in nuclear industry.

In this work, a crystal plasticity constitutive framework coupling with the probabilistic analysis concerning the competition between the cleavage and ductile void failure is proposed to explore the mechanical properties of steels including the DBT feature. The paper is organized as follows: In Section 2, a probabilistic model concerning the competition between the cleavage fracture and ductile void failure is proposed. In Section 3, a crystal plasticity constitutive model with temperature and irradiation effects is introduced systematically. In Section 4, the proposed model is used to study the mechanical properties of ferritic/martensitic steels, and numerical results under different irradiation conditions are presented. In Section 5, a detailed investigation on the DBT is carried out, and the mechanism of irradiation embrittlement is discussed. In Section 6, conclusive remarks are presented.

2. A probabilistic model for competition between cleavage and ductile fracture

For ferritic/martensitic steels, the carbide precipitate and temperature are two main factors influencing the failure modes. After irradiation, the steels would suffer irradiation damage which leads to the formation of micro-defects. Consequently, both the deformation behaviors and failure mechanisms of steels are affected by temperature and irradiation. Fig. 1 gives a schematic diagram about the influence of temperature and irradiation dose on the failure modes of ferritic/martensitic steels. In the absence of loading, there are a number of intact carbide particles in steels, and some micro-defects can form during the irradiation process [Figs. 1 (A) and (B)]. Carbides in ferritic/martensitic steels are the potential nucleation sources of cleavage fracture (Qian et al., 2018). At large strains, homogeneously distributed small carbide particles can nucleate and lead to the ductile void growth (Tvergaard and Needleman, 1993). Therefore, carbides can actually lead to both cleavage initiation and void nucleation. As shown in Figs. 1 (a-c), at low temperature the cleavage micro-cracks nucleate with minor plasticity. Therefore, a number of micro-cracks nucleate and no void is observed. As the temperature increases, void nucleation and growth develop rapidly and suppress the cleavage initiation. As a consequence, the number of voids increases gradually while the number of cleavage cracks decreases. The higher flow stress in irradiated materials makes more carbide particles break and the uniform plastic deformation is limited. These two features give rise to an increase on the number of the cleavage micro-cracks and a rapid decline in numbers of micro-voids as shown in Figs. 1 (d-f). Consequently, irradiation deteriorates the plastic deformation capacity of materials, and the materials behave in a brittle manner with more cleavage
micro-cracks nucleating. Therefore, the DBTT increases after irradiation. To thoroughly investigate the DBT, a probabilistic model is developed to quantitatively describe the contribution of cleavage cracking and ductile void growth.

Cracking of carbide precipitates promotes catastrophic cleavage fracture. However, if a void nucleates in a potential nucleation site, it can grow with the plastic deformation and contribute to the ductile void fracture. Therefore, increasing the probability of void nucleation can reduce the probability of cleavage failure, and the catastrophic cleavage fracture event can be delayed by void nucleation (Xia and Shih, 1996). For a potential nucleation site, it is clear that

\[ P_i^{\text{clea, nul}} + P_i^{\text{void}} + P_i^{\text{surv}} = 1. \]

where \( i \) denotes the ith stressed region, \( P_i^{\text{clea, nul}} \), \( P_i^{\text{void}} \) and \( P_i^{\text{surv}} \) represent the probability of cleavage initiation, void nucleation and surviving, respectively. To determine the relationship between \( P_i^{\text{clea, nul}} \), \( P_i^{\text{void}} \) and \( P_i^{\text{surv}} \), a conditional probability is adopted as

\[ P(A|B) = \frac{P(A \cap B)}{P(B)}. \]

where event A and event B express cleavage nucleation and no void initiation, respectively. In our study, event A is a subset of event B. The relationship between cleavage nucleation and void initiation can be determined as \( P(A) = P(A|B) \times P(B) \) or

\[ P_i^{\text{clea, nul}} = P_i^{\text{clea, nul(nv)}} (1 - P_i^{\text{void}}). \]

where \( P_i^{\text{clea, nul(nv)}} \) represents the probability of cleavage nucleation with no void initiation. Eq. (2.3) depicts the competing relation between cleavage initiation and void nucleation, recalling that the void nucleation can restrain the cleavage failure in a stressed region.

The porosity \( f \) is defined as the ratio between the void volume \( V_{\text{void}} \) and the total volume of the specimen \( V_{\text{total}} \) as

\[ f = \frac{V_{\text{void}}}{V_{\text{total}}}. \]

Both void nucleation and growth contribute to the evolution of \( f \). According to the normal distribution for void nucleation proposed by Chu and Needleman (1980), the evolution of porosity due to void initiation \( \dot{f}_{\text{void, nuc}} \) is

\[ \dot{f}_{\text{void, nuc}} = \frac{f_N}{s_N \sqrt{2\pi}} \exp \left( -\frac{1}{2} \left( \frac{\dot{\varepsilon}_p - \varepsilon_N}{s_N} \right)^2 \right) \dot{\varepsilon}_p, \]

where dots represent the time derivatives, \( f_N (= 0.00025) \) is a void nucleation parameter, \( s_N (= 0.02) \) and \( \varepsilon_N (= 0.08) \) are the standard deviations (Xia and Shih, 1996), and \( \dot{\varepsilon}_p \) represents the equivalent plastic strain. It is noted that the equivalent

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**Fig. 1.** A schematic diagram describing the influence of temperature and irradiation dose on the failure modes.
plastic strain $\varepsilon_p$ at every nucleation area is different. Therefore, the void porosities at the individual nucleation areas are different, and the distributions of void porosity are also different. Void nucleation in ferritic/martensitic steels is assumed to arise from the interfacial de-cohesion and cracking of carbides. The total volume of void due to the void nucleation is

$$V_{\text{void,nuc}} = P_{\text{void}}N_{\text{total}}\frac{4}{3}\pi r^3,$$  \tag{2.6}$$

where $P_{\text{void}}$ denotes the probability of void nucleation, and $N$ and $r$ represent the number density and average radius length of carbides, respectively. According to the void nucleation law proposed by Chu and Needleman (1980), the total volume of void due to void nucleation can be described as

$$V_{\text{void,nuc}} = f_{\text{void,nuc}}V_{\text{total}} = V_{\text{total}} \times \int \frac{f_N}{s_N\sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\varepsilon_p - \varepsilon_N}{s_N} \right)^2 \right] d\varepsilon_p. \tag{2.7}$$

Based on Eqs. (2.6) and (2.7), the probability of void nucleation $P_{\text{void}}$ can be derived as

$$P_{\text{void}} = \frac{1}{N^2 \frac{4}{3}\pi r^3} \int \frac{f_N}{s_N\sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\varepsilon_p - \varepsilon_N}{s_N} \right)^2 \right] d\varepsilon_p. \tag{2.8}$$

It is indicated that $P_{\text{void}}$ depends on the carbide precipitate and plastic deformation of metallic materials. Until now, we have derived the expression of $P_{\text{void}}$, further discussions on the cleavage process are as follows.

A catastrophic cleavage process includes two independent parts: cleavage nucleation and crack propagation. As for the probability of cleavage microcrack nucleation, several experiments were carried out to explore the initiation of fracture at carbide particles in spheroidized carbon tool steels (Gurland, 1972; Kaechele and Tetelman, 1969). It was found that the probability of cleavage microcrack nucleation had linear relationship with the plastic strain $\varepsilon_p$ and yield stress $\sigma_y$ as shown in Fig. 2. Therefore, a linear relationship is derived here to describe the yield stress and plastic strain dependent probability of cleavage microcrack nucleation as

$$P_{\text{clea,nul(nv)}} = \begin{cases} \kappa (\sigma_y(T) - \sigma_{y,\text{critical}})\varepsilon_p, & \sigma_y(T) \geq \sigma_{y,\text{critical}}, \\ 0, & \sigma_y(T) < \sigma_{y,\text{critical}}, \end{cases} \tag{2.9}$$

where $\kappa$ is the nucleation coefficient, $\sigma_y(T)$ is the temperature dependent yield stress of steels, and $\sigma_{y,\text{critical}}$ is the nucleation critical stress.

Till now, the probability of void nucleation and cleavage crack nucleation without plasticity has been analyzed. Based on Eq. (2.3), at $\sigma_y(T) \geq \sigma_{y,\text{critical}}$, the actual probability of cleavage initiation accounting for the inhibition effect of void nucleation on cleavage fracture for a potential nucleation site is

$$P_{\text{clea,nul}}^b = P_{\text{clea,nul(nv)}} (1 - P_{\text{void}})$$

$$= \kappa (\sigma_y(T) - \sigma_{y,\text{critical}})\varepsilon_p \times \left[ 1 - \frac{1}{N^2 \frac{4}{3}\pi r^3} \int \frac{f_N}{s_N\sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\varepsilon_p - \varepsilon_N}{s_N} \right)^2 \right] d\varepsilon_p \right]. \tag{2.10}$$

Besides the cleavage initiation, the cleavage propagation is another important factor influencing the cleavage process. It is noted that cleavage fracture in ferritic/martensitic steels usually takes place on the cleavage plane ($\{001\}$ plane) of BCC materials. With a premise of no void initiation and plasticity (conditional probability discussed above), the total deformation.
process can be treated as brittle deformation. Based on the classical Griffith theory for penny-shaped cracks (Kroon and Faleskog, 2002), the critical crack size \( l_{\text{crit}} \) of cleavage propagation can be calculated at a given stress field as (Bordet et al., 2005)

\[
l_{\text{crit}} = \frac{\pi E \gamma_p}{2(1-\nu^2) (\sigma_{[001]}^{\text{CS}})^2},
\]

(2.11)

where \( E \) is the Young's modulus, \( \gamma_p \) represents the surface energy of cleavage plane, \( \nu \) is the Poisson ratio of carbides, and \( \sigma_{[001]}^{\text{CS}} \) is the threshold cleavage strength.

As described in the Beremin model (Beremin, 1983), the probability of nucleated cleavage micro-cracks treated as Griffith cracks is described by an inverse power law as

\[
g(I) = \frac{\xi_1}{I^\xi_2},
\]

(2.12)

where \( I \) is the micro-crack length, and \( \xi_1 \) and \( \xi_2 \) are material parameters. Therefore, the total probability of cleavage propagation is

\[
P_{\text{clea,prop}} = \chi \int_{I_{\text{crit}}}^{I_{\text{max}}} (\sigma_{[001]}^{\text{CS}}) g(I) dI,
\]

(2.13)

where \( \chi \) is introduced as a scale parameter enforcing that the maximum of \( P_{\text{clea,prop}} \) is 1, and \( I_{\text{crit}}(\sigma_{[001]}^{\text{CS}}) \) denotes the maximum nucleated micro-crack length determined by the threshold stress \( \sigma_{[001]}^{\text{CS}} \). Here \( \sigma_{[001]}^{\text{CS}} \) is approximately equal to the yield stress \( \sigma_y \). \( I_{\text{max}}(\sigma_{[001]}^{\text{MAX}}) \) is the shortest crack length calculated by the maximum stress \( \sigma_{[001]}^{\text{MAX}} \) on cleavage plane. Substituting Eqs. (2.11) and (2.12) into Eq. (2.13), a stress-dependent probability of cleavage propagation can be obtained as

\[
\begin{align*}
&P_{\text{clea,prop}} = 0, \\
&P_{\text{clea,prop}} = \frac{(\sigma_{[001]}^{\text{MAX}})^{\mu_c} - (\sigma_{[001]}^{\text{CS}})^{\mu_c}}{(\sigma_{[001]}^{\text{MAX}})^{\mu_c} - (\sigma_{[001]}^{\text{CS}})^{\mu_c}} \cdot \frac{\sigma_{[001]}^{\text{MAX}}}{{\sigma_{[001]}^{\text{CS}}}}, \quad \sigma_{[001]}^{\text{MAX}} < \sigma_{[001]}^{\text{CS}}, \\
&P_{\text{clea,prop}} = 1, \quad \sigma_{[001]}^{\text{MAX}} \geq \sigma_{[001]}^{\text{CS}}.
\end{align*}
\]

(2.14)

where \( m_c (= 2\xi_2 - 2) \) is the Weibull shape factor characterizing the particle dispersion and \( \sigma_{[001]}^{\text{U}} = [ - m_c / (2\xi_1) ]^{1/\mu_c} \cdot \left[ \pi E \gamma_p / 2(1-\nu^2) \right]^{1/2} \). At \( \sigma_{[001]}^{\text{MAX}} = \sigma_{[001]}^{\text{U}} \), \( P_{\text{clea,prop}} = 1 \). Therefore, we have \( \chi = (\sigma_{[001]}^{\text{U}})^{\mu_c} / (\sigma_{[001]}^{\text{MAX}})^{\mu_c} - (\sigma_{[001]}^{\text{CS}})^{\mu_c} \). It means that as the maximum tensile stress on the cleavage plane \( \sigma_{[001]}^{\text{MAX}} \) reaches \( \sigma_{[001]}^{\text{U}} \), the cleavage crack must propagate. The stress-dependent probability of cleavage propagation can then be expressed as

\[
\begin{align*}
&P_{\text{clea,prop}} = 0, \\
&P_{\text{clea,prop}} = \frac{(\sigma_{[001]}^{\text{MAX}})^{\mu_c} - (\sigma_{[001]}^{\text{CS}})^{\mu_c}}{(\sigma_{[001]}^{\text{MAX}})^{\mu_c} - (\sigma_{[001]}^{\text{CS}})^{\mu_c}} \cdot \frac{\sigma_{[001]}^{\text{MAX}}}{{\sigma_{[001]}^{\text{CS}}}}, \quad \sigma_{[001]}^{\text{MAX}} < \sigma_{[001]}^{\text{CS}}, \\
&P_{\text{clea,prop}} = 1, \quad \sigma_{[001]}^{\text{MAX}} \geq \sigma_{[001]}^{\text{CS}}.
\end{align*}
\]

(2.15)

Since the probability of both cleavage nucleation and propagation evolves during the deformation process, the actual failure probability of a potential site is

\[
P_{\text{failure}} = P_{\text{clea,prop}} \times P_{\text{clea,nul}} = \sum_{n=1}^{N} \left[ P_{\text{clea,nul}}^{i} (\epsilon_{p,n}) - P_{\text{clea,nul}}^{i} (\epsilon_{p,n-1}) \right] \times P_{\text{clea,prop}} (\epsilon_{p,n}).
\]

(2.16)

where \( \epsilon_{p,n} \) and \( \epsilon_{p,n-1} \) represent the accumulated equivalent plastic strain at previous and current loading steps, respectively. The term \( \left[ P_{\text{clea,nul}} (\epsilon_{p,n}) - P_{\text{clea,nul}} (\epsilon_{p,n-1}) \right] \) denotes the probability increment of micro-crack nucleation, and \( P_{\text{failure}} \) is the total failure probability of ith stressed region.

The whole sample consists of multiple potential cleavage regions, and all stressed regions in good condition can guarantee the overall structure integrity based on the weakest-link theory. In a consequence, the overall failure probability is

\[
P_{f} = 1 - \exp \left( - \sum_{i} P_{\text{failure}}^{i} \right)
\]

\[
= 1 - \exp \left[ - \int_{V_0} \left( \sum_{n=1}^{N} \left[ P_{\text{clea,nul}}^{i} (\epsilon_{p,n}) - P_{\text{clea,nul}}^{i} (\epsilon_{p,n-1}) \right] \times P_{\text{clea,prop}} (\epsilon_{p,n}) \right) \frac{dV}{V_0} \right].
\]

(2.17)

where \( V_0 \) is the average volume of one grain.

In this section, a probabilistic model describing the competition between cleavage and ductile void failure is introduced. To systematically explore the mechanical behaviors and DBT feature, a constitutive framework is presented in the following section.
3. Constitutive relation with the probabilistic model

As discussed above, the probabilistic model involves the cleavage stress and plastic strain of steels, thus it is coupled with the constitutive relation of materials. In this section, a constitutive relation coupling with the probabilistic model is introduced.

Adopting the framework of the classical crystal plasticity theory (Asaro and Rice, 1977; Hill, 1966; Hill and Rice, 1972), the deformation gradient $\mathbf{F}$ can be decomposed into elastic and plastic parts as

$$
\mathbf{F} = \mathbf{F}^e \cdot \mathbf{F}^p,
$$

(3.1)

where the subscripts e and p denote quantities associated with the elastic and plastic deformation, respectively. As the plastic deformation is assumed to be dominated by the slipping of dislocations, the derivative of the plastic deformation gradient $\mathbf{F}^p$ with respect to time can be given by

$$
\dot{\mathbf{F}}^p = \left( \sum_{\alpha=1}^{N_s} \gamma^\alpha \mathbf{S}^\alpha \otimes \mathbf{n}^\alpha \right) \mathbf{F}^p,
$$

(3.2)

where the dot represents the first derivative to the loading time, $\gamma^\alpha$ is the shearing slip rate on the $\alpha$th slip system, $N_s$ is the total number of slip systems, and the vectors $\mathbf{s}^\alpha$ and $\mathbf{n}^\alpha$ represent the slip direction and normal direction of the $\alpha$th slip plane, respectively. The superscript $\alpha$ is used to denote a quantity associated with the $\alpha$th slip system. For BCC materials, there are $N_s = 24$ slip systems characterized by the Miller indexes $(110) < 111 >$ and $(112) < 111 >$.

Recalling the Green strain tensor $\mathbf{E}^e$ expressed as

$$
\mathbf{E}^e = \frac{1}{2} \left( (\mathbf{F}^e)^T \cdot \mathbf{F}^e - \mathbf{I} \right),
$$

(3.3)

with $\mathbf{I}$ as the second-order unit tensor, the second Piola-Kirchhoff stress $\mathbf{T}^{(1)}$ is given by

$$
\mathbf{T}^{(1)} = \mathbf{C} : \mathbf{E}^e,
$$

(3.4)

where $\mathbf{C}$ denotes the fourth-order stiffness tensor.

To characterize the shear strain rate $\dot{\gamma}^\alpha$ on the slip system $\alpha$, the resolved shear stress (RSS) $\tau^\alpha$ is introduced as

$$
\tau^\alpha = \mathbf{T}^{(1)} : \mathbf{S}^\alpha,
$$

(3.5)

where $\mathbf{S}^\alpha = (\mathbf{s}^\alpha \otimes \mathbf{n}^\alpha + \mathbf{n}^\alpha \otimes \mathbf{s}^\alpha) / 2$ is the Schmid tensor. Taking into account the applied mean stress $\sigma_m$ and the porosity $\mathbf{f}$, the effective RSS $\tau^\alpha_{eff}$ acting on the slip system $\alpha$ can be derived as (Faleskog et al., 1998; Gurson, 1977; Han, 2013; Tvergaard and Needleman, 1984)

$$
\left( \frac{\tau^\alpha_{eff}}{\tau^\alpha} \right)^2 + \lambda \left( \frac{\sigma_{eq}}{\tau^\alpha} \right)^2 + 2q_1 f \cosh \left( q_2 \sqrt{\frac{3}{20} \frac{\sigma_{eq}}{\tau^\alpha}} \right) - q_1 f^2 = 1,
$$

(3.6)

where $q_1$ and $q_2$ are heuristic factors (Tvergaard and Needleman, 1984), $\lambda$ is a new parameter to characterize the relative contribution of the RSS on the slip system $\alpha$. Here, $\lambda = 6.456$, $q_1 = 1.471$ and $q_2 = 1.325$ are taken as Han (2013). $\sigma_{eq}$ and $\sigma_m$ are the Von Mises equivalent stress and the mean stress, respectively. If there is no void ($f = 0$), Eq. (3.6) reduces to $\tau^\alpha_{eff} = \tau^\alpha$.

As the plastic deformation develops, the porosity $f$ evolves. Both the rates of void nucleation and void growth contribute to the evolution of porosity and are assumed to obey a simple linear relation as

$$
\dot{f} = \dot{f}_{\text{void\_growth}} + \dot{f}_{\text{void\_nuc}},
$$

(3.7)

where the void nucleation rate $\dot{f}_{\text{void\_nuc}}$ is described by Eq. (2.5), and the void growth rate $\dot{f}_{\text{void\_growth}}$ depends on the plastic deformation rate $\dot{\varepsilon}_p$ as (Chakraborty and Biner, 2015)

$$
\dot{f}_{\text{void\_growth}} = (1 - f) \dot{\varepsilon}_p.
$$

(3.8)

The equivalent plastic strain $\dot{\varepsilon}_p$ is accumulated by the shear strain on each slip system $\dot{\gamma}^\alpha$. According to the normality rule, the plastic strain rate tensor $\dot{\varepsilon}_p$ can be expressed as

$$
\dot{\varepsilon}_p = \sum_{\alpha=1}^{N_s} \dot{\gamma}^\alpha \mathbf{S}^\alpha,
$$

(3.9)

where the shearing slip rate $\dot{\gamma}^\alpha$ is closely related to the dislocation motion. The mobilities of screw and edge dislocations in BCC crystals show a strong difference at low temperature. According to the work of Monnet et al., 2013, the flow stress at low temperature is mainly controlled by the mobility of screw dislocations, while the forest dislocation interactions dominate the flow stress as the temperature increases.
At low temperature, several dislocation-dynamics simulations (Monnet et al., 2004; Naamane et al., 2010) indicate that the flow stress is controlled by the effective stress on screw dislocation, regardless of the mobility law of non-screw dislocations, which is called ‘friction regime’. Naamane et al., 2010 proposed that the velocity of screw dislocations can be expressed as

\[ t^\alpha = H s^\alpha \exp \left( - \frac{\Delta G(\tau^\alpha)}{k_B T} \right) \text{sign}(\tau^\alpha). \]  

(3.10)

where \( H(=2 \times 10^{11} \text{s}^{-1}) \) is a frequency factor (Monnet et al., 2013), \( l_s^\alpha \) is the average length of the screw dislocation segments depending on the microstructure information (Monnet et al., 2013), \( k_B(=8.6 \times 10^{-5} \text{eV/K}) \) is the Boltzmann constant, \( T \) is the absolute temperature, and \( \Delta G \) is the effective RSS dependent activation energy for double-kink nucleation as

\[ \Delta G(\tau^\alpha) = \Delta G_0 \left( 1 - \sqrt{\frac{\tau^\alpha}{\tau_0}} \right) \]  

(3.11)

with two fitting parameters \( \Delta G_0 = 1.0 \text{ eV} \) and \( \tau_0 = 750 \text{ MPa} \). Taking into account both the contribution of screw dislocations and non-screw dislocations, the shear rate equation \( \dot{\gamma}_\text{friction} = 2 \rho_m b H s^\alpha \exp \left[ - \frac{\Delta G_0}{k_B T} \left( 1 - \sqrt{\frac{\tau^\alpha}{\tau_0}} \right) \right] \text{sign}(\tau^\alpha) \) (Monnet et al., 2013) can be derived as

\[ \dot{\gamma}_\text{friction} = 2 \rho_m b H s^\alpha \exp \left[ - \frac{\Delta G_0}{k_B T} \left( 1 - \sqrt{\frac{\tau^\alpha}{\tau_0}} \right) \right] \text{sign}(\tau^\alpha). \]  

(3.12)

At high temperature, the flow stress is mainly controlled by the thermally activated jog drag in the dislocation microstructure, which is termed as the ‘drag regime’ here (Monnet et al., 2013). Moreover, the shear strain rate can be given by

\[ \dot{\gamma}_\text{drag} = \gamma_0 \frac{\tau^\alpha}{\tau_c} \text{sign}(\tau^\alpha). \]  

(3.13)

where \( \gamma_0 \) is the reference strain rate, \( m \) is the strain rate sensitivity, and the critical resolved shear stress \( \tau_c^\alpha \) (CRSS) represents the hardening and softening effects which will be discussed later.

In general, the flow stress at certain temperature is regulated by both friction and drag regimes. A mixed rule shall be adopted to consider the coupling of these two regimes. It is further assumed that these two regimes are independent. The total time increment \( \Delta t \) is the sum of the time increment \( \Delta t_\text{drag} \) associated with dislocation movement by jog drag and the time increment \( \Delta t_\text{friction} \) with the jog-free screw dislocation movement (Monnet et al., 2013). As discussed above, we have

\[ \Delta t = \Delta t_\text{drag} + \Delta t_\text{friction} = \frac{1}{\dot{\gamma}_\text{drag}} = \frac{1}{\dot{\gamma}_\text{drag}} + \frac{1}{\dot{\gamma}_\text{friction}}. \]  

(3.14)

We now derive an expression to depict the characterization and evolution of the CRSS \( \tau_c^\alpha \). Recent years, the linear superposition model (Xiao et al., 2016; Yu et al., 2018) and root-sum-square model (Hiratani and Bulatov, 2004; Tan et al., 2016) have been widely accepted to calculate the CRSS. Roughly speaking, the root-sum-square model is suitable for analyzing the hardening mechanisms of different obstacles with comparable contributions; while the linear superposition method has a good performance in describing the hardening behavior of microstructures with different strengths. In ferritic/martensitic steels, there are mainly five strengthening mechanisms including (i) the dislocation forest hardening \( \tau_{\text{dis}}^\alpha \), (ii) Hall-Petch effect induced hardening \( \tau_{\text{hp}}^\alpha \), (iii) precipitation hardening \( \tau_{\text{p}}^\alpha \), (iv) solid solution hardening \( \tau_{\text{s}}^\alpha \) and (v) intrinsic lattice hardening \( \tau_l^\alpha \). A linear superposition law is adopted here to describe these five hardening mechanisms as

\[ \tau_c^\alpha = \tau_{\text{dis}}^\alpha + \tau_{\text{hp}}^\alpha + \tau_{\text{p}}^\alpha + \tau_{\text{s}}^\alpha + \tau_l^\alpha \]  

\[ = \mu b \sum_{\beta=1}^{N_t} K_{\alpha\beta} \rho_{\text{dis}}^\beta + k_{\text{hp}} d^{-\frac{1}{2}} + h_p \mu b \sqrt{\rho_{\text{p}} d_p} + K_t W_s + (A - B \cdot T)^2. \]  

(3.15)

where \( \mu \) is the temperature-dependent shear modulus, \( b \) is the magnitude of the Burgers vector, \( \rho_{\text{dis}} \) signifies the dislocation density, \( K_{\alpha\beta} \) is the dislocation interaction matrix as

\[ K_{\alpha\beta} = \chi_n \left[ \omega_1 + (1 - \omega_2) \delta_{\alpha\beta} \right] \]  

(3.16)

with \( \chi_n \) denoting the dislocation hardening coefficient, \( \omega_1 \) and \( \omega_2 \) two coefficients of interaction between forest dislocations, and \( \delta_{\alpha\beta} \) the Kronecker Delta. Here we adopt \( \omega_1 = 1.5 \) and \( \omega_2 = 1.2 \) to physically indicate the interaction difference on different slip systems (Chen et al., 2018). \( k_{\text{hp}} \) and \( d \) in the second term of Eq. (3.15) represent the Hall-Petch hardening coefficient and the average grain size, respectively. \( h_p \), \( \rho_p \) and \( d_p \) are the hardening coefficient, volume density and average size of precipitations, respectively. \( K_t \) and \( W_s \) signify the hardening coefficient and the concentration of solid solutes, respectively. \( A \) and \( B \) are two fitting parameters to describe the temperature-dependent intrinsic lattice friction.
During the plastic deformation, both the generation and annihilation of dislocations could contribute to the evolution of CRSS on activated slip systems. According to previous theoretical work (Chen et al., 2018; Cheong and Busso, 2004; Mecking and Kocks, 1981), the evolution of dislocation density $\rho^\alpha_{\text{dis}}$ can be expressed as

$$\dot{\rho}^\alpha_{\text{dis}} = \left( k_1 \sum_{\beta=1}^{N_l} \rho^\beta_{\text{dis}} - k_2 \rho^\alpha_{\text{dis}} \right) |\dot{\gamma}^\alpha|, $$

(3.17)

where the first term in parentheses denotes the generation rate of dislocation density, and the second term in parentheses signifies the dislocation annihilation rate. Here, $k_1$ and $k_2$ are two parameters describing dislocation generation and annihilation, respectively. In addition, the spatial distribution of dislocation density usually evolves as the plastic strain continues, and shall be different in different unit cells.

For ferritic/martensitic steels with irradiation, the dislocation loops are the primary irradiation defects (Terentyev and Martin-Bragado, 2015). It is mentioned that some precipitate phases can also form during irradiation, and their effect on the DBT are neglected in this work. The dislocation loops can impede the slipping of dislocations and lead to an increase of the yield and flow stresses. Therefore, the CRSS with consideration of the effect of dislocation loops on dislocation behaviors can be described as

$$\tau^\alpha_c = \tau^\alpha_{\text{dis}} + \tau^\alpha_{\text{hp}} + \tau^\alpha_p + \tau^\alpha_s + \tau^\alpha_f + \tau^\alpha_t,$$

(3.18)

where $\tau^\alpha_i$ represents the contribution of dislocation loops. Besides, due to the complexity of slip systems and the special feature plane of dislocation loops, the dislocation-defect interaction process is usually spatially dependent. A recently proposed tensorial model (Barton et al., 2013; Xiao et al., 2016) describing the dislocation-defect interaction is adopted here to depict the dislocation loop induced hardening as

$$\tau^\alpha_t = h_l \mu b \left( \sum_{\beta=1}^{N_l} N^\alpha : H^\beta \right),$$

(3.19)

where $h_l$ is the loop hardening coefficient, $N^\alpha (= n^\alpha \otimes n^\alpha)$ is a tensor describing the normal direction of the $\alpha$th slip system, and $N_l (=4)$ is the total number of the habit planes of dislocation loops. $H^\beta$ indicates the defect descriptor tensor which can be expressed as

$$H^\beta = \rho_1 \cdot 3d_i \cdot M^\beta,$$

(3.20)

$$M^\beta = I - m^\beta \otimes m^\beta,$$

(3.21)

where $\rho_1$ and $d_i$ are the initial number density and average size of dislocation loops, respectively, and $m^\beta$ is the unit normal vector of the defect habit plane.

As the plastic deformation continues, the dislocation loops can be absorbed by the slipping dislocations, which leads to the evolution of the microstructure and flow stress. The corresponding evolution law (Barton et al., 2013; Xiao et al., 2016) is formulated as

$$\dot{H}^\beta = -\eta \sum_{\alpha=1}^{N_l} (N^\alpha : H^\beta) M^\beta |\dot{\gamma}^\alpha|,$$

(3.22)

where $\eta$ is the annihilation efficiency.

The component of the second Piola-Kirchhoff stress $T^{(1)}$ determined by Eqs. (3.1)-(3.8) is substituted into Eqs. (2.11) and (2.14) to calculate the probability of cleavage cracking $P_{\text{clea, nul}(\text{MF})}$, and the plastic strain $\varepsilon^p$ calculated by Eqs. (3.9)-(3.14) is substituted into Eqs. (2.8) and (2.13) to obtain the probability of ductile void growth $P_{\text{void}}$. The overall failure probability derived from Eqs. (2.8), (2.11), (2.13) and (2.14) is used to calculate the fracture toughness of steels. Until now, a probabilistic model coupling with a temperature-dependent crystal plasticity framework has been built to investigate the competition between the cleavage initiation and ductile void nucleation and the mechanical behaviors of ferritic/martensitic steels. It is recognized that the DBTT is sensitive with temperature.

In the current work, the probability of brittle cleavage failure or ductile void growth is physically related to three terms, the distribution of microcrack size, the distribution of void volumetric fraction, and the constitutive relation. As the first term relies on the size distribution of carbides, it is independent of temperature. For the second and third terms, the distribution and evolution of void volumetric fraction are related to the temperature as the void volumetric fraction evolves with the temperature-dependent plastic strain continues (Eq. 2.5); the constitutive relation takes into account the temperature effect through temperature-dependent plastic deformation and strengthening mechanisms (Eqs. 3.14 and 3.15). Though the thermal effect on the DBTT is introduced in the second and third terms from a viewpoint of energy dissipation, the effect of the thermal stress fluctuation on the brittle crack formation and propagation as well as the plastic deformation is not analyzed here. For brittle materials, a recent theoretical study indicates that the brittle crack growth can be modeled as a separation process of atomic or molecular bonds due to external force in the presence of thermal fluctuation on the force transmission.
via bonds and adjusting the activation energy for bond rupture (Freund, 2014). Thermally activated processes could also regulate the dislocation motions by adjusting the activation energy tilted by the stress fluctuation. As Eq. (3.14) indicates, the 'friction regime' plays a leading role at the low temperature. \( \gamma_{\text{friction}} \) would decrease as the activation energy \( \Delta G \) decreases, and the corresponding stress can increase significantly. This can promote the nucleation and propagation of microcracks, which accelerates the failure of materials. As the effect of thermal fluctuation or the random force to the DBTT requires more sophisticated microscopical parameterization and small scale modeling of brittle and ductile fracture (Freund, 2014; Ponson and Bonamy, 2010; Santucci et al., 2004), a thorough and sound theoretical analysis is called for in future investigations.

In the following sections, we discuss the simulation results.

4. Mechanical properties of ferritic/martensitic steels without and with irradiation

A temperature-dependent crystal plasticity model accounting for the temperature and irradiation effects combined with a probabilistic model is proposed to describe the DBT in Sections 2 and 3. Our model can be applied to study ferritic/martensitic steels and polycrystal metals or alloys such as stainless steels, Fe-Cr alloys and pressure vessel steels (Bai et al., 2016; Gumruk et al., 2013; Xiao et al., 2016). Eurofer’97 is a typical ferritic/martensitic steel, and it is widely used as structural materials in nuclear reactors. In the following, taking the Eurofer’97 steel as an example of ferritic/martensitic steels, a polycrystal model is adopted to study the mechanical behaviors and DBT phenomenon with the irradiation effect. Different from the elasto-viscoplastic self-consistent method developed by Duan et al. (2005) and Xiao et al. (2015), a crystal plasticity finite element method (FEM) is adopted here to solve the problem with complex boundary and loading conditions (Wei et al., 2014). This model is implemented in ABAQUS as a User Material subroutine. C3D8R elements are used in modeling single and polycrystals, employing linear interpolation and reduced integration. A cube embedded with a crack having a dimension of 50 \( \mu \text{m} \times 20 \mu \text{m} \times 60 \mu \text{m} \) is shown in Fig. 3. The system has 7271 meshed elements and 200 grains. The initial grain orientation is randomly distributed and the average grain size is approximately 8.3 \( \mu \text{m} \), which falls in the reported range of 6.7 \( \mu \text{m} \) - 11 \( \mu \text{m} \) (Fernandez et al., 2004). As shown in Fig. 3(b), uniform quasi-static displacement loading (denoted by red arrows) is applied on two remote edges parallel to the intersection of the initial edge crack and the free surface, and displacement constraints are applied on the (red) dashed line to prevent rigid body motion. Initiation of cleavage is typically observed to occur at distance one to five CTOD (crack tip opening displacement) ahead of a crack tip. In this work, we focus on the ductile-to-brittle transition region, and the corresponding CTOD \( \delta \) is around 10 to 14 microns based on the approximate relation \( \delta = K_{\text{Ic}}^2/(2E\sigma_y) \) (Sarzosa et al., 2015) with \( K_{\text{IC}} = 60 \text{ MPa} \cdot \text{m}^{1/2} \), \( E = 200 \text{ GPa} \), and \( \sigma_y = 700 \text{ MPa} \). An appropriate domain size of the FEM model for this case is no less than 60 microns, and the size of our FEM model in the current work can satisfy this condition. However, it is noted that the domain considered here is an absolute minimum, a much larger domain is preferred for modeling to justify the comparisons with experimental results obtained from standard size specimens.

4.1. Parameter calibration

The Eurofer’97 steel is Heat 83698, and its chemical composition (wt%, balance Fe) is 8.82Cr-1.1W-0.37Mn-0.19V-0.068Ta-0.10C. The microstructure of Eurofer’97 is full lath martensite phase (van der Schaaf et al., 2000). Detailed heat

Fig. 3. (a) A crack tip region contains many carbides as potential sites of micro-crack nucleation. (b) Schematic of a cracked polycrystal containing 7271 C3D8R elements.
treatment conditions can be found in Fernandez et al., 2004. The strain rate is $1 \times 10^{-3}$ s$^{-1}$, the average grain size is $D_g = 6.7$ µm ~ 11 µm (Fernandez et al., 2004), and the average block size is taken as $d = 0.067D_g$ (Galindo-Nava and Rivera-Diaz-del Castillo, 2015). The initial mobile dislocation density is $1.2 \times 10^{14}$ m$^{-2}$ (Aktaa and Petersen, 2009). For ferritic/martensitic steels, the $\text{M}_{23}\text{C}_6$ precipitates usually exist on boundaries (Xia et al., 2011), and the corresponding hardening effect is integrated into the Hall-Petch relationship. The density and size of carbides are $4.86 \times 10^{10}$ m$^{-3}$ and 22 nm, respectively (Liu et al., 2013). $A = 16.48$ MPa$^{1/2}$ and $B = 0.045$ MPa$^{1/2}$K$^{-1}$ in Eq. (3.15) are parameters for the lattice friction (Butt, 2007; Xiao et al., 2016; Yu et al., 2018). $K_s = 700$ MPa is used to calculate the solute atoms induced hardening (Xiao et al., 2016). The reference plastic strain rate $\dot{\gamma}_0$, strain rate sensitivity $m$ and Burger’s vector length $b$ are $1 \times 10^{-3}$ s$^{-1}$, 0.05 and 0.248 nm, respectively (Xiao et al., 2016).

For Eurofer’97, it is reported that Cr solutes have minor effects on the elastic constants of Fe-Cr alloys in the range of Cr concentrations up to 10% (Speich et al., 1972). Therefore, the elastic constants of BCC irons are adopted for Eurofer’97. The temperature-dependent elastic constants can be given by an empirical formula as (Adams et al., 2006)

$$C_{ij}(T) = c_{ij} - \frac{s_{ij}}{\exp \left( \frac{T}{T_E} \right) - 1},$$

where $c_{ij}$ denote the elastic constants at 0 K, $T_E$ is the effective Einstein temperature, and $s_{ij}$ are the parameters depending on the strength of anharmonic interactions. Table 1 gives the values of these parameters. The shear modulus can be obtained as $\mu = \sqrt{C_{44} \cdot (C_{11} - C_{12})/2}$. Rest parameters used in the calculations such as these pertaining to the probabilistic cleavage model and these associated with irradiation are listed in Tables 2 and 3.

### 4.2. Temperature dependent mechanical behaviors of ferritic/martensitic steels

Based on the proposed constitutive framework in Section 3, we first investigate the temperature-dependent mechanical responses of the Eurofer’97 steel without irradiation to validate our model. As shown in Fig. 4, the simulation results agree well with experimental data (Spatig et al., 2007). The yield stress $\sigma_y$ exhibits strong temperature-dependent feature, decreasing rapidly as the temperature increases from a relatively low value to room temperature. Since $\sigma_y$ is closely related to the CRSS of slip systems, this temperature-dependence feature in Fig. 4 can attribute to the hardening contribution of intrinsic lattice friction according to Eq. (3.15). Stress-strain relationships at different temperature are presented in Fig. 5. The stress $\sigma$ and the strain $\varepsilon$ in Fig. 5 are correspondingly determined by Eqs. (3.4) and (3.9). Our simulation results agree well with the experiments (Spatig et al., 2007). We also present the shear strain rate of slip systems in Fig. 6. It is shown that the ‘friction regime’ is the main deformation behavior at low temperature, while the ‘drag regime’ determines the deformation behavior at high temperature. The critical temperature is found to be about 143 K.
Mechanical behaviors of ferritic/martensitic steels with irradiation

In this subsection, the mechanical behavior of Eurofer’97 with irradiation is analyzed. After irradiation, amounts of dislocation loops can be detected in Eurofer’97. The detailed irradiation information (Matijasevic et al., 2008) is given in Table 4. The coefficients in Eqs. (3.19) and (3.22) related to the irradiation hardening terms are chosen as $h_l = 0.76$ and $\eta = 80$, respectively.

Fig. 7 shows the yield stress $\sigma_y$ of Eurofer’97 under different irradiation doses at 593 K. Our simulation results match well with the experimental results (Lucon et al., 2004), and the irradiation hardening effect becomes more evident as the irradiation dose $\Phi$ increases. Fig. 8 presents our theoretical results and experimental data (Chaouadi, 2008) on stress-strain relationships under different irradiation doses at 593 K. The higher the irradiation dose, the lower the strain hardening rate. As the irradiation dose reaches 0.60 dpa, the flow stress even decreases and the plasticity localization appears as the plastic deformation continues. This phenomenon is mainly due to the annihilation of irradiation defects during the deformation process.

The excellent consistency with the experimental results on the mechanical behaviors of Eurofer’97 shown in Figs. 7–8 demonstrates the validity and accuracy of our probabilistic model proposed in Section 2 and the constitutive model in...
Fig. 6. The shear strain rate of Eurofer'97 at different temperatures 73 K, 113 K, 143 K, 173 K, 223 K and 297 K. $\dot{\gamma}_{\text{friction}}$ in Eq. (3.12) denotes the shearing slip rate associated with the 'friction regime', and $\dot{\gamma}_{\text{drag}}$ in Eq. (3.13) is associated with the 'drag regime', and $\dot{\gamma}_{\alpha}$ is the total shearing slip rate.

Section 3. In next section, we further investigate the temperature-dependent macroscopic fracture toughness to explore the DBT mechanism.

5. Ductile-to-brittle transition phenomenon and irradiation embrittlement

To explore the DBT feature of ferritic/martensitic steels, we analyze the fracture toughness of materials via different temperatures. The simulation results of the fracture toughness $K_{IC}$ are obtained as the following procedures: (a) at a certain
temperature, a uniform strain rate is applied and the failure probability increases correspondingly, (b) calculating the \( J \)-integral and converting it to the fracture toughness, (c) repeating steps (a)-(b) at different temperatures.

By the Master Curve Approach (Wallin, 1984; 2011), an exponent type expression and a reference temperature \( T_0 \) are introduced to describe the fracture toughness data. Our simulation results in Fig. 9 agree well with the experimental data (Spatig et al., 2007) and the fitting lines obtained by the Master Curve Approach. Here we only present the simulation results of \( P_f = 5\% \) and \( P_f = 95\% \) instead of 1\% and 99\% for comparison, since the numerical errors of the latter in simulations do not converge. The experimental data of the fracture toughness of Eurofer'97 at low temperature are extremely limited, since Eurofer'97 steels mainly behave as a brittle material and fail by cleavage. At low temperature, the fracture toughness of Eurofer'97 approaches a constant. As the temperature increases, the void nucleation becomes active and restrains the cleavage initiation and propagation, leading to a great improvement on the fracture toughness.

Fig. 10 compares our simulation results with the experiment data (Lucon et al., 2004) at different irradiation doses. It is indicated that the irradiation reduces the fracture toughness and makes the lower bound of the fracture toughness maintain at a very low level, which can be understood as follows. Firstly, the hardening induced by the irradiation defects increases the flow stress significantly, which promotes the cleavage crack development even at high temperature. Secondly, the irradiation-induced plasticity localization impedes the global void nucleation and growth, meaning that the hindering effect from ductile void growth on the cleavage nucleation and propagation is weakened.

To analyze the influence of the irradiation effect on the fracture toughness, all simulation results without or with irradiation are shown in Fig. 11. It is indicated that the fracture toughness with irradiation decreases significantly compared with the case without irradiation. Fig. 12 shows the slope of the fracture toughness curves \( dK_f/dT \) with or without irradiation.

Fig. 9. Temperature-dependent fracture toughness of Eurofer’97 without irradiation. Symbols indicate the experimental data (Spatig et al., 2007).

Fig. 10. Temperature-dependent fracture toughness of Eurofer’97 with irradiation: (a) 0.74 dpa and (b) 1.62 dpa. Symbols represent the experimental results (Lucon et al., 2004).

There is a linear relationship between the $dK_f/dT$ and the temperature in a log-log diagram, which is consistent with the result by the Master Curve Approach.

To quantitatively investigate the irradiation influence on the DBTT, the irradiation-induced yield stress increasing $\Delta \sigma_y$ and DBTT ($\Delta T$) are presented in Fig. 13. The temperature at which $K_f = 100$ MPa - $m^{1/2}$ is defined as the DBTT and denoted as $T^{100}$. It is shown that the DBTT ($T_{0\text{dpa,exp}}^{100} = 148$ K) without irradiation is very close to the experimental data as $T_{0\text{dpa,exp}}^{100}$ reported by Chaouadi (2008). Table 5 shows the relation between the irradiation hardening $\Delta \sigma$ and the irradiation embrittlement $\Delta T$. It can be seen that $\Delta T/\Delta \sigma_y \approx 0.30$ K/MPa falls into the range of experimental results reported by Kurtz et al., 2009.

Table 5

<table>
<thead>
<tr>
<th>Irradiation doses $\Phi$ (dpa)</th>
<th>$\Delta \sigma_y$ (MPa)</th>
<th>$\Delta T$ (K)</th>
<th>$\Delta T/\Delta \sigma_y$ (K/MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.74</td>
<td>146.396</td>
<td>35.0</td>
<td>0.239</td>
</tr>
<tr>
<td>1.62</td>
<td>224.051</td>
<td>78.0</td>
<td>0.348</td>
</tr>
</tbody>
</table>

At high temperature, beyond the ductile-to-brittle transition region, the failure mechanism of steels is mainly controlled by void nucleation-growth-coalescence mechanism but not cleavage microcrack propagation. Therefore, at high temperature the probability of void nucleation and void growth play dominant roles in regulating the mechanical properties of steels and the failure mechanism, meanwhile the cleavage fracture is inhibited by the void nucleation. With the help of more experimental observation and evidence at the microscopic scale, a thorough theoretical framework taking into account void-related ductile fracture, particularly at high temperature, certainly deserves further detailed investigations in the future.
Fig. 11. Temperature-dependent fracture toughness $K_J$ of Eurofer'97 without or with irradiation effect. Symbols denote experimental data (Lucon et al., 2004; Spatig et al., 2007).

Fig. 12. $\log_{10}(dK_J/dT)$ as a function of $\log_{10}(T)$ without or with irradiation effect. Symbols are calculated by the simulation results from Figs. 11. Lines denote the linear fitting results.

Fig. 13. The relations between the fracture toughness $K_J$ and temperature $T$ from which the ductile-to-brittle transition temperature under different irradiation doses are determined.
6. Conclusions

In this work, we propose a probabilistic model coupling with the temperature dependent constitutive relationship to describe the competition between the cleavage and ductile void failure of ferritic/martensitic steels with irradiation effects. This model not only predicts the temperature-dependent mechanical properties of ferritic/martensitic steels with or without irradiation but also precisely describes the significant variation of fracture toughness with temperature called the DBT phenomenon. The irradiation effects include not only rise in the yield and flow stresses (irradiation hardening) but also an increase on the DBTT (irradiation embrittlement). Different from widely used phenomenological models like the Master Curve Approach and statistical modelling based on the Beremin model, our probabilistic model physically describe the cleavage nucleation-propagation process and the influence of ductile void growth, and it gives a better description for the DBT. The main conclusions are as follows.

(1) At low temperature, the fracture toughness of ferritic/martensitic steels is relatively low as the cleavage is the main failure mechanism. At high temperature, the cleavage nucleation and crack propagation is suppressed, the ductile void growth gives rise to a relatively high fracture toughness. The probability of cleavage nucleation

\[ p_{\text{clea}, \text{nuL}} = p_{\text{clea}, \text{nuL} \text{vir}} (1 - p_{\text{void}}) \]

indicates a competition between the cleavage and ductile void failure is used to explain the DBT. An essential feature of the proposed probabilistic model is that it enables a sound and meaningful description of the inherent scatter of experiment data on the fracture toughness.

(2) Temperature dependent mechanical behaviors with and without irradiation effects are explored. The difference of intrinsic lattice hardening at different temperatures is the main reason of the discrepancy on the yield and flow stresses. In the DBT region, the material deformation is controlled by a mixed deformation regime, i.e., the friction regime at low temperature and drag regime at high temperature. The existence of irradiation defects leads to irradiation hardening, and the annihilation of irradiation defects also brings material softening and plasticity localization.

(3) One of the irradiation effects is an increase of the DBTT. The underlying mechanism is that the irradiation defects induced hardening makes the flow stress increase greatly which can promote the development of cleavage micro-crack, and the irradiation-induced plasticity localization weakens the hindering effect from ductile void growth on the cleavage nucleation and propagation. Irradiation hardening and embrittlement phenomenon coexist, and the ratio between the irradiation-induced higher DBTT and the irradiation-induced yield stress \( \Delta T / \Delta \sigma \approx 0.30 \) K/MPa reported in this work agrees with the experimental results (Kurtz et al., 2009).

Though we take Eurofer'97 for example, our model can be applied for other ferritic/martensitic steels or polycrystalline metals such as stainless steels, Fe-Cr alloys and pressure vessel steels (Bai et al., 2016; Gumruk et al., 2013; Xiao et al., 2016).

Conflicts of Interest

The authors have no conflicts of interest to disclose.

CRediT authorship contribution statement

Lirong Chen: Conceptualization, Methodology, Software, Validation, Formal analysis, Writing - original draft. Wenbin Liu: Methodology, Writing - review & editing. Long Yu: Methodology, Writing - review & editing. Yangyang Cheng: Investigation, Writing - review & editing. Ke Ren: Investigation, Writing - review & editing. Haonian Sui: Investigation, Writing - review & editing. Xin Yi: Writing - review & editing, Supervision, Project administration, Funding acquisition. Huiying Duan: Writing - review & editing, Supervision, Project administration, Funding acquisition.

Acknowledgements

The authors are grateful to Prof. Huajian Gao at Nanyang Technological University for insightful discussions on the theoretical framework of this paper. Financial support for this work was provided by the National Natural Science Foundation of China (Grant Nos. 11632001, 11521202, U1830121), Science Challenge Project (No. TZ2018001), and National Science and Technology Major Project (2017-VI-0003-0073).

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