

Lifetime Prediction and Type-IV Failure Analysis in Weldments of Creep-resistant Ferritic Alloys

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Dedication

This doctoral dissertation is dedicated to my parents, my beloved husband, and my parents-in-law for their sincere love, encouragement, full support and unconditional trust in all my pursuits, and all beloved ones who have unconditionally loved and supported me.

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ABSTRACT

A number of computational methodologies have been proposed to investigate deformation and damage mechanism of various structural materials and weldments under extreme loading conditions, and also to provide valuable insights on the development of materials with improved performance. Creep strength enhanced ferritic (CSEF) steels containing 9-12wt% chromium have been extensively used in fossil-fuel-fired power plants. Despite their excellent creep resistance at high temperatures, premature failures are often found in the fine grained heat-affected zone (HAZ) of the welded components after years of service, which is referred as Type IV failure. Experiment measurements capture this so-called Type IV failure is preceded by the strain localization in the fine grained HAZ. Here we aim to develop an Integrated Computational Materials Engineering (ICME) approach to determine the micromechanical and microstructural origins of the above deformation and failure process. First, a microstructure-based finite element model is developed for studying the strain localization phenomenon, with the deformation processes resulting from a synergy of thermally activated dislocation movements, diffusional flow, and grain boundary sliding. The comparison of the digital image correlation (DIC) measurement and numerical simulations facilitates the understanding of the effect of pre-welding tempering on the evolution of the strain localization in the HAZ of P91 steels. To meet the design lifetime (>30 years) of thermal power plants, it is crucial to get the fundamental understanding the long-term creep fracture behaviors of power plant steel weldments. Therefore, in the current work an integrated microstructure-micromechanics-based finite element method is presented to analyze the long-term creep fracture behavior

(Type IV crack), in which we account for the physical fracture mechanisms at different length scales, including nucleation of grain boundary cavities, their growth, the emergence of microcracks and their evolution to the ultimate failure. The methodology demonstrates excellent computational capabilities in modeling the Type IV failure and also providing high-quality creep rupture life prediction for the CSEF steel and its weldments. These methodologies will be efficient tools to evaluate the very-long-term creep and damage behavior of many other high temperature alloys and their weldments.

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1 INTRODUCTION

1.1 Background and Motivation

1.1.1 Type IV failure in creep resistant steel weldments

To fulfill the current and future demands for environmental friendly and cost-effective energy sources, the thermal and nuclear power plants are required to operate at higher temperature and stress levels, which raises power efficiency and reduces fuel consumption and emission of greenhouse gases. Creep resistant 9-12% steels, developed to withstand the severe service conditions, have been used as one of the major structural materials for thick section components in the Ultra Supercritical (USC) power plants due to their outstanding creep resistance at high temperatures. Welded components made from these advanced steels usually have been put into practical applications under high temperature (500°C to 650°C) and low applied stresses (~ 35 MPa). Nevertheless, premature failures commonly occur in the heat-affected zone (HAZ) of welded joints, which is known as Type IV failure [1-3], as shown in Fig. 1.1. In general, the service cracking is classified into four categories according to its position and orientation in the weldments, as shown in Fig. 1.2. Type I crack and Type II crack occur in the weld metal, with the former arrested in the weld metal and the latter preferentially propagating into the HAZ and the base metal. Type III crack forms in the coarse grained heat-affected zone (CGHAZ) and may grow into the base material. Type IV cracking occurs in the fine grained heat-affected zone (FGHAZ) or intercritical heat-affected zone (ICHAZ). It is a kind of detrimental crack that happens

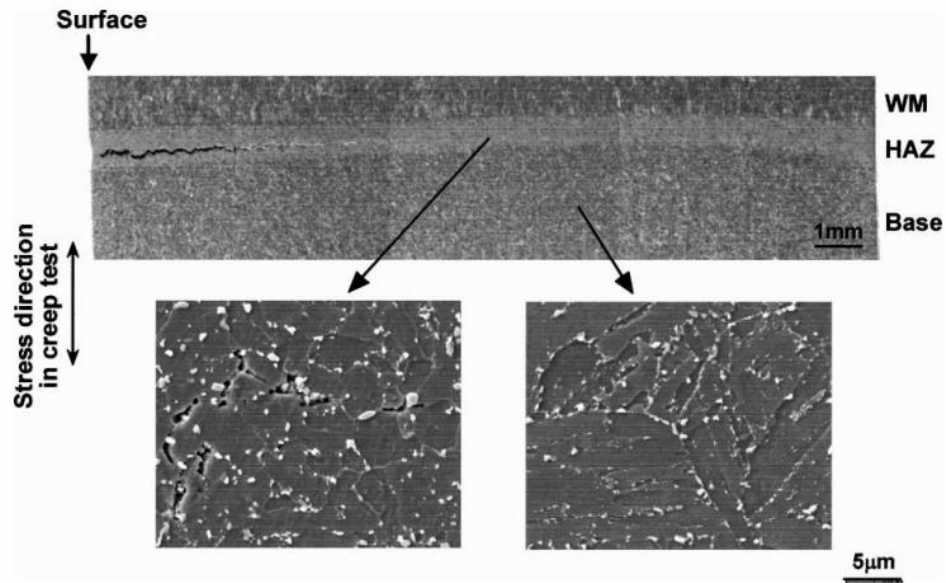


Figure 1.1 Type IV crack profile and microstructure of creep crack in EBW joint of P122 after creep rupture testing at 923K and 60MPa ($t_r=7300$ h) [4].

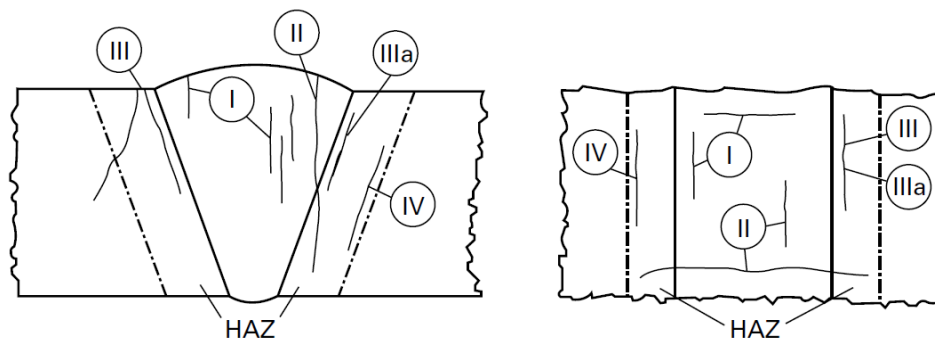


Figure 1.2 Schematic plots of cracking modes in weldments of heat-resistant steels [1].

at low stress levels, always leading to premature failure of welded joints during service exposure.

It is well acknowledged the Type IV failure is preceded by the locally accumulated strain in the HAZ [1-3, 5-7]. By using digital image correlation technique, Yu et al. [5] measured the full field deformation of modified 9Cr-1Mo steel cross-welds and captured the strong creep strain localization in the fine grained HAZ. Their experiments showed the reduction of pre-weld tempering temperature from 760°C to 650°C lead to an order of magnitude decrease of the steady-state creep rate for the fine grained HAZ, where the improvement in creep properties were correlated with the hardness and microstructure changes of the two pre-weld tempering specimens [5, 8]. Extensive studies have been performed to identify the causes for the deteriorated creep performance of the welded joints. Many of these report the sharp microstructure and material property gradients in the HAZ result in significant creep strength degradation [4, 6-12]. Furthermore, the grain size, orientation of the fine grained HAZ and the constraint from base metal and weld metal can lead to high triaxial stresses that may contribute to the creep damage [10, 13].

Although many creep tests and microstructure characterizations have been performed for CSEF steel welded structures, the underlying deformation mechanisms, which link the microstructure, and material properties with creep performance, have not been fully understood. The current work pertains to developing a microstructure-informed mechanisms-based finite element model to illustrate the deformation mechanisms (fracture mechanisms) responsible for the strain localization (Type IV failure) in the fine grained HAZ and to investigate the effects of pre-weld tempering on the evolution of creep and

creep fracture of ferritic steel welds. Currently, the thermal and nuclear power plants are designed for 30 years, and a further attempt is being made to extend the design life of the power plants to 40 or even 60 years through introduction of advanced heat resistant materials [1]. However, it is impractical to perform such long-term creep rupture tests in laboratory-condition due to the considerable time and experiment costs. Therefore, a clear understanding of the long-term creep rupture behavior (Type IV failure) as well as reliable lifetime prediction methodologies of welded joints of CSEF steels becomes necessary.

1.1.2 Elastic-plastic indentation for HCP Single Crystals

Strengths and failure resistance of crystalline materials can be manipulated by microstructural design through various thermomechanical processing techniques, but even for advanced engineering alloys, their strengths are still one or two orders of magnitude smaller than the theoretical value because of crystalline defects. Moreover, a general trend of “smaller being stronger” has been routinely observed in small scale mechanical property measurements such as indentation hardness and micropillar compression tests [14-16]. It is thus imperative to determine the conditions for the crystalline materials to reach the theoretical strengths and to quantitatively evaluate these theoretical values by convenient experimental techniques. Most tests by compressing pillars with micrometer-sized diameter or stretching nanowires are still unable to reach these ideal strengths because of pre-existing dislocations or other defects [14], or the presence of free surfaces or ledges that leads to the heterogeneous dislocation nucleation [17]. These limitations can be avoided by spherical nanoindentation tests where the stressed volume inside the bulk can

be easily made far below micrometers, which can also be easily and conveniently repeated for the statistical investigations.

In this study, the pop-in loads required for homogeneous dislocation nucleation in HCP single crystals such as Mg, Hf, and Ti will be investigated as a function of crystallographic orientation and elastic anisotropy, as motivated by the following observations. First, HCP single crystals oftentimes have multiple slip systems in operation, and the macroscopic plastic properties, including critical resolved shear stress (CRSS) and hardening moduli, are very sensitive to the temperature and c/a ratio. The CRSS ratios of various slip systems can be directly measured by uniaxial or other simple tests [18, 19], but can only be indirectly determined from indentation hardness tests [20, 21]. It should be noted that crystalline materials under indentation will generally display indentation size effects, with the CRSS being the asymptote at one end and the pop-in asymptote at the other end. It is thus of crucial importance to examine whether the pop-in loads can be used to determine the ratios of theoretical strengths of various slip systems. Second, microstructural characterizations of deformation behavior at small scales are tedious experiments, such as transmission electron microscopy (TEM) [22-24]. In situ TEM tests of Mg nanowires [22] reveal interesting synergistic activation of multiple slip systems and most interestingly the simultaneous initiation of a large number of twin partials. The experiments usually suffer the complication of surface dislocation nucleation and are also restricted to certain crystalline orientations. Third, due to the spatio-temporal limitations, it is more desirable for molecular simulations to compare to experimental measurements at small stressed volumes. For example, Barrett et al. [25] showed the breakdown of Schmid

law in homogeneous and heterogeneous dislocation nucleation in Mg single crystals under uniaxial stresses. As explained earlier, a direct comparison to these simulations works by TEM or other characterization techniques is extremely challenging, as opposed to the relatively convenient pop-in measurements. The objective of this work is to examine whether nanoindentation pop-in tests can be used to identify the incipient plasticity and to calculate the theoretical strength of HCP single crystals when there are multiple candidate sets of slip systems.

1.2 Outline

This thesis work is organized as follows. In Chapter 2, we will present the fundamental deformation and damage mechanisms of crystalline materials at high temperatures, including diffusional flow, grain boundary sliding and dislocation creep, as well as the creep fracture mechanisms, such as transgranular creep fracture, intergranular creep fracture and rupture. In Chapter 3, we aim to develop a microstructure-informed and micromechanics-based constitutive model, which is capable of explicitly modeling the weldment microstructure, elucidating the underlying deformation mechanisms and establishing the relationship between microstructure, material heterogeneities and the creep behavior of CSEF steel welds. In Chapter 4, a micromechanical constitutive model will be presented to systematically study the Type IV failure in CSEF steel welded joints, especially to illustrate the creep cavitation and damage development of Grade 91 weld joints, and to establish the correlation between the cavity evolution and the creep rupture life. In Chapter 5, the incipient plasticity of HCP single crystals, including Mg, Ti and Hf,

will be investigated by the calculation of indentation Schmid factors based on the anisotropic elastic Hertz contact theory. The last chapter presents the conclusions and future suggestions.

2 DEFORMATION AND DAMAGE MECHANISM

2.1 Introduction

Plastic flow is determined by the kinetic process that occurs on the atomic scale, including the glide motion of dislocation lines, coupled dislocation glide and climb, diffusional flow of individual atoms, and grain boundary sliding (involving diffusion and defect motion), among many others [26]. These deformation mechanisms are given in two groups: low-temperature plasticity and high-temperature plasticity. In the low temperature range, plastic deformation is controlled by the propagation of dislocation lines on highest packing density planes, and plastic flow is always hindered by obstacles, such as other dislocations, precipitates or solute atoms, and grain boundaries, which leads to increased strength. At high temperatures, creep behavior as the rate-dependent plastic deformation depends critically on the micro- and nano-structures. In polycrystalline metals, the creep deformation results from a synergy of thermally activated dislocation movements, diffusion flow and grain boundary sliding. Each of the three mechanisms may occur independently, but from geometric point of view, grain boundary sliding usually requires accommodation from either dislocation creep or diffusional flow. The competition between the grain-interior and grain-boundary mechanisms has been extensively studied. It is found that diffusional flows controlled by grain boundary diffusion (Coble creep) [27] and by lattice diffusion (Nabarro-Herring creep) [28] dominate under low applied stress regime, dislocation creep limited by lattice or dislocation core diffusion dominates at high stress

level, and grain boundary sliding is more important at intermediate stress regime especially in materials with fine grain sizes.

2.2 Creep deformation and deformation mechanism map

As the mobility of atoms increases rapidly with temperature, the diffusion-controlled process is often associated with creep as the dominant plastic deformation mechanism at high temperatures, including the diffusional creep, dislocation creep and grain boundary sliding. The characterized creep strain-time curve contains three stages: the primary creep during which the creep rate decreases with time; the steady-state creep with a nearly constant creep rate which is resulted from a balance of competing processes of strain hardening and recovery; and the tertiary creep in which void formation and necking begin to develop and lead to the final failure. Studies in the past were mainly focused on the development of deformation mechanisms for steady-state creep, which can be generally described by the following equation:

$$\dot{\epsilon} = \frac{ADGb}{kT} \left(\frac{b}{d}\right)^p \left(\frac{\sigma}{G}\right)^n \quad (2.2.1)$$

where $\dot{\epsilon}$ is the tensile creep rate; σ is the flow stress; T is the absolute temperature; G is the shear modulus; d is the grain size; p is the inverse grain size exponent; n is the stress exponent, which is equal to $1/m$ (where m is the strain-rate-sensitivity exponent); A is a dimensionless constant and D is the diffusion coefficient, given by

$$D = D_0 \exp(-Q/kT) \quad (2.2.2)$$

where Q is the activation energy for the diffusion flow. Each diffusional creep mechanism can be described by Eq. (2.1.1) with specific values of D , p and n . The diffusional creep mechanisms and their corresponding rate equations are summarized as follows.

2.2.1 Diffusional Creep

The diffusional creep at high temperature is a result of stress-driven migration of vacancies (or atoms). When vacancies move through the lattice, the corresponding Nabarro-Herring creep [28] is given by

$$\dot{\epsilon}_{NH} = A_{NH} \frac{D_l \sigma \Omega}{d^2 kT} \quad (2.2.3)$$

where Ω is the atomic volume, D_l is lattice self-diffusion coefficient and A_{NH} is a dimensionless constant which depends on the shape of grain. The Coble creep [27] involves vacancy flow along grain boundaries, and the rate equation is described by

$$\dot{\epsilon}_C = A_C \frac{D_{gb} \delta \sigma \Omega}{d^3 kT} \quad (2.2.4)$$

where A_C is a dimensionless constant, D_{gb} is the grain-boundary diffusion coefficient, and δ is the grain boundary thickness. Note that Nabarro-Herring creep and Coble creep are of the same stress exponent $n = 1$, but Coble creep ($p = 3$) shows a stronger size dependence than the Nabarro-Herring creep ($p = 2$). The activation energy of grain boundary diffusion is much lower than that of lattice diffusion, and therefore the required temperature at which Coble creep dominates is lower than that of Nabarro-Herring creep. In fine-grained materials, the diffusional creep rate increases monotonically with decreasing grain size,

and grain boundary diffusion governed creep becomes one of the dominant deformation mechanism due to the significantly increased volume fraction of grain boundaries materials [29, 30].

2.2.2 Dislocation creep

Dislocation creep, at the atomic level, is the result of the diffusion of single vacancies to or from the dislocation climb, rather than the dislocation motion itself. It is found that in dislocation creep, dislocation glide accounts for most of the plastic strain, but its creep rate is determined by dislocation climb, which is controlled by lattice or dislocation core diffusion. The rate equation for dislocation creep can be described in the generalized power-law equation,

$$\dot{\epsilon}_D = \frac{A_D D G b}{kT} \left(\frac{\sigma}{G} \right)^n \quad (2.2.5)$$

where A_D is a dimensionless constant, D is the lattice or dislocation core diffusivity. In the majority of alloys, at high temperatures ($T > 0.5 T_M$), climb is required when the gliding dislocation is held by physical obstacles, in which transport of matter is through lattice diffusion D_l , and the stress exponent n varies from 4 to 5. It is usually seen in the dispersion-strengthened alloys, the stress exponent is very high $n > 8$, and it is resulted from the existence of threshold stress [31]. At lower temperature or higher stresses, the dislocation core diffusion (with diffusivity D_c) contributes significantly to the overall diffusive transport of matter, and becomes the dominant deformation mechanism. The dislocation creep is the favorable deformation mechanism at high stress regime.

2.2.3 Grain boundary sliding

Grain boundary sliding is characterized by a stress exponent of $n = 2$,

$$\dot{\epsilon}_{gbs} = \frac{A_{gbs}DG}{kT} \left(\frac{b}{d}\right)^p \left(\frac{\sigma}{G}\right)^2 \quad (2.2.6)$$

and the diffusion coefficient is derived either from lattice diffusion or from grain boundary diffusion, with grain size dependence $p = 2$ or 3 , respectively. It is important to note that grain boundary sliding cannot occur in absence of other deformation mechanisms. It requires accommodation processes from diffusional flow, dislocation slip, or grain boundary migration. Many quantitative models have been developed to describe the grain boundary sliding with accommodated plastic flow (e.g., [32, 33]). Grain boundary sliding contributes to the plastic deformation in solids of all grain sizes, and it becomes the dominant mechanism especially in materials of small grain sizes at high temperatures.

2.2.4 Deformation mechanism map

Frost and Ashby [26] constructed the deformation maps for various materials based on superposition of the above rate equations, revealing the dominant deformation mechanisms in different ranges of stresses and temperatures. As a hindsight, the grain boundary sliding mechanism was not treated explicitly in their work. For a typical polycrystalline material with micrometer grain size, the low-temperature plasticity is controlled by dislocation glide. At high temperature, power-law creep, diffusional flow and grain boundary sliding as three independent flow mechanisms compete to be the dominant

deformation mechanism for different ranges of stresses and temperatures. The strain rate of polycrystalline materials can be obtained by summing the rate equations,

$$\dot{\epsilon} = \dot{\epsilon}_{\text{diffu}} + \text{greatest of } (\dot{\epsilon}_{\text{plas}}, \dot{\epsilon}_{\text{D}}) + \dot{\epsilon}_{\text{gbs}} \quad (2.2.7)$$

where $\dot{\epsilon}_{\text{diffu}}$ is the diffusional creep rate, involving both Nabarro-Herring creep and Coble creep, and $\dot{\epsilon}_{\text{plas}}$ represents strain rate by dislocation glide at low temperatures. It should be noted in each deformation mechanism the strain rate is governed by the faster one, that is, the contribution of dislocation motion is either from dislocation glide or from power-law creep, at low temperature regime dislocation glide is important, otherwise power-law creep contributes more to the total plastic deformation.

Based on the material properties of pure nickel (taken from Frost and Ashby [26]), contour of constant strain rate is plotted with the axes $\log_{10}(\sigma_s/G)$ and T/T_M as shown in Fig. 2.1. The deformation map for pure nickel is divided into 3 principle fields: low-temperature plasticity, power-law creep and diffusional flow field. The power-law creep appears at high stress level, and this field is subdivided into two regions, one is core-diffusion controlled creep at low temperature and the other is lattice-diffusion controlled dislocation creep at high temperature. Diffusional flow is important at high temperature and low stress regime, in which grain boundary diffusion controlled Coble creep dominating at lower temperatures and lattice diffusion controlled Nabarro-Herring creep dominating at higher temperatures. The deformation mechanism map provides a simple and direct way to distinguish which deformation mechanism is dominant under given field of stress and temperature.

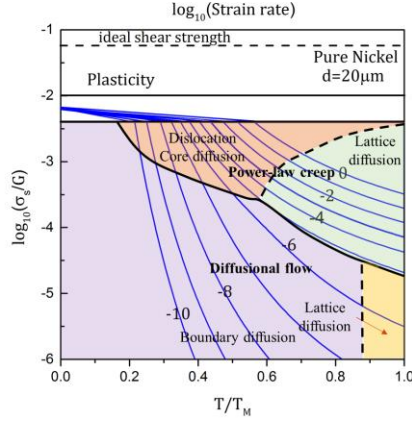


Figure 2.1 Deformation mechanism map for a pure nickel with grain size of 20 μm , with parameters extracted from Frost and Ashby [26].

2.2.5 Grain size effect

Once we are dealing with crystalline solids with microstructure gradients, we may ask a question: how will the grain sizes affect the deformation mechanisms? To answer this question, it is useful for us to construct a deformation mechanism map, showing the dominant deformation mechanism when the grain size varies from micrometer to nanometer. Fig. 2.2 plots the deformation map for pure nickel based on the superposition of rate equations as discussed in Section 2.2, with the material parameters taken from Frost and Ashby [26]. At grain size $d_1 = 20\mu\text{m}$, the deformation map clearly shows three principle fields, including low-temperature plasticity, power-law creep, and diffusional flow governed regions. The power-law creep consists of core-diffusion controlled creep at low temperature and the lattice-diffusion controlled dislocation creep at high temperature. Diffusional flow is important at high temperature and low stress regime, including grain boundary diffusion controlled Coble creep and lattice diffusion controlled Nabarro-Herring creep. When grain size decreases to 0.5 μm , the diffusional flow expands at the expense of

power-law creep, and grain boundary diffusion becomes dominant, as a result, the lattice diffusion controlled dislocation creep shrinks and Nabarro-Herring creep disappears from the deformation map. As the grain size decreases further to 10nm, grain boundary diffusion (Coble creep) contributes most to the total deformation, and dislocation activities are severely confined due to the small lattice geometry. It is clearly seen, in the high temperature regime, grain boundary diffusion gradually becomes the dominant deformation mechanism when grain sizes decreases from 20 μm to 10nm. In the low-temperature plasticity field, the strength increases as the grain size decreases from 20 μm to 0.5 μm following the grain boundary strengthening Hall-Petch relationship, but as the grain size decreases further to 10nm, the strength shows softening behavior due to the lack of strengthening mechanism in absence of dislocation multiplication. It should be noted that grain boundary sliding does not appear in the deformation mechanism map.

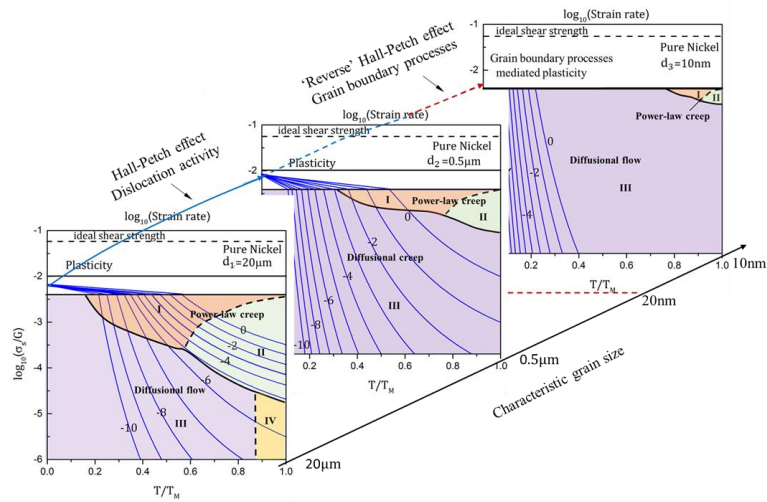


Figure 2.2 Deformation mechanism maps for pure nickel with grain sizes of 20 μm , 0.5 μm and 10nm.

2.3 Creep fracture and fracture mechanism map

Crystalline solids exhibit several modes of fracture depending on loading conditions, i.e., stress and temperature. In low temperature regime, it may fail by cleavage, or by a brittle intergranular fracture, or it may fail in a ductile way. In the high temperature regime, it may fail by various creep fracture ways, such as transgranular fracture, intergranular fracture and rupture. As creep testing condition changes, the fracture model may change from transgranular fracture in short-term creep to intergranular fracture in long-term crack. In this thesis, our emphasis is on the creep fracture mechanism at high temperatures, as the service condition of Type IV failure is usually over 823K. In the following section, different creep fracture mechanisms and fracture mechanism map will be discussed in details.

2.3.1 Transgranular, intergranular creep fracture and rupture

Fig. 2.3 Schematically shows the three creep fracture mechanisms [34]. From Fig.2.3 (a)-(c): (a) brittle intergranular fracture, (b) intergranular or transgranular fracture with some ductility, and (c) rupture after 100% reduction in area. The fracture ductility changes substantially with the fracture mechanics. There are two types of brittle intergranular creep fracture as shown in Fig. 2.3(a). One is by coalescence of cavities formed on grain boundaries aligned roughly normal to the applied stress. The other is wedge cracking formed at triple grain boundary junctions by stress concentration which is resulted by grain boundary sliding. The growth of intergranular cavity is controlled by diffusion and power-law creep. The intragranular creep cavities nucleate at inclusions as

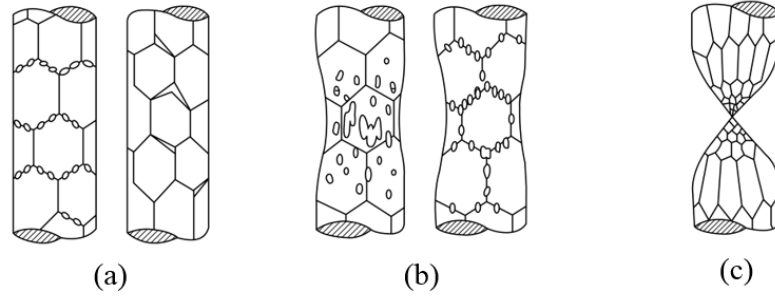


Figure 2.3 Representative fracture modes at high temperature, (a) Brittle intergranular fracture, (b) transgranular and intergranular creep fracture (growth of voids by both power-law creep and GB diffusion), and (c) rupture due to dynamic recrystallization [34].

shown in Fig. 2.3(b), and they grow as material creeps, until they coalesce to form a crack path. Recrystallization occurs when deformation becomes localized in neck or shear band during rupture, as shown in Fig. 2.3(c).

2.3.2 Fracture mechanism map

Ashby and his coworkers [34, 35] also proposed the concept of fracture mechanism map, which provides us with the information of the dominant mechanism operating under different loading condition. Fig. 2.4 shows an example for FCC metals. In this fracture mechanism map, there is no cleavage fracture field, with axes of normalized stress σ/G and homogeneous temperature T/T_m . The ideal strength represents the stress which overcome the interatomic force in a perfect crystal. The crystalline solids will separate on a plane normal to the stress axis. At the stresses lower than ideal strength, fracture takes place in a ductile, transgranular way, which is ductile transgranular fracture. At high temperatures, three fracture mechanisms are important, including transgranular creep

fracture, intergranular creep fracture and rupture. At around 50% of the melting temperature, transgranular (shorter term) creep fracture is more important at high stress regime, and intergranular (longer term) creep fracture caused by the coalescence of grain boundary cavities is dominant in the low stress regime. Wedge cracking is sometimes observed in the transition region between these two fracture mechanisms. At high temperature and high stress condition, rupture occurs by dynamic recrystallization, allowing extensive deformation localized in a neck, and failure eventually happens when the cross-section area decreases to zero. Fig. 2.5 shows an example for 1Cr-1Mo-0.25V steel for a turbine rotor, plotted for stress-temperature and stress-time to rupture, respectively [1]. The fracture mechanism map provides us with useful guidelines for assessment of damage evaluation and remaining life estimation of components in service.

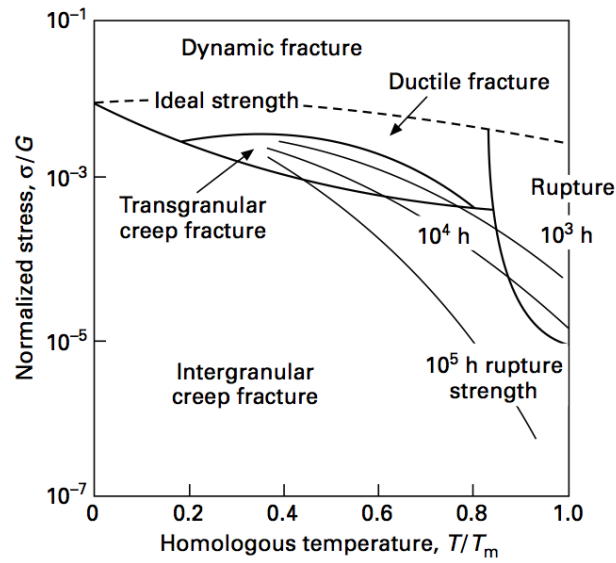
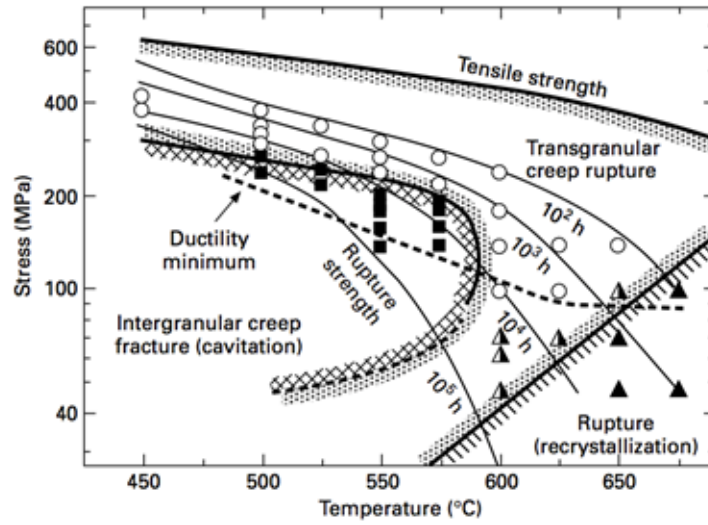
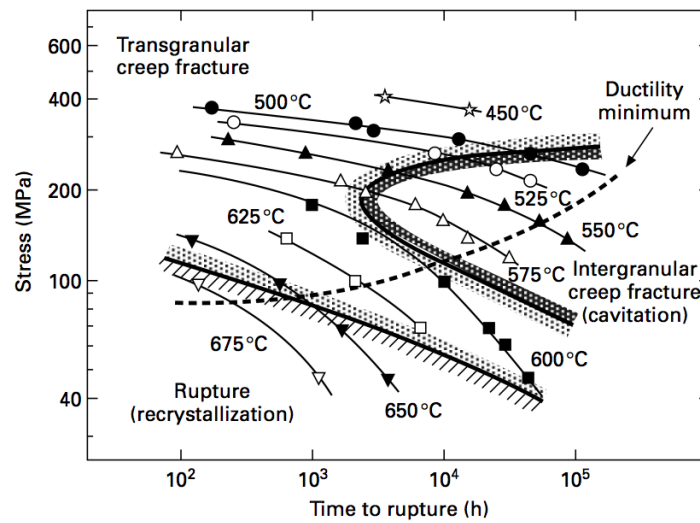


Figure 2.4 Schematic plot of fracture mechanism map for contours of time to rupture for FCC metals [1].



(a)



(b)

Figure 2.5 Fracture mechanism maps for 1Cr-1Mo-0.25V steel, (a) stress vs. temperature and (b) stress vs. time to rupture [1].

3 MICROMECHANICAL ORIGIN FOR STRAIN LOCALIZATION IN HAZ OF CREEP RESISTANT STEELS

3.1 Introduction

Creep strength enhanced ferritic (CSEF) steels with 9-12wt% Cr are widely used in ultra super critical (USC) fossil fire power plants because of their excellent creep resistance and good thermal properties at high temperatures. Welded components made from these advanced steels usually have been put into practical applications under high temperature (500 °C to 650 °C) and low applied stresses (~35MPa). In the welded components during long-term service, premature fractures mainly occur in the fine grained heat-affected zone (HAZ), where the peak temperature is just above A_{C3} during the welding thermal cycle [2, 3]. This so-called Type-IV failure limits the long-term creep performance of CSEF steel weldments. It is well acknowledged the Type IV failure is preceded by the locally accumulated strain in the HAZ [1-3, 5-7]. By using digital image correlation technique, Yu et al. [5] measured the full field deformation of modified 9Cr-1Mo steel cross-welds and captured the strong creep strain localization in the fine grained HAZ. Their experiments showed the reduction of pre-weld tempering temperature from 760°C to 650°C lead to an order of magnitude decrease of the steady-state creep rate for the fine grained HAZ, where the improvement in creep properties were correlated with the hardness and microstructure changes of the two pre-weld tempering specimens [5, 8]. Extensive studies have been performed to identify the causes for the deteriorated creep performance of the welded joints. Many of these report the sharp microstructure and material property

gradients in the HAZ result in significant creep strength degradation [4, 6-12]. Furthermore, the grain size, orientation of the fine grained HAZ and the constraint from base metal and weld metal can lead to high triaxial stresses that may contribute to the creep damage [10, 13]. Although many creep tests and microstructure characterizations have been performed for CSEF steel welded structures, the underlying deformation mechanisms, which link the microstructure, material properties with creep performance, have not been fully understood. The current work pertains to developing a microstructure-informed mechanisms-based finite element model to illustrate the deformation mechanisms responsible for the strain localization in the fine grained HAZ and to investigate the effects of pre-weld tempering on the evolution of creep deformation of ferritic steel welds.

Recently, there have been some finite-element based constitutive models proposed to study the high temperature creep behavior of CSEF steel weldments. Shinozaki and Kuroki [13] modeled the creep deformation of P122 steel weldment by compiling a multi-material model consisting of four zones, including the weld metal (WM), coarse grained heat-affected zone (CGHAZ), fine grained heat-affected zone (FGHAZ) and base metal (BM), where the creep deformation of each zone follows the Norton's law. Their work showed the FGHAZ has high hydrostatic stress and equivalent strain, which can promote nucleation and growth of creep voids in the tertiary creep stage. Similar multi-material models with creep deformation described by the Norton's law were also applied to investigate the creep behavior of 9%Cr advanced steel weldments [6, 36]. In order to investigate the creep response of CSEF steel welds under multiaxial stress conditions, Yaguchi et al. [37] numerically studied the stress/strain distribution of the welded structure

under internal pressures by using a Bailey-Norton law based finite element model. The multiaxial creep tests show similar results as the uniaxial creep tests where the highest creep strain and stress multiaxiality occur at the mid-thickness of HAZ. A viscoplastic continuum damage model, which was first developed for understanding the creep behavior of low chromium steel and its welded joints [38-40], recently has been applied to P91 and P92 steels [41, 42] and their weldments [43, 44]. By including hardening effect and intergranular damage via internal state variables, it provides satisfactory computational results for the creep strain, however, there are too many none mechanisms-based parameters to be estimated which strongly influence the predicted creep performance. Basirat et al. [45, 46] coupled a dislocation-based creep model with a continuum damage model for investigation of the creep behavior of modified 9Cr-1Mo steel and its weld joints, in which the evolution of dislocations was considered as the main driving mechanism and the effects of precipitate coarsening, solid solution depletion and void growth are incorporated by adding damage terms into the Orowan's equation. An alternative finite element approach for modeling the creep deformation was proposed by Kimmins and Smith [47], allowing for the relaxation of constraint by the sliding of adjacent elements. Their numerical calculations suggest that the cross-weld specimens with grain boundary relaxation provide good agreement with experimental observations. Although many computational approaches have been utilized to study the high temperature creep behavior of CSEF steel weldments, most of them are Norton's creep law-based or dislocation-based creep models, which only account for the deformation mechanisms at high stress regime and neglect those (e.g., grain boundary sliding and diffusional creep) operating at lower

stress regime. During practical service of fossil fire power plants, the materials deform at low stresses ($< 40\text{MPa}$). Therefore, it is crucial to get the fundamental understanding of the long-term (low stress) creep behavior of CSEF weldments for safe design. The present work aims to develop a comprehensive micromechanics-based computational model capable of predicting weld creep performance over a wide range of stress and temperature of interest. A typical ferritic steel weldment shows heterogeneous microstructures in the base metal, fine-grained HAZ, coarse-grained HAZ and weld metal, and there are corresponding heterogeneities in the creep properties. Most of the current computational models account for the heterogeneous material properties by compiling multiple regions, with each region represented by a bulk material [6, 13, 36, 37, 43, 44, 46]. Different from those in literature, the present work will propose a microstructure-based computational model that can explicitly consider the microstructure and simulate the creep deformation of CSEF steel weldments on the grain length scale.

3.2 Microstructure-informed model

To consider the microstructure heterogeneities of ferritic steel weldments, as shown in Fig. 3.1, we construct a two-dimensional digital microstructure by using Voronoi tessellation method in an open source software Neper [48]. The Voronoi tessellation method was implemented to obtain a more realistic microstructure by manipulating the location of the Voronoi seeds. A Voronoi tessellation is a partition of a domain D into n regions R_i corresponding to n distributed seed Q_i , according to

$$R_i = \{x \in D: \|Q_i - x\| < \|Q_j - x\| \ \forall j \neq i, j = 1, 2, \dots, n\}. \quad (3.2.1)$$

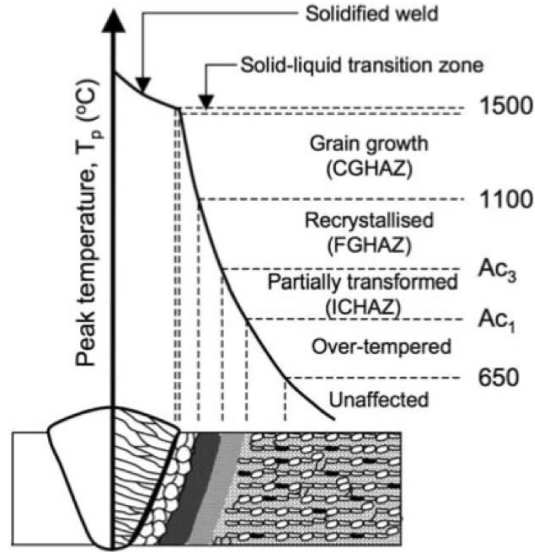


Figure 3.1 Schematic representation of microstructure of weldments [2].

The generated digital microstructure agrees well with experimental sample in its topological and structural properties. As a result of the welding thermal cycle, the microstructure of base metal is altered and the heat-affected zone with microstructure gradients is formed.

As shown in Fig. 3.2, the microstructure shows strong grain size gradients in weld metal (WM), coarse grain heat-affected zone (CGHAZ), fine grain heat-affected zone (FGHAZ), intercritical heat-affected zone (ICHAZ) and the base metal (BM). As both ICHAZ and FGHAZ essentially have fine-grained microstructures after post weld heat treatment, in the present study they are referred as FGHAZ without differentiation. The two-dimensional microstructure contains 750 grains, with random crystallographic orientations in each individual grain. Note the colors in Fig. 3.2 only represent the boundaries of each grain with no specific meaning of grain orientations.

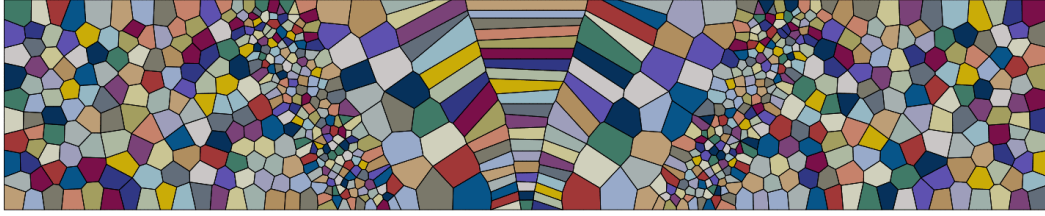


Figure 3.2 Two-dimensional digital microstructure model for ferritic steel weldment with grain size gradients in the base metal (BM), fine grained heat-affected zone (FGHAZ), coarse grained heat-affected zone (CGHAZ), and weld metal (WM).

As we concern the creep behavior of ferritic steel weldments under low applied stresses and high temperatures, our focused region is the fine-grained HAZ where creep strain accumulates significantly and Type IV failure takes place during the long-term applications [4-6, 9, 36, 49]. In the present study, the average grain sizes of FGHAZ and the other regions (BM, CGHAZ and WM) are assumed to be $1\mu\text{m}$ and $5\mu\text{m}$, respectively. Taking advantage of the digital microstructure, we are capable of considering the heterogeneous material properties at the scale of individual grains, e.g., heterogeneous grain boundary diffusivity and slip anisotropy, etc. The digital microstructure generally captures the main characterized features of ferritic steel weldments. Our work here is among the first to explicitly model weldment microstructure and grain size distribution, which play a significant role in the overall and local deformation of weldments [2, 3].

3.3 Constitutive laws and finite element method

High temperature creep deformation of crystalline material results from a synergy of thermally activated dislocation movements, diffusion flow and grain boundary sliding (GBS). Each of the three mechanisms may occur independently and compete to be the

dominant deformation mechanism. Deformation mechanism maps [26] show the dominant mechanisms for various materials in different ranges of stresses and temperatures. For a typical polycrystalline material, the plastic flow at high temperature is mediated by Coble creep through grain boundary diffusion [27] or Nabarro-Herring creep through lattice diffusion [28, 50] under low applied stresses, by dislocation creep through lattice or dislocation core diffusion at high stresses, and by grain boundary sliding at intermediate stress regime especially in fine grained materials. Bower and Wininger [51] developed a comprehensive finite element framework to model the grain boundary sliding, grain boundary diffusion and migration, as well as thermally activated dislocation creep of polycrystalline materials. Their simulation results reflect a deformation-mechanism transition from dislocation creep controlled plasticity in materials with coarse grain sizes at high strain rates to grain boundary sliding and diffusion dominated plasticity in fine grained materials at low strain rates. The mechanisms-based finite element methods were also used to investigate the deformation of nanocrystalline materials [52-54], in which grain boundary deformation, e.g., grain boundary sliding and diffusion, was found to play significant roles in the determination of the macroscopic response of small-grained materials. The continuum levels finite element simulations show the unique advantage in analyzing the microstructure evolution, grain-scale deformation, and the global-local deformation relationships of polycrystalline materials.

In the following, we will present a mechanisms-based constitutive model for analysis and prediction of the high temperature creep deformation of CSEF steel weldments. The computational framework accounts for the combined effects of grain

interior dislocation creep and diffusional creep as well as grain boundary sliding, i.e., is to couple a creep constitutive model for the grain interior deformation with a viscous interface model for grain boundary sliding.

3.3.1 Constitutive equation for grain interior

It is commonly accepted that the main plastic deformation of grain interior results from diffusional creep and dislocation creep at high temperatures. The steady-state creep rates of different mechanisms are generally described by the well-known Mukherjee-Bird-Dorn equation [55]:

$$\dot{\epsilon}_{ss} = \frac{ADEb}{kT} \left(\frac{b}{d}\right)^p \left(\frac{\sigma}{E}\right)^n, \quad (3.3.1)$$

where $\dot{\epsilon}_{ss}$ is the steady state creep rate; σ is the applied stress; k and T are the Boltzmann's constant and the absolute temperature, respectively; E is the Young's modulus; d is the grain size; p is the inverse grain size exponent; n is the stress exponent; A is a microstructure dependent constant; and D is the diffusion coefficient represented by Arrhenius law,

$$D = D_0 \exp(-Q/kT), \quad (3.3.2)$$

where Q is the activation energy for the diffusion process, and D_0 is the diffusion pre-exponents. Each creep mechanism can be characterized by Eq. (3.3.1) with specific values of diffusivity D , activation energy Q , inverse grain size dependence p and stress exponent n . For diffusional creep, they are lattice diffusion controlled Nabarro-Herring creep and

grain boundary diffusion governed Coble creep. As the Nabarro-Herring creep only occurs at extremely high temperature ($\sim 0.8T_M$) [26], in the present analysis solely Coble creep is considered as the operating diffusional flow. The rate equation of Coble creep is characterized by stress exponent $n = 1$ and inverse grain size exponent $p = 3$ via Eq. (3.3.1). With the strong grain size dependence, Coble creep may contribute significantly to the strain accumulation in fine-grained HAZ. For the dislocation creep, dislocation glide accounts for most of the plastic strain, but its creep rate is determined by dislocation climb, which is controlled by lattice or dislocation core diffusion. In the majority of alloys, at high temperatures the dislocation climb is required when the gliding dislocation is held by physical obstacles, in which transport of matter is through lattice diffusion. The dislocation creep governed by lattice diffusion is considered as another contribution to the grain interior deformation, and its rate is usually characterized by stress exponent $n \geq 4$ and inverse grain size exponent $p = 0$ via Eq. (3.3.1). The creep rate study and material parameter calibration for CSEF steel and its weldments will be discussed in section 2.3.

Based on the above discussions, we will develop a creep constitutive model for grain interior deformation accounting for the lattice diffusion governed dislocation creep and the grain boundary diffusion controlled Coble creep. The strain rates are decomposed into elastic and plastic parts,

$$\dot{\epsilon}_{ij} = \dot{\epsilon}_{ij}^e + \dot{\epsilon}_{ij}^p. \quad (3.3.3)$$

The elastic deformation follows the generalized Hooke's law,

$$\dot{\varepsilon}_{ij}^e = \frac{1+\nu}{E} \left(\dot{\sigma}_{ij} - \frac{\nu}{1+\nu} \dot{\sigma}_{kk} \delta_{ij} \right). \quad (3.3.4)$$

As the creep deformation mechanisms are independent of each other, the strain produced by each mechanism contributes additively to the total creep deformation. The plastic strain rate is the summation of Coble creep rate and dislocation creep rate, and it is generalized to multiaxial stress state as followings:

$$\dot{\varepsilon}_{ij}^p = \left[A_{\text{dis}} \frac{EbD_l}{k_B T} \left(\frac{\sigma_e}{\sigma_0} \right)^n + A_{\text{coble}} \frac{EbD_{\text{gb}}}{k_B T} \left(\frac{b}{d} \right)^3 \left(\frac{\sigma_e}{E} \right) \right] \frac{3S_{ij}}{2\sigma_e}, \quad (3.3.5)$$

where the two terms represent the contribution of dislocation creep and Coble creep, respectively, S_{ij} is the deviatoric stress tensor $\sigma_{ij} - \sigma_{kk}\delta_{ij}/3$, and σ_e is the von Mises stress $\sqrt{3S_{ij}S_{ij}/2}$. The diffusivity coefficients for the dislocation creep D_l and Coble creep D_{gb} obey the Arrhenius law,

$$D_l = D_{0l} \exp(-Q_l/RT), \quad (3.3.6a)$$

$$D_{\text{gb}} = D_{0\text{gb}} \exp(-Q_{\text{gb}}/RT), \quad (3.3.6b)$$

where the pre-exponents for lattice diffusion D_{0l} and grain boundary diffusion D_{gb} , and the activation energies for lattice diffusion Q_l and grain boundary diffusion Q_{gb} all can be found in the literature [1, 26]. The only unknowns, the dimensionless material constants A_{dis} , A_{coble} and the stress exponent n for dislocation creep, will be determined via calibration with experimental creep data in section 2.3.

In order to represent the anisotropic nature of crystal slips induced by crystallographic orientation effects of each individual grain, we introduce a micromechanical Taylor factor [56]. It is defined as the ratio between the local crystallographic shear $\sum \gamma^{\text{local}}$ and the local von Mises strain $\langle \epsilon_{\text{VM}}^{\text{local}} \rangle$ within each grain,

$$M = \frac{\sum \gamma^{\text{local}}}{\langle \epsilon_{\text{VM}}^{\text{local}} \rangle}, \quad (3.3.7)$$

where $\sum \gamma^{\text{local}}$ and $\langle \epsilon_{\text{VM}}^{\text{local}} \rangle$ are numerically calculated by using a separate crystal plasticity [57] finite element analysis. The results for the micromechanical Taylor factors are shown in Fig 3.3. High values of the Taylor factor indicate the grain with certain crystallographic orientation is kinematically soft, where the crystal slips are preferable to occur. In the weldment, dislocation creep strain percolation follows grains which are kinematically soft and avoids grains those are hard. To incorporate the grain orientation effects into creep deformation, we modify the creep rate by adding the micromechanical Taylor factor to the dislocation creep term,

$$\dot{\epsilon}_{ij}^{\text{p}} = \left[A_{\text{dis}} \bar{M}^I \frac{EbD_l}{k_B T} \left(\frac{\sigma_e}{\sigma_0} \right)^n + A_{\text{coble}} \frac{EbD_{\text{gb}}}{k_B T} \left(\frac{b}{d} \right)^3 \left(\frac{\sigma_e}{E} \right) \right] \frac{3S_{ij}}{2\sigma_e}, \quad (3.3.8)$$

where $\bar{M}^I$ is the normalized micromechanical Taylor factor for the I_{th} grain, $\bar{M}^I = M^I / \max(M^1, M^2, \dots, M^I, \dots, M^N)$, and N is the total number of grains within the polycrystalline model. The numerical procedure of the grain interior creep constitutive model is implemented in the commercial finite-element software ABAQUS [58] via a user-defined material model (UMAT).

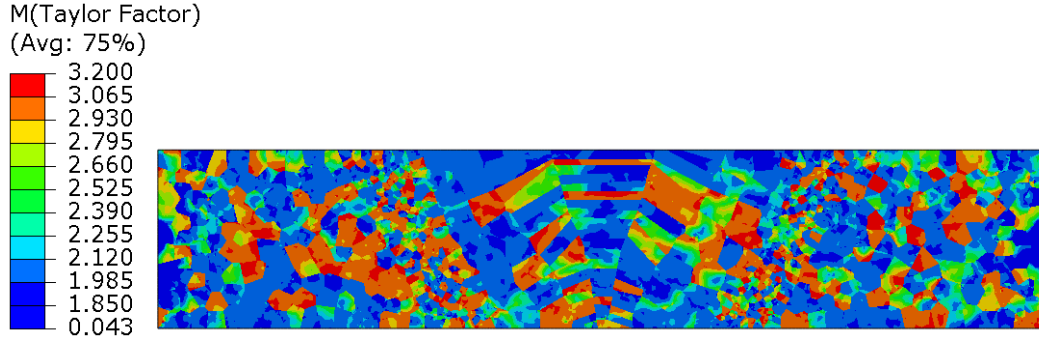


Figure 3.3 Contour plot of micromechanical Taylor factor for ferritic steel weldment to represent the crystallographic orientation of each individual grain (each grain assigned with random orientations).

3.3.2 Constitutive model for grain boundary

Grain boundary sliding (GBS) is one of the competing mechanisms that contribute to the creep deformation and damage of ferritic steel weldments [1, 3, 45-47]. In general, GBS, controlling the strain rate sensitivity in the intermediate stress regime, is the main deformation mechanism for superplasticity of polycrystalline materials [33]. In the literature GBS is usually considered as a rate contribution to the grain interior deformation and characterized by Eq. (3.3.1) with grain size dependence $p = 2, 3$ and stress exponent $n = 2$ [59]. Even though this treatment of GBS provides quantitative creep rate, it has no obvious effect on the stress state and cavity formation of polycrystalline materials. It is well acknowledged GBS on the other hand significantly influences the stress multiaxiality which has direct effects on the creep cavitation and crack formation [13, 37]. Furthermore, in consideration of large microstructure gradients of ferritic steel weldments, it requires explicit modeling of grain boundary sliding in the welded structure.

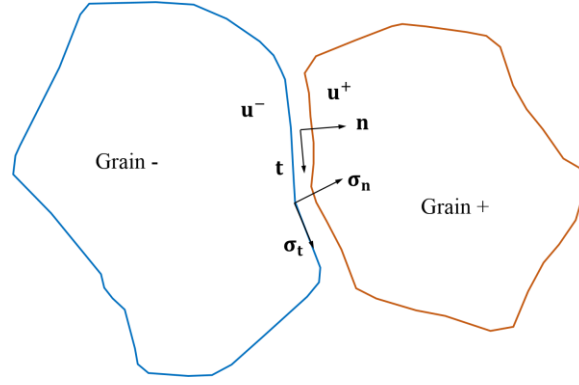


Figure 3.4 A representative grain boundary with displacement $\mathbf{u}^+$ and $\mathbf{u}^-$ across the boundary, normal $\mathbf{n}$ and tangential $\mathbf{t}$ directions, as well as normal σ_n and tangential σ_t tractions.

Grain boundary sliding is driven by shear tractions acting tangentially to the grain boundary. In our analysis, we assume that grain boundary sliding is a thermally activated process, and obey the Newtonian viscous law,

$$\dot{u}_t = \frac{\Omega \eta_0 \exp(-Q_{\text{gbs}}/RT)}{k_B T} \sigma_t, \quad (3.3.9)$$

where $u_t = (\mathbf{u}^+ - \mathbf{u}^-) \cdot \mathbf{t}$ denotes the relative tangential displacement across the grain boundary in response to the local shear traction σ_t , as shown in Fig. 3.4, η_0 is a characteristic sliding velocity, Ω is the atomic volume and Q_{gbs} is the activation energy for grain boundary sliding. The numerical procedure of grain boundary sliding is implemented in ABAQUS [58] by developing a user defined elements (cohesive zone model), in which the relative sliding velocity of two adjacent grains is related to the local shear stress acting on the grain boundary (Eq. 3.3.9). From geometric point of view, GBS cannot occur in a polycrystalline solid in absence of some other deformation mechanisms. It usually requires

accommodation from diffusional flow, grain boundary migration or dislocation creep, to diminish the incompatible velocity discontinuity across the GB [33, 51, 60]. In the present work, the coupling between GBS, dislocation creep, and diffusional flow accommodates the discontinuous velocity field naturally as a consequence of enforcing compatibility and equilibrium on the overall deformation using the finite element method.

3.4 Calibration of material parameters

Applying the proposed constitutive models to investigate the high temperature creep deformation of CSEF steel weldments, we need to estimate reasonable values for the material constitutive parameters. Most of the them can be found in the literature [1, 7, 26, 61], and only several (e.g., dimensionless coefficient A_{dis} and A_{Coble} , and stress exponent n) are not readily available. These unknown material parameters will be determined through calibration with experimental creep rate data. The creep deformation of CSEF steel and its weldments has been experimentally studied by numerous researches (e.g., [5-7, 36, 49, 61-64]). Most laboratory experiments performed short-term creep tests at high applied stresses, however, the knowledge of long term creep at low stress level is required in practical application of power plant components. The NIMS [64] and Shrestha et al.'s [61] creep data of Grade 91 steels, as shown in Fig. 3.5, are selected as they cover both the long-term creep (grain boundary diffusion controlled Coble creep) and the short-term creep (lattice diffusion governed dislocation creep). It is observed the creep rate of Shrestha et al. [61] is about one order of magnitude higher than that of the NIMS data [64] especially in the low stress regime. This kind of creep rate scatter for Grade 91 steels is commonly

reported in the literature [65], which can be resulted from difference in chemical composition and heat treatment conditions, etc. In the present work, the NIMS creep strain rate vs. stress curve is used as a reference dataset to calibrate the unknown material parameters for the computational model. As discussed in section 2.3, the grain interior creep deformation mechanisms are independent of each other and the strain caused by each mechanism contributes additively to the total creep strain. Therefore, the mechanism giving the highest value of creep rate dominates creep deformation at a given stress and temperature. This assumption allows us to do calibration for material parameters in the low stress (< 60 MPa) and high stress regimes, respectively, as shown in Fig. 3.5. The calibration of Coble creep coefficient is performed for stresses below 60 MPa, where the diffusional creep is expected to be dominant. By fitting the low stress zone with Coble creep (stress exponent $n = 1$), the dimensionless coefficient A_{Coble} is determined as 5.7306×10^{-10} . The calibrated material parameters for dislocation creep are obtained by fitting the power-law creep rate with the experimental data in high stress regime. The stress exponent for the dislocation creep, i.e. the slope of the $\log(\dot{\epsilon}) - \log(\sigma)$ curve, is identified as $n \approx 8$ by using least square method. Correspondingly, the dimensionless coefficient for dislocation creep A_{dis} is determined as 1.1462×10^{-9} . The representative values for the material parameters used as model inputs are listed in the Table 3.1.

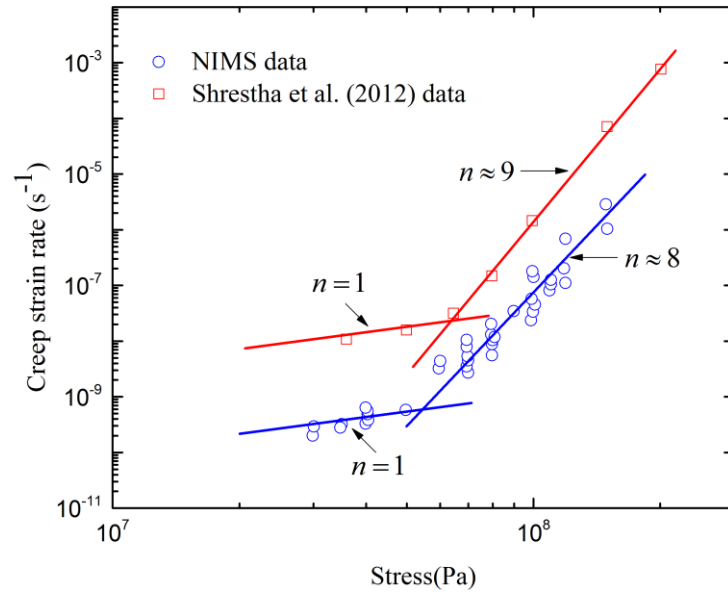


Figure 3.5 Stress dependence of steady state creep rate for Grade 91 ferritic steel at 923K.

Table 3.1 Representative values for material parameters used in the computational model. Parameters related to the thermal activation processed are fitted from the NIMS data.

Parameter	Value
Atomic volume, Ω	$1.18 \times 10^{-29} \text{m}^3$
Melting temperature, T_M	1810K
Burgers vector, b	$2.48 \times 10^{-10} \text{m}$
Young's modulus, E_0	223GPa
Young's modulus at 923K, E	90.1GPa
Poisson's ratio, ν	0.3
Grain boundary diffusion pre-exponent, $D_{0\text{gb}}$	$0.0044 \text{m}^2/\text{s}$
Grain boundary diffusion activation energy, Q_{gb}	174 KJ/mole
Coble creep coefficient, A_{coble}	5.7306×10^{-10}
Lattice diffusion pre-exponent, $D_{0\text{l}}$	$0.021 \text{m}^2/\text{s}$
Lattice diffusion activation energy, Q_{l}	500 KJ/mole
Dislocation creep coefficient, A_{dis}	1.1462×10^{-9}
Reference stress, σ_0	60 MPa
Stress exponent, n	8
Grain boundary sliding pre-exponent, η_0	40 m/s
Average grain size in FGHAZ, d	1 μm
Average grain size in the other zones, d	5 μm

3.5 Application of the constitutive model to ferritic steel weldment

The full field creep deformation of Grade 91 steel weldments through two pre-welding temper conditions was measured by using digital image correlation (DIC) techniques [5], in which one is pre-welding tempered at 760°C for 1h (standard) and the other is at 650°C for 1h (non-standard). Fig. 3.6 and Fig. 3.7 shows the DIC results for the strain field of the standard and nonstandard Grade 91 steel weldments loaded and hold at 650°C/70MPa for 85 hours. The strain maps exhibit inhomogeneous creep deformation, and particularly significant creep strain localization was observed in the standard pre-weld tempered specimen. In this section, we will apply the proposed computational model to investigate the micromechanical and microstructural origin for the creep deformation and strain localization phenomenon in the CSEF cross-welds, and also to discuss the effects of pre-welding temper condition on the strain localization evolution.

In the recent years, finite element method has been successfully used to investigate the mechanical behavior for the polycrystalline materials [51-54]. It can both qualitatively and quantitatively reveal insights on the micromechanical interactions, local and overall deformation of material systems. In the present work, a creep constitutive model is proposed to describe the grain interior deformation, including Coble creep and dislocation creep, and a viscous interface model is used for grain boundary sliding. Some representative simulations will be presented to show our capability of modeling the creep deformation of ferritic steel weldments. The numerical simulations are validated and compared with the strain field measurement [5]. By taking advantage of this mechanisms-

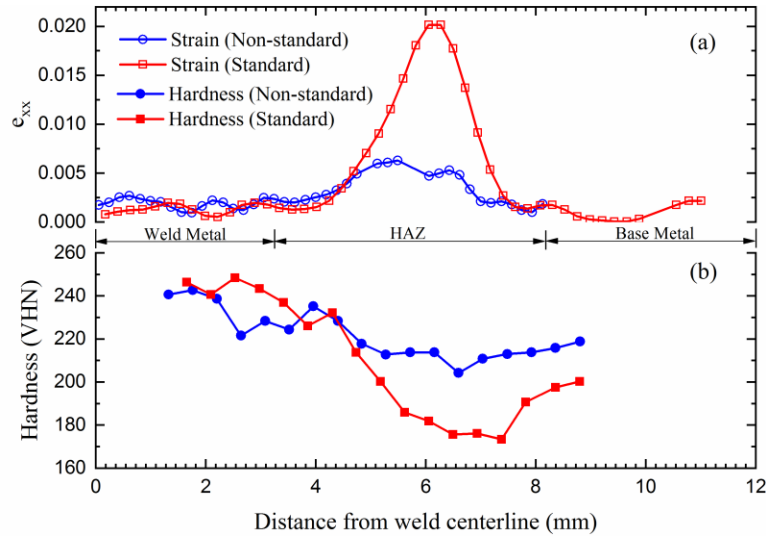


Figure 3.6 (a) Distribution of transverse creep strain, and (b) hardness profile for the Grade 91 steel weldments [5].

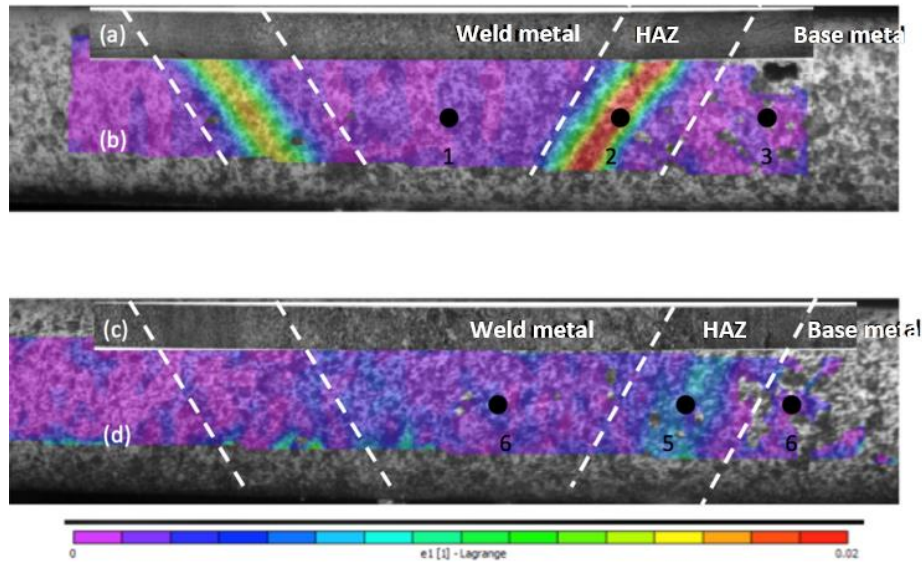


Figure 3.7 Full field strain maps obtained using DIC and metallographs for standard pre-weld tempering condition (b, a) and non-standard pre-weld tempering condition (d, c) Grade 91 steel weldments after 85 hrs creep at 70 MPa and 923K [5].

based finite element model, we will quantify the contribution of Coble creep, dislocation creep and grain boundary sliding to the total plastic deformation step-by-step. The following simulations are of same boundary and loading conditions as the experimental creep tests [5]: the microstructure model as shown in Fig. 3.2 is fixed on the left side, loaded and hold at 650°C/70MPa for 85 hours on the right side along the transverse direction.

3.5.1 Coble creep and grain size effect

The microstructure of CSEF steel weldment, as shown in Fig. 3.2, presents strong grain size gradients in the BM, CGHAZ, FGHAZ and WM. Fine grain in the FGHAZ is commonly considered as one of the important factors responsible for the strain localization in the heat-affected zone [1-3]. In this section, the following modeling strategy is employed to investigate the grain size effects on the creep deformation of ferritic steel welds. The different regions in whole weldment are assumed to be of same strength as the base metal, and the present simulation only accounts for the grain interior deformation to exclude the contribution from grain boundary sliding.



Figure 3.8 Contour plot of the strain distribution for Grade 91 steel weldment after 85 hrs creep at 70 MPa and 923K, only considering the grain size effects.

Fig. 3.8 plots the numerical results for the strain field of the whole weldment under 70 MPa loading and holding for 85 hours at 923K. The strain map shows most of the deformation is concentrated in the FGHAZ. The creep strain of fine-grained HAZ (~0.3%) is about two times higher than that of the base metal and weld metal (~0.1%), which is due to the fine grains in this region. Considering the grain interior deformation mechanisms, the dislocation creep is independent of grain size, whereas the creep rate of Coble creep is proportional to d^{-3} (d is the grain size), i.e., the Coble creep rate increases with the decreased grain size. Therefore, the present numerical simulation counts the contribution of Coble creep to the total strain accumulation in the fine grained HAZ. It is illustrated the grain size dependent Coble creep plays an important role in the high temperature creep deformation and strain concentration in the FGHAZ of CSEF steel weldments.

3.5.2 Dislocation creep and hardness variation effect

Hardness of CSEF steel weldments shows minimum value in the vicinity of fine grained or intercritical heat-affected zone [4-7, 9, 13, 36]. The softening zone produced during the welding heat cycles accelerates the deformation and damage development of the ferritic steel weldments. Yu et al.'s [5] measured the hardness of the standard and non-standard pre-welding tempered Grade 91 steel weldments. Fig. 3.6(a) shows the profiles of hardness data along different positions of the welds, where the fusion line was taken to be zero for the distance measurement. The hardness profiles reveal the minimum hardness of the non-standard and standard conditions is about 210 VHN (93% base metal hardness) and 170 VHN (77% base metal hardness), respectively, and the low hardness region is the same region that has high creep deformation. So far the quantitative correlation between

material hardness and creep deformation of cross-welds is still not fully understood. The following numerical simulations, accounting for the grain interior deformation, are employed to study the effect of hardness on creep behavior of ferritic steel weldments. Dislocation creep is strongly dependent on the material strength, as shown in Eq. (3.3.8) its creep strain rate is expressed as a function of the reference stress σ_0 , which is a representation of material strength and proportional to the hardness. In the present simulation the strain rate of dislocation creep is correlated with hardness measurement via the reference stress σ_0 . The contour plots of the strain field for the standard and nonstandard weldments after 85 hours of creep are shown in Fig. 3.9, with the contour maximum limits as 6.0×10^{-3} and minimum as 0.0. It is observed there is stronger strain localization in the fine-grained HAZ of standard condition than that of the non-standard condition. As the strain rate of dislocation creep is proportional to $(1/\sigma_0)^8$, it can be deduced that the dislocation creep rate of the fine-grained HAZ is increased by $(1/0.93)^8$ and $(1/0.77)^8$, respectively, compared to that of the base metals of the non-standard and standard condition welded structure. It is indicated the softer FGHAZ of standard pre-welding tempered weldment brings higher creep strain. The degraded creep behavior was correlated with microstructure characterizations [5, 8]: both standard and non-standard specimens contain $M_{23}C_6$ (M=Cr, Fe) and MX (M=Nb, V; X=C, N) precipitates, however, the distribution is quite different. There are sparse and large carbides and even carbide free zone in the FGHAZ of standard specimen, which makes the material less strengthened and results in the high creep deformation. Compared with the standard condition, FGHAZ of the non-standard condition shows more uniformly distributed precipitates, especially with

finer $M_{23}C_6$ carbides on the prior austenite grain boundaries and martensite block boundaries. The change in precipitate distribution leads to the improvement of the creep properties and lower creep deformation of non-standard pre-welding tempered welds. Comparing the numerical results with those obtained in section 5.1, it is observed that hardness reduction results in more strain concentration in the fine-grained HAZ (e.g., standard condition 0.58%). Besides the Coble creep, dislocation creep with dependence on material strength also plays an important role in the high temperature deformation and strain localization in the CSEF steel welded structures. The modeling sequence of section 5.1 and 5.2 helps gradually quantify the contribution of Coble creep and dislocation creep to the total strain accumulation in HAZ of ferritic steel weldments.

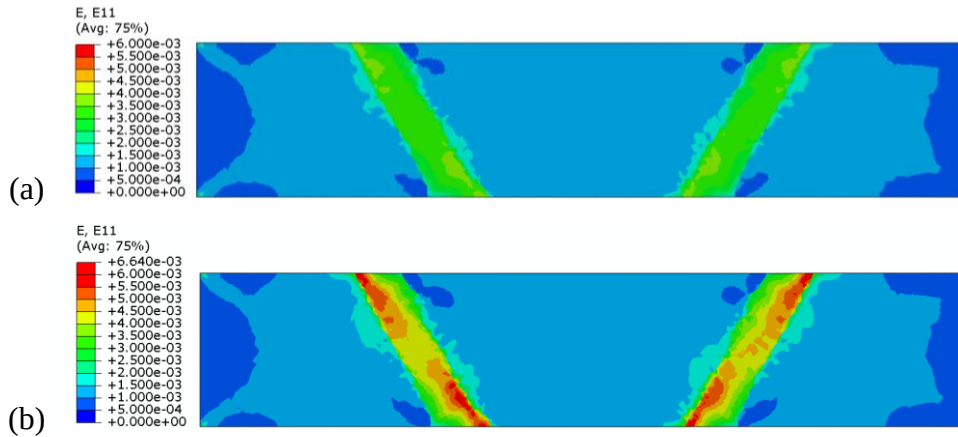


Figure 3.9 Contour plot of the full field strain in presence of the variation of both grain size and hardness, (a) for non-standard condition weldment with 7% hardness reduction in HAZ, and (b) for standard condition weldment with 23% hardness reduction in HAZ, after 85 hrs creep at 70 MPa and 923K.

3.5.3 Grain boundary sliding

In addition to the grain interior creep deformation, we include the contribution of grain boundary sliding to investigate the high temperature deformation response of the ferritic steel weldments. Fig. 3.10 plots the simulation results of strain field for the non-standard and standard weldments after 85 hours creep. The average strain in the fine grained HAZ of the standard and non-standard conditions is about 1.52% and 0.45%, respectively. These numerical results of creep strain show quantitative agreement with the experimental measurement as shown in Fig. 3.6(a). Compared the strain field results with those obtained in section 5.2, it is found grain boundary sliding brings more creep strain accumulation in the fine grained HAZ. This can be induced by the general effect of grain boundary sliding that plays a significant role in the creep deformation of small-grained materials at intermediate stresses. FGHAZs of both standard and nonstandard conditions essentially have fine grained microstructures, nevertheless, GBS results in more creep deformation in the standard condition ($\sim 0.84\%$) than the non-standard condition. This illustrates GBS is more active in the softer fine grained HAZ of the standard condition, and also implies the strong interaction between GBS and grain interior creep deformation. Because of the artificial construction of grain morphology, there are some strain concentrations in the vicinity of the grain boundary triple junctions in the weld metal and coarse grained HAZ as shown in Fig. 3.10. In practical creep tests, such strain localization is not present due to the topological compatibility of real microstructures. Even though digital microstructure does not reproduce the exact microstructure, it generally captures the main characterized features of ferritic steel weldments.

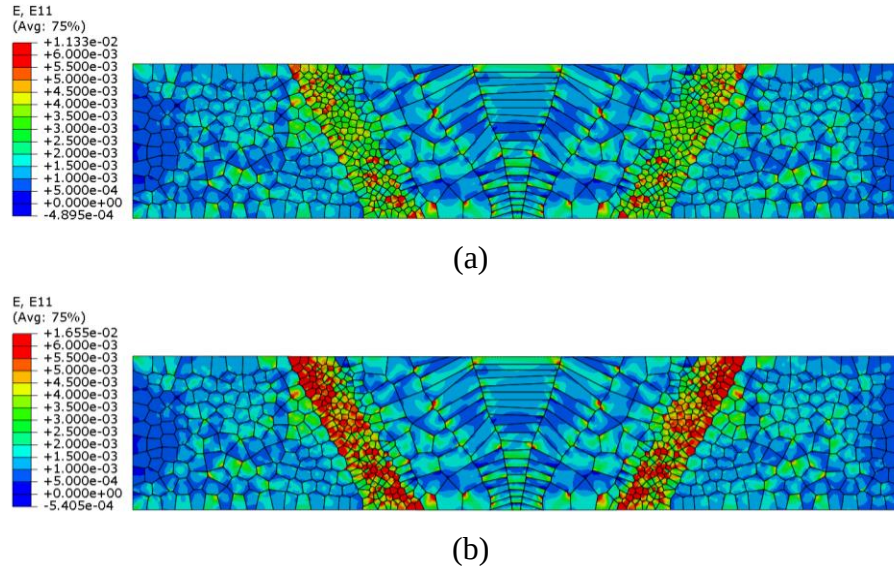


Figure 3.10 Contour plot of strain distribution after 85 hrs creep at 70 MPa and 923K (a) for non-standard condition weldment, and (b) for standard condition weldment, involving the contribution of the grain size dependent Coble creep, material strength dependent dislocation creep as well as grain boundary sliding.

In the CSEF steel weldment, it is the interplay between the response of grain interior and grain boundaries that dictates the overall deformation. The microstructure-informed constitutive model enables us to numerically study the competition among the thermally activated diffusional flow, dislocation motion and grain boundary sliding. Fig. 3.11 illustrates the contribution of Coble creep, dislocation creep and grain boundary sliding to the total creep deformation of ferritic steel weldments (with the strain extracted from a path along half-height of the weldment). For the non-standard condition, diffusional Coble creep and grain boundary sliding provide equally 45% of the creep strain in the fine grained HAZ, with the dislocation creep providing the reminder 10%. For the standard condition, grain boundary sliding acting as the dominant deformation mechanism provides approximately 65% of the creep strain in the FGHAZ, dislocation creep becomes more important (20%)

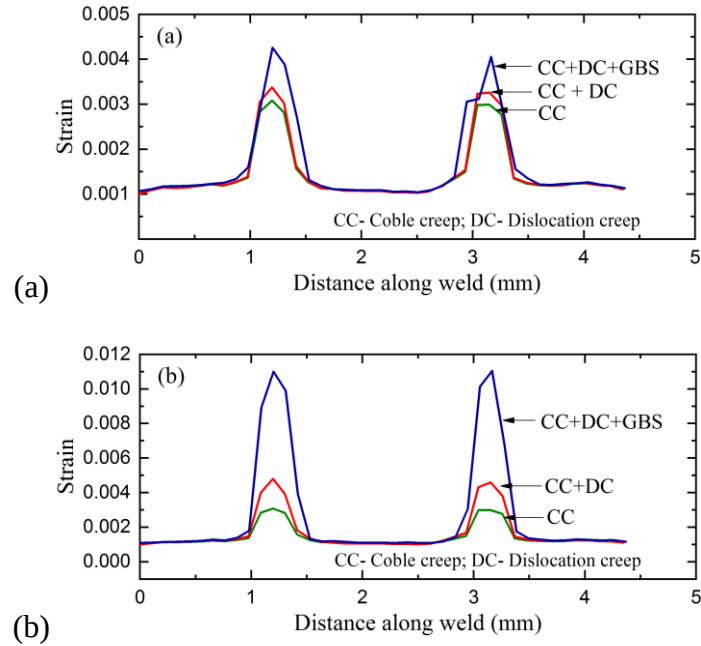


Figure 3.11 The quantitative contribution of Coble creep, dislocation creep and grain boundary sliding to the total creep strain concentration in the fine grained HAZ, (a) for the non-standard pre-weld tempering condition and (b) for the standard pre-weld tempering condition.

with the reduced hardness, and Coble creep provides the remaining 15% of the creep strain. Compared our numerical results with those obtained by DIC technique [5], it is found the strain concentration of fine-grained HAZ predicted by the computational model is lower than that of the experimental measurement. This is due to the underestimation of the creep deformation for the following reasons: (a) The dislocation creep rate is multiplied by a micromechanical Taylor factor which has a value less than 1 (to represent the grain orientation effects); and (b) The entire creep deformation of a material commonly contains three stages, including the primary creep, secondary (steady-state) creep and tertiary creep. For engineering design of high temperature components for long-term application, the steady-state regime is of more practical significance. Therefore, in the present work the

primary creep is neglected due to its short effective time range, which leads to the underestimated creep strain.

The high constraint of the weak HAZ from the adjacent stronger WM and BM is one of the key factors for the Type-IV failure. The weakest part tries to deform transversely under high strains, however, it is constrained from doing so by the adjacent stronger materials. As a result, a multiaxial stress state predominates. The stress triaxiality factor is defined as the ratio between the hydrostatic pressure σ_h , and equivalent von-Mises stress σ_e ,

$$TF = \frac{\sigma_h}{\sigma_e} = \frac{1/3 (\sigma_1 + \sigma_2 + \sigma_3)}{\frac{1}{2} \sqrt{(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2}} \quad (5.1)$$

where σ_1 , σ_2 and σ_3 are principle stresses. The average stress triaxiality factors for the standard FGHAZ, nonstandard FGHAZ and BM are calculated as 0.829, 0.796 and 0.401, respectively. According to the vacancy diffusion theory, it is controlled by the hydrostatic stress gradients, i.e., vacancies diffuse from regions of lower triaxiality to those of higher triaxiality. Thus, the high triaxial stress fields in HAZ are expected to result in vacancy accumulation and creep void formation in this region [1]. The location of Type IV cracking is found to be consistent with the region where the stress triaxiality factor is high [6, 13, 37, 66]. Therefore, evaluating the stress multi-axiality is important for predicting the Type-IV failure of CSEF steel weldments.

The present work shows the HAZ region has a combination of strain concentration and high stress triaxiality, which possibly leads to early cavity nucleation, its growth and

further coalescence towards to the critical failure. The computational approach for investigation of deformation and damage mechanisms responsible for Type-IV failure of CSEF steel weldments, as well as the lifetime prediction will be presented in the Part II of our series work.

3.6 Summary

We have developed a microstructure-informed mechanisms-based finite-element model to numerically study the high temperature deformation behavior of CSEF steel weldments. A creep constitutive model which accounts for the dislocation creep and Coble creep (diffusional creep) is used for the grain interior plasticity, and a Newtonian viscous model is employed to describe grain boundary sliding. The numerical results of strain field distribution show encouraging quantitative agreement with DIC measurement, particularly illustrating the effect of pre-welding tempering on the evolution of strain localization in HAZ of ferritic steel weldments. We found that the thermally activated dislocation creep, diffusional creep as well as grain boundary sliding all contribute to the high temperature deformation of ferritic steel weldments, and their relative significance to the total strain accumulation in the fine grained HAZ is quantified. For the non-standard pre-welding tempering condition, Coble creep and grain boundary sliding provide equally 45% of the creep strain in the fine grained HAZ, with the dislocation creep providing the reminder 10%. For the standard pre-welding tempering condition, grain boundary sliding acting as the dominant deformation mechanism provides approximately 65% of the creep strain in the FGHAZ, dislocation creep and Coble creep provides remaining 20% and 15%,

respectively. The effects of weldment heterogeneities, including the large grain size gradients in the microstructure and the variation of material hardness, on high temperature creep deformation are numerically studied. The computational simulations provide valuable insights of the micromechanical and microstructural origins for the strain localization in fine-grained HAZ of CSEF steel weldments.

4 TYPE-IV FAILURE IN WELDMENTS OF CREEP-RESISTANT FERRITIC ALLOY: INTERGRANULAR CREEP FRACTURE

4.1 Introduction

Creep and creep damage behaviors are the most important considerations for design of structural components operating at high temperatures. In particular, Type IV crack always leads to premature failure and limits the lifetime of CSEF steel welded joints during high temperature service exposure. It is essential to develop fundamental understanding of the microstructure and physical mechanisms responsible for Type IV failure. So far, there have been extensive finite element based numerical methods proposed to investigate the Type IV creep fracture behavior of weldments of CSEF steels. The existing models can be generally classified into three main categories. Firstly, finite element models with emphasis on the creep deformation of the welded joints of CSEF steels have been developed in absence of creep damage analysis [4, 6, 7, 13, 36, 37]. These studies can be used to predict the crack initiation prediction based on the strain accumulation and stress multiaxiality distribution, whereas most of them are not capable of elucidating and simulating the creep damage processes. Secondly, at the macroscopic level, the classic fracture mechanics based finite element models have been developed to simulate the creep crack growth behavior. For creep materials at high temperatures, the crack tip stress and strain rate fields are usually characterized by the parameter C^* , which is the path independent integral of the energy release rate. The general idea is to identify the appropriate load parameter C^* , so that the measured crack growth rates can be transferred from the laboratory to the

component in service. Yatomu and Tabuchi [67] proposed a combined creep fracture mechanics and node-release damage model to investigate the creep damage behavior of P92 steel weldments, in which the creep crack growth behavior is discussed with the C^* via Nikbin, Smith and Webster (NSW) [68] and modified NSW model [69]. Similar uncoupled damage model with creep fracture mechanics model was also presented to analyze the creep crack growth behavior of P92 welded joints by Zhao et al. [70]. In above mentioned studies, the stress and strain fields near the crack tip are independent of creep damage, that is, the creep rate cannot be accelerated by the damage evolution, which is not the fact in the real condition. Thirdly, continuum damage models, incorporating cavitation or damage by means of micromechanism-based or phenomenological internal variables, have also been utilized for modeling the creep damage of ferritic steel welded joints. By including hardening effect and intergranular damage to creep rate models, the continuum damage models have been developed for simulating the creep deformation evolution and analyzing the rupture lifetime of creep resistant steel weldments [40, 43, 44]. Hyde et al. [71] employed an coupled creep/damage model for investigating the creep crack growth behavior in P91 steel weld, with crack growth tracked by the evolution of the damage parameter. Zhao et al. [66] simulated the crack growth behavior of different sub-regions in P92 steel welded joint by employing a modified Karchanov-Rabotnov continuum damage model, in which the creep crack growth rate is correlated with steady state creep integral parameter C^* . The above damage models have been successfully employed to study the damage development and crack growth for CSEF steel weldments, nevertheless, they cannot address the actual failure mechanisms and the discreteness of fracture near the crack

tips, such as cavity nucleation, growth and coalescence, which are responsible for the creep fracture. From a material design point of view, it is important to know how the physical mechanisms and their interactions affect the creep fracture behavior. Moreover, considering the fact, service life of creep resistant steel weldments depends more on the early stage damage such as cavity nucleation and growth rather than on the crack growth at the later stage [72, 73]. It is essential to understand the micromechanics for creep cavitation so as to study the Type IV failure and provide reliable remaining life prediction for the CSEF steel welded joints.

At high temperature and relatively low stresses, the creep life of CSEF steel welded joints is usually limited by the Type IV failure, which belongs to intergranular creep fracture. This kind of creep fracture in polycrystalline materials starts with nucleation of creep cavities on grain boundaries. The cavity growth is contributed by the typical high temperature mechanisms, such as diffusion and dislocation creep, until they coalesce and form microcracks along grain facets. The final intergranular fracture occurs by linking up the facet microcracks with the main crack. In the current study, the creep cavitation and damage development for the CSEF steel welded joints will be investigated by using a micromechanical creep fracture model. A pioneer work was proposed by Hull and Rimmer [74] concerning the growth of one single cavity by grain boundary diffusion. Then the modeling of cavity growth was modified by Needleman and Rice [75], in which the contribution of the creep deformation to the cavity growth was incorporated and its coupling with grain boundary diffusion was studied. The grain boundary cavity nucleation law and a smeared-out representation of discrete cavity distribution on grain boundaries

was proposed [76, 77]. Onck and van der Giessen complied the cavity growth model with the cavity nucleation law and performed a series of simulations for analyzing the intergranular creep fracture behavior of polycrystalline aggregates [78-83].

4.2 Digital microstructure

In the past two decades, numerous researches have been carried out to investigate the main causes for the Type IV crack. Although the mechanisms are not fully understood, many of these reports the sharp microstructure and creep property gradients, due to the welding thermal cycles, promote the Type IV failure in welded joints (e.g., [4, 6, 9, 10]). To consider the microstructure heterogeneities of ferritic steel weldments, we construct a two-dimensional digital microstructure by using Voronoi tessellation method in an open source software NEPER [26]. The Voronoi tessellation method was implemented to obtain a more realistic microstructure by manipulating the location of the Voronoi seeds. The generated digital microstructure agrees well with experimental sample in its topological and structural properties. As a result of the welding thermal cycle, the microstructure of base metal is altered and the heat-affected zone with microstructure gradients is formed. As shown in Fig. 4.1, the microstructure shows strong grain size gradients in weld metal (WM), coarse grain heat-affected zone (CGHAZ), fine grain heat-affected zone (FGHAZ), intercritical heat-affected zone (ICHAZ) and the base metal (BM). As both ICHAZ and FGHAZ essentially have fine-grained microstructures after post weld heat treatment, in the present study they are referred as FGHAZ without differentiation. The two-dimensional microstructure contains 750 grains, with random crystallographic orientations in each

individual grain. Note the colors in Fig. 4.1 only represent the boundaries of each grain with no specific meaning of grain orientations. As we concern the creep behavior of ferritic steel weldments under low applied stresses and high temperatures, our focused region is the fine-grained HAZ where Type IV failure takes place during the long-term applications [3, 4, 8, 9, 14, 27]. In the present study, the average grain sizes of FGHAZ and the other regions (BM, CGHAZ and WM) are assumed to be $1\mu\text{m}$ and $5\mu\text{m}$, respectively. Taking advantage of the digital microstructure, we are capable of considering the influences of heterogeneous material properties at the scale of individual grains, e.g., orientation and shape of all grains, and heterogeneous grain boundary diffusivity, etc. The digital microstructure generally captures the main characterized features of ferritic steel weldments. Our current work is among the first to explicitly model weldment microstructure and grain size distribution, which play a significant role in the overall and local deformation of weldments.

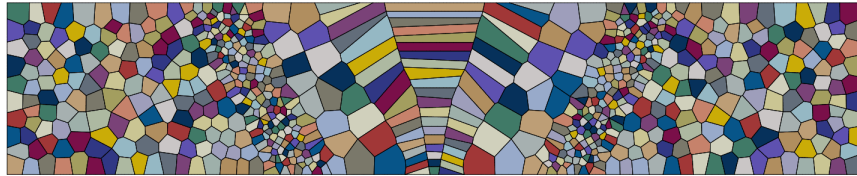


Figure 4.1 Two-dimensional digital microstructure model for ferritic steel weldment with grain size gradients.

4.3 Constitutive model

The failure mechanism of Type IV cracking is governed by creep cavitation at high temperatures. According to the fracture mechanism map [35], a material typically exhibits three types of fracture modes in the creep regime: intergranular creep fracture, transgranular creep fracture and rupture. Rupture only takes place at extremely high temperatures. For structural material used around 50% of their melting temperature, the transgranular and intergranular creep fracture due to cavity coalescence are important mechanisms under such creep conditions. The former appears at high stress (short term creep fracture) and the latter dominates at lower stress (long term creep fracture). Type IV failure, as a long-term creep fracture, happening at high temperature and low stress conditions, belongs to the intergranular creep fracture. Microstructure examinations also confirmed Type IV failure occur at grain boundaries, with the preferential nucleation sites for creep voids being the grain boundary particles associated with inclusions or second phase particles [4, 6, 9, 10, 84, 85]. Therefore, we employ the following micromechanics-based intergranular creep fracture model [76, 79, 86, 87] to simulate the Type IV cracking, and to investigate the microstructure origin, deformation and damage mechanisms responsible for the Type IV failure. The constitutive description includes physics at all relevant length scales, i.e., grain boundary cavity nucleation and growth, viscous grain boundary sliding, microcracking by the coalescence of cavities, and microcracks link up to form macroscopic cracks finally leading to premature failure. A user-defined element (UEL) subroutine and a user-defined material properties (UMAT) subroutine are utilized to implement the rate-dependent cohesive behavior of the grain boundary and the creep

deformation of the grain interior, respectively. The constitutive equations of the micromechanics model are summarized as follows.

4.3.1 Grain interior: creep model

The material inside the grains is assumed to be deformed by dislocation (power-law) creep in addition to the elastic deformation, and the total strain rate is the sum of elastic and creep strain rate,

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^e + \dot{\varepsilon}_{ij}^p. \quad (4.3.1)$$

These two components can be obtained from

$$\dot{\varepsilon}_{ij}^e = \frac{1+\nu}{E} \left(\dot{\sigma}_{ij} - \frac{\nu}{1+\nu} \dot{\sigma}_{kk} \delta_{ij} \right), \quad (4.3.2)$$

$$\dot{\varepsilon}_{ij}^p = \dot{\varepsilon}_0 \left(\frac{\sigma_e}{\sigma_0} \right)^n \frac{3S_{ij}}{2\sigma_e}, \quad (4.3.3)$$

where E and ν are Young's modulus and Poisson's ratio, respectively, δ_{ij} is the Kronecker delta, $\dot{\varepsilon}_0$ and σ_0 are the reference strain rate and stress, $\sigma_e = \sqrt{3S_{ij}S_{ij}/2}$ is the von Mises stress, S_{ij} is the deviatoric stress, and n is the stress exponent.

The micromechanical Taylor factor [56] is introduced to represent the slip anisotropy induced by crystallographic orientation of each individual grain. It is defined as the ratio between the local accumulated shear $\sum \gamma^{\text{local}}$ and the local von Mises strain $\langle \varepsilon_{\text{VM}}^{\text{local}} \rangle$,

$$M = \frac{\sum \gamma^{\text{local}}}{\langle \varepsilon_{\text{VM}}^{\text{local}} \rangle}, \quad (4.3.4)$$

where $\sum \gamma^{\text{local}}$ and $\langle \varepsilon_{\text{VM}}^{\text{local}} \rangle$ are numerically calculated by using a modified crystal plasticity model [57]. The results for the Taylor factors are presented in Fig 4.2. High values of the Taylor factor indicate the grain with certain crystallographic orientation is kinematically soft, where the crystal slips are preferable to occur. During deformation, dislocation creep strain percolation follows grains which are kinematically soft and avoids grains those are hard. To incorporate the grain orientation effects into creep deformation, we modify the creep rate as follows,

$$\varepsilon_{ij}^p = \varepsilon_0 \left(\frac{\sigma_e}{\sigma_0} \right)^n \frac{3S_{ij}}{2\sigma_e} \cdot \bar{M}^I, \quad (4.3.5)$$

where $\bar{M}^I$ is the normalized micromechanical Taylor factor for the I_{th} grain, $\bar{M}^I = M^I / \max(M^1, M^2, \dots, M^I, \dots, M^{N_g})$, and N_g is the total number of grains within the polycrystalline model. The numerical procedure of the grain interior creep constitutive model is implemented in the commercial finite-element software ABAQUS [39] via a user-defined material model (UMAT).

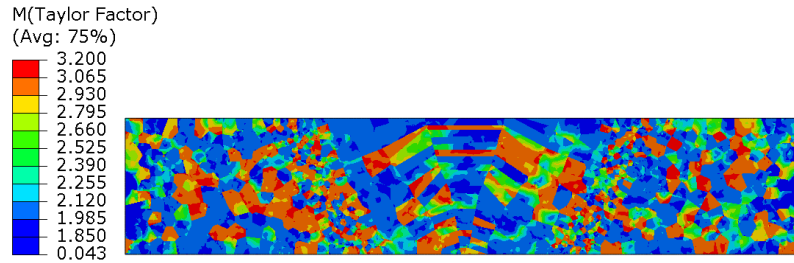


Figure 4.2 Contour plot of micromechanical Taylor factor for ferritic steel weldment to represent the crystallographic orientation of each individual grain (each grain assigned with random orientations).

4.3.2 Grain boundary cavitation

The creep cavitation process at grain boundaries involves the nucleation, growth and coalescence of cavities. The cavities on a grain boundary are characterized by the spherical-caps shape with radius a , half-spacing b , and cavity tip angle ψ , as shown in Fig. 4.3(a). During cavity growth the cavity tip angle ψ keeps a constant value of about 75° [78]. The cavity volume V is computed as

$$V = \frac{4}{3}\pi a^3 h(\psi), \quad (4.3.6)$$

where h is the spherical-caps shape parameter,

$$h(\psi) = \frac{[(1 + \cos \psi)^{-1} - 1/2 \cos \psi]}{\sin \psi}. \quad (4.3.7)$$

It is difficult to explicitly model each individual cavity on grain boundaries, and therefore a smeared-out representation of grain boundary cavities [88] is introduced to simplify the problem, in which the discrete distribution of cavities on each grain boundary is replaced by a continuous varying separation $u_n = V/(\pi b^2)$, as shown in Fig. 4.3(b). The rate of normal separation varies continuously,

$$\dot{u}_n = \frac{\dot{V}}{\pi b^2} - \frac{2V\dot{b}}{\pi b^3}, \quad (4.3.8)$$

which is determined by the volumetric growth rate $\dot{V}$, and the rate of change of the cavity spacing $\dot{b}$.

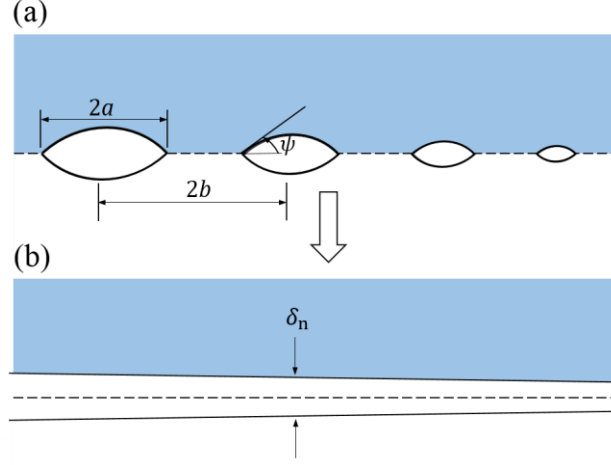


Figure 4.3 Schematic drawing (a) the geometry of cavities in the spherical-caps shape located at the grain boundary and (b) the smeared-out representation of grain boundary cavitation in terms of a continuous varying normal separation.

4.3.3 Cavity nucleation

The nucleation of cavities during high temperature exposure is a complex process that takes place at the very small length scales. Experiment observations show that density of cavities increases in proportion to the creep strain and it depends highly on the grain boundary microstructure, such as the distribution of second-phase particles or segregation impurities [4, 6, 9, 10]. Due to the complexity of the nucleation process and lack of detailed experimental measurements, the physical description of cavity nucleation is not readily available. In the present work, a phenomenological model proposed by Tvergaard [76] is adopted, in which the cavity nucleation rate is a function of the effective creep rate $\dot{\epsilon}_e^c$ and normal stress σ_n near the grain boundary,

$$\dot{N} = F_n \left(\frac{\sigma_n}{\Sigma_0} \right)^2 \dot{\epsilon}_e^c \quad \text{for } \sigma_n > 0, \quad (4.3.9)$$

where Σ_0 is a reference stress, F_n is the material parameter that incorporates the microstructural features that influence cavity nucleation rate at a grain boundary, and $\dot{\epsilon}_e^c = \dot{\epsilon}_0(\sigma_e/\sigma_0)^n$. It has been shown from experiments that nucleation of cavities on some grain boundaries only occurs in the late stage of creep life [58], i.e., there exists a threshold before the cavity nucleation takes place. To account for the threshold, a parameter that combines the stress and strain accumulation has been proposed [87],

$$S = \left(\frac{\sigma_n}{\Sigma_0}\right)^2 \epsilon_e^c \text{ for } \sigma_n > 0. \quad (4.3.10)$$

The cavity nucleation can be triggered only when the parameter S reaches a threshold value S_{thr} , which is defined in terms of the initial cavity density N_i as

$$S_{\text{thr}} = \frac{N_i}{F_n}. \quad (4.3.11)$$

With continuous cavity nucleation on grain boundaries, the cavity spacing decreases and the changing rate is determined by

$$\frac{\dot{b}}{b} = \frac{1}{2}(\dot{\epsilon}_I + \dot{\epsilon}_{II}) - \frac{1}{2} \frac{\dot{N}}{N}, \quad (4.3.12)$$

where $\dot{\epsilon}_I$ and $\dot{\epsilon}_{II}$ are in-plane principle logarithmic strain rate at the grain boundary and N is the cavity density, which is defined as the number of cavities per unit undeformed grain boundary.

4.3.4 Cavity growth

The cavities grow by both the diffusion of atoms from their surface into the grain boundary layer and also the creep deformation of the surrounding grains. The cavity growth relations in the present work are based on the pioneering work of Needleman and Rice [75]. The volumetric cavity growth rate $\dot{V}$ can be expressed as

$$\dot{V} = \dot{V}_1 + \dot{V}_2, \quad (4.3.13)$$

where $\dot{V}_1$ is the contribution of grain boundary diffusion, given by

$$\dot{V}_1 = 4\pi D \frac{\sigma_n - (1-f)\sigma_s}{\ln(1/f) - \frac{1}{2}(3-f)(1-f)}, \quad (4.3.14)$$

and $\dot{V}_2$ represents the cavity growth induced by creep deformation,

$$\dot{V}_2 = \begin{cases} \pm 2\pi \dot{\epsilon}_e^c a^3 h(\psi) \left[\alpha_n \left| \frac{\sigma_m}{\sigma_e} \right| + \beta_n \right]^n, & \text{for } \pm \frac{\sigma_m}{\sigma_e} > 1 \\ 2\pi \dot{\epsilon}_e^c a^3 h(\psi) [\alpha_n + \beta_n]^n \frac{\sigma_m}{\sigma_e}, & \text{for } \left| \frac{\sigma_m}{\sigma_e} \right| < 1 \end{cases}, \quad (4.3.15)$$

where σ_s is the sintering stress, which is usually small and can be neglected, $\alpha_n = 3/(2n)$, and $\beta_n = (n-1)(n+0.4319)/n^2$. In Eq. (4.3.14), f is the effective cavity volume fraction given by

$$f = \max \left[\left(\frac{a}{b} \right)^2, \left(\frac{a}{a+1.5L} \right)^2 \right], \quad (4.3.16)$$

where L dictates the coupling of diffusion and creep deformation to the cavity growth and it is described through a stress and temperature dependent length scale

$$L = \left[D \frac{\sigma_e}{\dot{\epsilon}_e^c} \right]^{1/3}, \quad (4.3.17)$$

D is the grain boundary diffusion parameter and defined by

$$D = \frac{D_{b0} \delta_b \Omega}{kT} \exp \left(-\frac{Q_b}{RT} \right), \quad (4.3.18)$$

where $D_{b0} \delta_b$ is the diffusion coefficient of grain boundary, Ω is the atom volume, Q_b is the activation energy of grain boundary diffusion, T is absolute temperature, k is Boltzmann constant, and R is gas constant.

The cavity growth rate can be calculated from the cavity volume change

$$\dot{a} = \dot{V} / (4\pi a^2 h(\psi)). \quad (4.3.19)$$

4.3.5 Grain boundary sliding

Grain boundary sliding (GBS) is one of the competing mechanisms that contribute to the creep deformation and damage of ferritic steel weldments [1, 47]. GBS is driven by shear tractions acting tangentially to the grain boundary. In the present analysis, grain boundary sliding is assumed to be a thermally activated process and governed by Newtonian viscous flow,

$$\dot{u}_t = \frac{\Omega \eta_0 \exp(-Q_{\text{gbs}}/RT)}{kT} \tau \quad (4.3.20)$$

where η_0 is a characteristic sliding velocity, Q_{gbs} is the activation energy for grain boundary sliding, and $\dot{u}_t$ is the relative sliding velocity of adjacent grains due to the shear stress τ .

4.4 Numerical simulation

4.4.1 Finite element implementation

The interface mechanical behavior is usually described by the cohesive laws that relates the normal and tangential tractions with the corresponding displacements. There are a variety of methods for implementing the cohesive laws in ABAQUS, and the development of cohesive element is the most versatile one. In the present work, a rate-dependent cohesive element is developed to simulate the grain boundary cavitation and GBS by implementing a user-defined element subroutine (UEL) in ABAQUS [58]. The derivation of the tangent stiffness matrix for the cohesive element is described below.

In the tangential direction, the relationship between the shear stress and tangential displacement obeys the Newtonian viscous flow, as presented in Eq. (4.3.20). The partial derivative of the incremental shear stress with respect to the incremental tangential displacement is

$$\frac{\partial \Delta \tau}{\partial \Delta u_t} = \frac{kT}{\Omega \eta_0 \exp(-Q_{\text{gbs}}/RT)} \frac{1}{\Delta t} \quad (4.4.1)$$

where Δt is the time increment.

In the normal direction, the traction vs. separation relation is governed by the constitutive laws of creep cavitation, including cavity nucleation, growth and their coalescence on grain boundaries. Substituting Eq. (4.3.9), (4.3.12), (4.3.14), (4.3.15) into Eq. (4.3.8) yields the normal separation rate as a function of the normal traction,

$$\dot{u}_n = A\sigma_n^2 + B\sigma_n + C, \quad (4.4.2)$$

where

$$A = \frac{V}{\pi b^2} \frac{1}{N} \frac{F_n}{\Sigma_0^2} \dot{\epsilon}_e^c, \quad (4.4.3a)$$

$$B = \frac{1}{\pi b^2} \frac{4\pi D}{\ln(1/f) - \frac{1}{2}(3-f)(1-f)}, \quad (4.4.3b)$$

$$C = \frac{\dot{V}_2}{\pi b^2} - \frac{V}{\pi b^2} (\dot{\epsilon}_I + \dot{\epsilon}_{II}). \quad (4.4.3c)$$

The three terms on the right side of Eq. (3.4.2) represent contributions of cavity nucleation, grain boundary diffusion and the creep deformation to the total normal separation of the grain boundary.

Taking the partial derivative of the incremental stress with respect to the incremental displacement yields the material Jacobian matrix

$$\begin{Bmatrix} \Delta\sigma_n \\ \Delta\tau \end{Bmatrix} = \begin{bmatrix} \frac{1}{(2A\sigma_n + B)\Delta t} & 0 \\ 0 & \frac{kT}{\Omega\eta_0 \exp(-Q_{\text{gbs}}/RT)\Delta t} \end{bmatrix} \begin{Bmatrix} \Delta u_n \\ \Delta u_s \end{Bmatrix} \quad (4.4.4)$$

In order to calculate the creep fracture behavior, the numerical analysis requires the knowledge of stress and strain at the Gaussian integration points of cohesive elements, but also those of the grains adjacent to the grain boundaries. Therefore, the COMMON BLOCK technique is introduced for data storage and acquiring between UMAT and UEL subroutines, i.e., the information of stress and strain is stored when the UMAT is called for computing the grain interior deformation, and it will be acquired by UEL for calculating the traction-separation behavior of grain boundaries.

4.4.2 Material parameters

The material parameters for grain interior creep deformation are adopted from our Part I work (Chapter 3). The reference stress, stress exponent, reference strain rate are given by $\sigma_0 = 0.001E$, where E is the Young's modulus at 923K [7], $n = 8$ and $\dot{\epsilon}_0 = 2.975 \times 10^{-8} \text{ s}^{-1}$, respectively. For the grain boundary elements, the values of materials properties are listed in Table 4.1. Among these parameters, the reference stress Σ_0 in the nucleation law is taken as that suggested by Onck et al [87], the grain boundary viscosity η_0 , atomic volume Ω and the activation energy of grain boundary diffusion Q_{gbs} are taken from literature [26, 51]. The only unknowns, grain boundary diffusion parameter $D_{\text{bo}}\delta_{\text{b}}$ and cavity nucleation parameter F_{n} , will be determined by fitting the simulation results with the experimental creep life for Grade 91 steel and its weldments [8, 65, 89]. The initial cavity density and radius are $N_I = 40N_R$ and $a_I = 6.7 \times 10^{-4} R_0$, where R_0 is the half facet length and $N_R = 1/\pi R_0^2$, respectively. The cavity half spacing is related with the initial cavity density as $b_I = 1/\sqrt{\pi N_I} R_0 = 0.16R_0$. The sintering stress σ_s is usually relatively

small and can be neglected. The two crucial parameters that govern the cavity nucleation F_n and diffusive growth D ($D_{b0}\delta_b$), are specified by dimensionless parameters F_n / N_R and L/R_0 , respectively, with L defined as $L = (D\sigma_e/\dot{\epsilon}_e^c)^{1/3}$. As explained by Needleman and Rice [75], a relatively large value of L/R_0 implies the cavity growth is controlled by diffusion and constrained by the creep deformation of surrounding grains, whereas a small value of L/R_0 implies the contribution of creep deformation to the cavity growth becomes more important.

4.5 Results and discussion

The process of Type IV failure involves the cavity nucleation on grain boundaries, their growth, microcracking by coalescence, and the propagation of microcracks to the formation of macrocrack, which leads to the final intergranular creep fracture in the HAZ of welded joints. Previous experimental investigations [72, 73] have shown the cavity nucleation and growth continue up to the late stage of creep life, once the microcracks initiate and link up to form macrocracks, the welded joints will break up in a very short time. Therefore, it is crucial to understand the evolution of creep cavitation so as to provide reliable remaining life prediction for the CSEF steel welded joints.

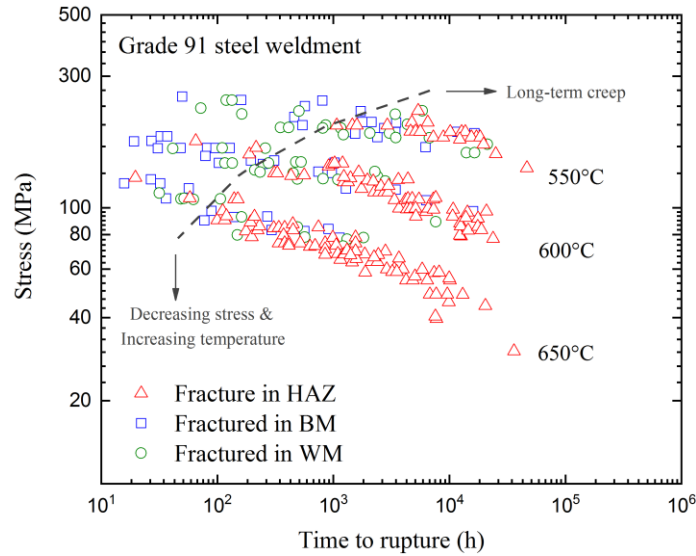


Figure 4.4 Double logarithmic plot of applied stress vs. time to rupture in terms of fracture locations (HAZ, BM and WM) for Grade 91 steel weldments [6, 8, 49, 65, 89].

4.5.1 Cavity evolution and creep life assessment

The micromechanics-based model will be applied to investigate the creep cavity evolution for Type IV failure, and to establish the correlation between the creep cavitation and rupture life of Grade 91 steel welded joints. Fig. 4.4 summarized the collected creep rupture data based on the fracture locations for the welded joints of Grade 91 steel [89]. It is observed the welds are mainly fractured in the base metal or weld metal at lower temperatures and higher stresses, while the fracture location shifts to the HAZ with increasing temperature or decreasing stress. In particular, for longer term creep, e.g., with rupture life more than 200 hrs at 650 °C, 900 hrs at 600 °C and 5000 hrs 550 °C, the Grade 91 steel welded joints are mainly fractured in HAZ, which is the well known Type IV failure. The slope of stress vs. rupture time curve is expected to change when the fracture location shifts from base metal or weld metal to the heat-affected zone, because the fracture

mechanism transfers from transgranular creep fracture to intergranular creep fracture with decreased stress or increased temperature. Nevertheless, the change of slope is not distinct in Fig. 4.4, which is due to the large data scatter and lack of long-term rupture data (with life more than 10^4 hrs) for Grade 91 steel welded joints. Such scatter band in the creep rupture data for the heat resistant steel and its welded joints were commonly reported in the literature [65, 90], which can be caused by the difference in the heat treatment conditions, material compositions and welding procedures, etc. For instance, Yu et al. [8] performed creep rupture tests for two types of Grade 91 steel welded joints at 650 °C and 70MPa, with one pre-weld tempered at 760 °C for 2 hrs and (denoted as standard condition) and the other at 650 °C for 2 hrs (nonstandard condition), and inspiringly they measured the lifetime was prolonged from 518 hrs to 2414 hrs when reducing the pre-weld tempering temperature from 760 °C to 650 °C. Both of the welded joints were fractured in the FGHAZ, and their creep rupture data are shown with the star point in Fig. 4.4, which are located at the lower (standard condition) and upper bounds (nonstandard condition) of the scatter band.

The creep rupture data which are fractured in the HAZ together with those for base material of Grade 91 steel are presented [65, 91], as shown in Fig. 4.5, for calibrating the material parameters (F_n and $D_{b0}\delta_b$) for both the fine grained HAZ and base metal used in the computational modeling. The numerical results for creep rupture life show quantitative agreement with the experimental data [8, 65, 89, 91]. The black dash and solid lines represent the simulated lower and upper bounds for the rupture life of welded joints, and the grey solid line is the simulated average value of the creep rupture life for the base metal

of Grade 91 steel, respectively. The unknown parameters for the computational model are calibrated as $(F_n/N_R)^{L-HAZ} = 5.027 \times 10^4$, $(F_n/N_R)^{H-HAZ} = 1.2174 \times 10^4$, $(L/R_0)^{L-HAZ} = 0.346$, $(L/R_0)^{H-HAZ} = 0.514$ for the fine-grained HAZ, where L-HAZ and H-HAZ are corresponding to the lower and upper bound, and $(F_n/N_R)^{BM} = 9.4248 \times 10^3$, $(L/R_0)^{BM} = 0.058$ for the base metal at 650°C, where the diffusion parameter $D_{b0}\delta_b$ is specified through the normalized length L/R_0 . The dimensionless length L/R_0 (the diffusion parameter $D_{b0}\delta_b$) is determined by the long-term creep rupture life ($> 10^4$ hrs) since atom diffusion dominates the creep cavitation at low applied stresses, while the cavity nucleation parameter F_n/N_R is calibrated with rupture data of relative shorter creep life

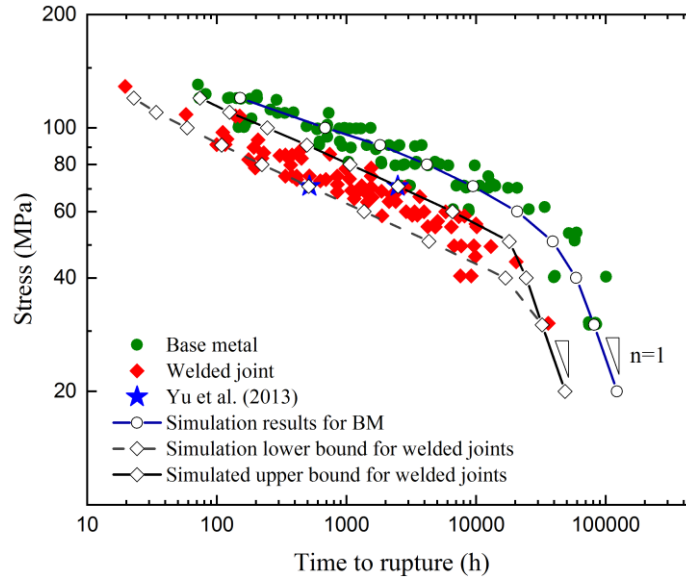


Figure 4.5 Stress vs. creep life behavior predicted by using the micromechanical model for both the base metal and welded joints of Grade 91 steel in comparison with the literature experimental data [6, 8, 65, 89, 91] at 650°C.

where the activity of cavity nucleation is prominent. It is observed that the reduction of creep rupture time accelerates in the long-term creep region ($> 10^4$ hrs) for both the base metal and welded joints, which is represented by a steeper slope in the stress vs. rupture life curve. Note that the mechanism origin of slope change at long-term creep is different from the one mentioned above that the failure mechanism transfers from transgranular creep fracture (fractured in weld and base metal at high applied stresses) to intergranular creep fracture (fractured in HAZ at lower applied stresses). Generally, this sharp slope transition indicates the micromechanics change of creep cavitation for intergranular creep fracture, i.e., the competition of diffusion and creep deformation to the cavity growth, and the activity of cavity nucleation and cavity growth. For the long-term creep region (rupture life $> 10^4$ hrs), it is observed the slope of $\log(\sigma)$ - $\log(t_r)$ equals to -1, which implies the rupture time is inversely proportional to the diffusional creep rate ($\dot{\epsilon} \propto \sigma$). This is consistent with the conclusion of the Hull and Rimmer model [74] that assumes the grains are effectively rigid and the creep cavitation is controlled by surface and grain boundary diffusion. Under low applied stresses, creep fracture is only controlled by atom diffusion induced cavity growth, where is no cavity nucleation and the contribution of creep deformation to the cavity growth can be neglected. The details of creep cavitation processes will be discussed in the following. Consequently, simple extrapolation based on short-term creep rupture data can seriously overestimate long-term creep life, which necessitates the micromechanical model capable of predicting rupture time for long-term creep regime.

Table 4.1 Material parameters for grain boundaries.

Parameter	Value
Atomic volume, Ω	$1.18 \times 10^{-29} \text{m}^3$
Melting temperature, T_M	1810K
Burgers vector, b	$2.48 \times 10^{-10} \text{m}$
Young's modulus, E_0	223GPa
Young's modulus at 923K, E	90.1GPa
Poisson's ratio, ν	0.3
Grain boundary diffusion pre-exponent for BM, $(D_{\text{gb}}\delta)_{\text{BM}}$	$5.317 \times 10^{-20} \text{m}^3/\text{s}$
Grain boundary diffusion pre-exponent for HAZ, $(D_{\text{gb}}\delta)_{\text{HAZ}}$	$1.139 \times 10^{-19} \text{m}^3/\text{s}$
Cavity nucleation parameter $(F_n/N_R)^{\text{BM}}$	9.4248×10^3
Cavity nucleation parameter $(F_n/N_R)^{\text{H-HAZ}}$	1.2174×10^4
Cavity nucleation parameter $(F_n/N_R)^{\text{L-HAZ}}$	5.027×10^4
Grain boundary diffusion activation energy, Q_{gb}	174 KJ/mole
Dislocation creep coefficient, A_{dis}	1.1462×10^{-9}
Reference stress, Σ_0	90.1 MPa
Stress exponent, n	8
Grain boundary sliding pre-exponent, η_0	40 m/s
Average grain size in FGHAZ, d	1 μm
Average grain size in the other zones, d	5 μm

The creep cavitation could be examined by several micromechanical variables, such as the cavity radius a , cavity half-spacing b and the ratio of a/b . During creep exposure, the cavities grow by both atom diffusion and the creep deformation of neighboring grains, and in the meanwhile the cavity number increases with accumulated creep strain, which attests to the enlargement of the existing cavities and nucleation of new cavities [72, 73]. As the cavity itself could not support load, the size of isolated cavities keeps growing while the spacing between neighboring cavities decreases. Eventually, the adjacent cavities join together and form microcracks on grain boundaries. The damage state is quantified by the ratio between the cavity size and half-spacing, i.e. a/b . Experiment observations show that the coalescence may occur earlier by ductile tearing or the cleavage of the ligament between the cavities, and here we assume coalescence occur when $a/b = 0.9$. The cavity growth is denoted by increasing cavity radius a , while cavity nucleation is denoted by decreasing cavity half-spacing b . Fig. 4.6 and Fig. 4.7 show the variation of cavity size a , half spacing b and the ratio of a/b with creep life for the FGHAZ of both the standard (lower bound) and nonstandard condition (upper bound). It is observed that cavity growth and nucleation rate increases with the applied stress. As shown in Fig. 4.6(b) and Fig. 4.7(b), the cavity half-spacing b and its changing rate decrease with creep time, that is, cavities continuously nucleate and saturate on the grain boundaries, which is consistent with the experiment measurement of cavity nucleation in FGHAZ [72]. Moreover, the cavity half-spacing b starts to decrease earlier and reaches a smaller final value upon cracking under higher applied stresses, which indicates it is easier for cavity nucleation and there is larger density of cavities on grain boundaries when the welded joints are under

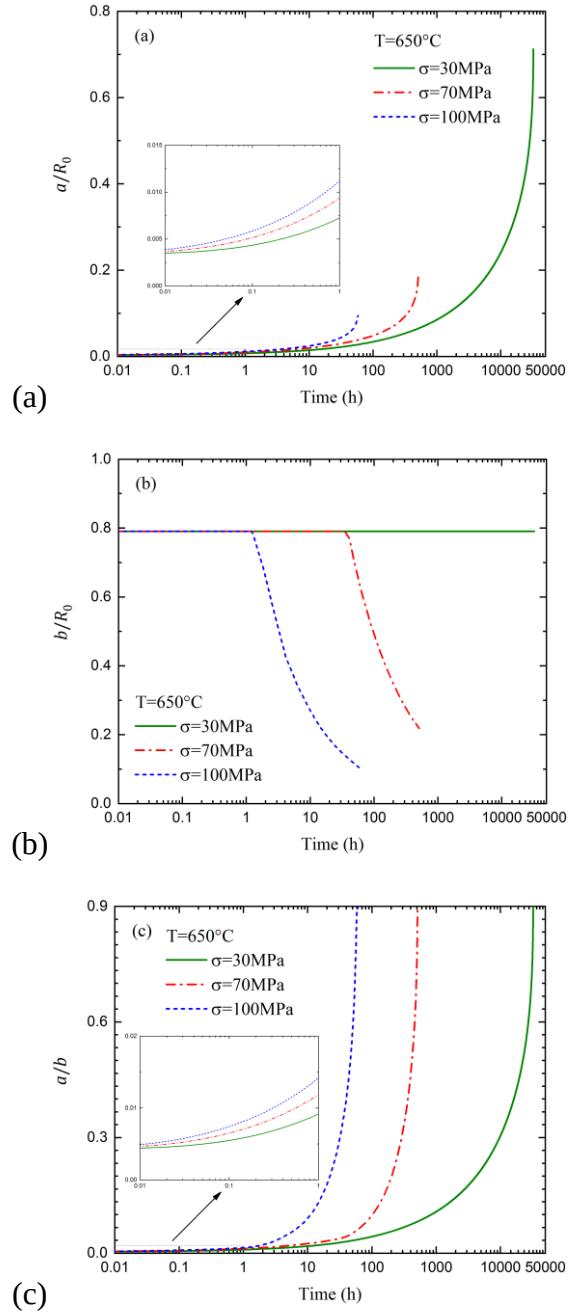


Figure 4.6 The creep cavitation examined by the evolution of micromechanical parameters of (a) cavity radius, (b) cavity half-spacing and (a) the damage ration a/b , in in terms of creep time for the standard condition.

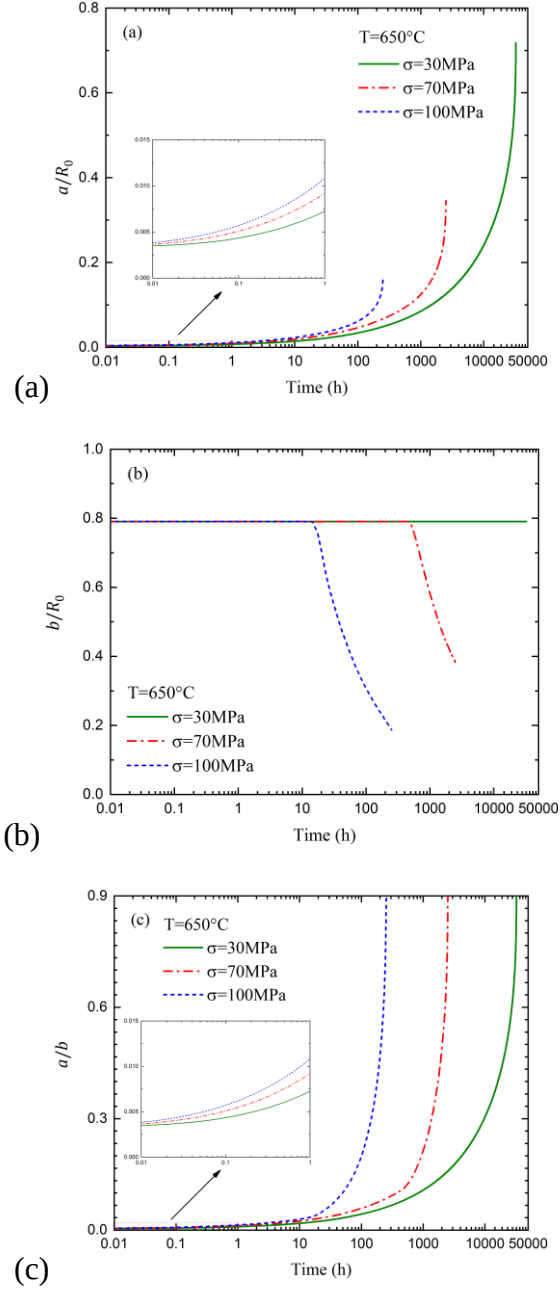


Figure 4.7 The creep cavitation examined by the evolution of micromechanical parameters of (a) cavity radius, (b) cavity half-spacing and (a) the damage ration a/b , in terms of creep time for the nonstandard condition.

higher applied stresses. Interestingly, the cavity half-spacing b keeps constant at low applied stresses ($< \sim 40\text{MPa}$), which indicates the stress is not high enough to trigger new cavity nucleation and only the growth of preexisting cavities leads to the microcracks and final failure on grain boundaries during long-term creep. In the present modeling we assume there is small and low density of preexisting cavities on each grain boundary, specified by $a_i = 6.7 \times 10^{-4} R_0$ and $b_i = 0.16 R_0$. The damage variable a/b as a function of creep life is plotted in Fig. 4.6(c) and Fig. 4.7(c) for the standard and nonstandard condition, respectively. It increases monotonically and reaches the damage value sooner for a higher applied stress, leading to shorter creep rupture life. Compared the creep cavitation of the standard condition (Fig. 4.6) with those of the nonstandard condition (Fig. 4.7), there is no significant difference in the growth of cavity size a , while the cavity half-spacing b decreases more rapidly in the standard condition as shown in Fig. 4.7(b), which is due to the higher cavity nucleation parameter in the FGHAZ of the standard condition, $(F_n/N_R)^{L-HAZ} = 5.027 \times 10^4$, $(F_n/N_R)^{H-HAZ} = 1.2174 \times 10^4$. This can be correlated with microstructure characteristics [8], especially the distribution of precipitated carbides on grain boundaries. In the standard pre-weld tempering condition, carbides in the FGHAZ region are only partially dissolved during the welding thermal cycle, and the large particles, such as $M_{23}C_6$ ($M = \text{Fe}, \text{Cr}$) favored on grain boundaries, coarsen more rapidly than those in the base metal or weld metal, which promotes creep cavity nucleation at grain boundaries. In the nonstandard condition, however, Yu et al. [8] showed the carbides $M_{23}C_6$ and MX in the nonstandard condition are completely dissolved into the matrix during welding thermal cycles, and after post-weld heat treatment, more uniformly

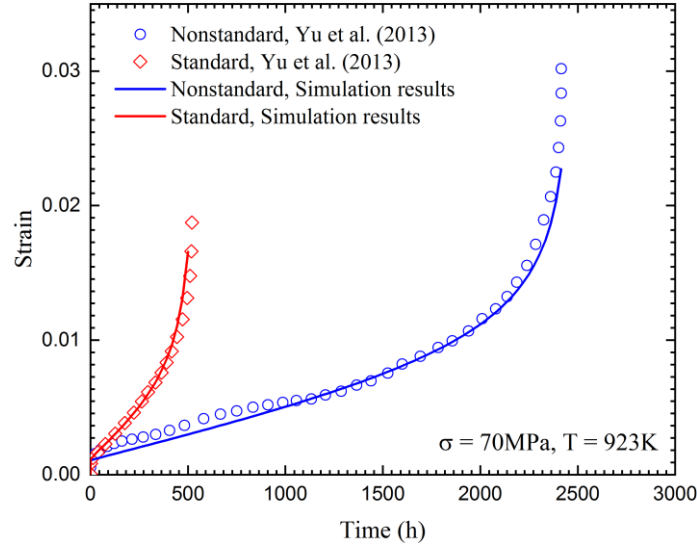


Figure 4.8 Comparison of simulated (lines) and experimental (symbols) [8] creep strain curves for welded joints of Grade 91 steel at 650°C and 70MPa.

distributed and finer $M_{23}C_6$ precipitated on the subgrain and grain boundaries, effectively stabilizes the grain boundary movements and postpones and inhibits the cavity nucleation during creep deformation. Our numerical simulations show consistent results with experimental measurements that the cavity nucleation is faster in the standard condition, and finally leads to the shortened creep rupture life. Fig. 4.8 shows the numerical results for creep curves in comparison with experiment measurements [8]. It is demonstrated that the micromechanics-based computational model processes the capability of modeling the creep strain evolution of welded joints, covering both the steady-state creep and the tertiary creep.

Base on the viewpoint of deformation mechanism, the separation of between adjacent grain boundaries can be categorized into diffusion-controlled and creep-controlled mechanism. The normal GB separation rate $\dot{u}_n$, as shown in Eq. (4.4.2), consists of three

terms. The second term is contributed by grain boundary diffusion, while both the first and third terms (i.e., cavity nucleation and creep) are controlled by the creep strain rate. Therefore, to determine whether the creep fracture is controlled by diffusion or creep, the components of the normal GB separation rate resulting from diffusion and creep deformation are examined during creep fracture process. Fig. 4.9 shows the variation of normal separation rate with creep life for applied stress of 40MPa, 70MPa and 100MPa. It is observed that the fracture process is controlled by diffusion for the three applied stresses, which results in the relative brittle fracture behavior of Type IV failure. Meanwhile, the contribution of creep deformation increases with increasing applied stress. The cavity growth results from both grain boundary diffusion and creep deformation of surrounding grains, where the competition of these two mechanisms to the cavity growth can be represented by the dimensionless parameter L/R_i . Fig.4.10 presents the contour plot of L/R_i as a function of normalized temperature T/T_M and applied stress σ/E , where T_M is the melting temperature. Under high temperature and low stress loading conditions, the value of L/R_i is large which implies cavity growth is dominated by diffusion, while under lower temperature and high applied stress, the value of L/R_i is low and the contribution of creep deformation to the cavity growth becomes more important. Though the numerical simulation may not represent the exact cavity evolution during creep exposure, it is consistent with the main features of experimental observations [72, 73]. In practical condition, the cavity nucleation and growth may also be related with kinetics of microstructural changes, e.g., coarsening of the precipitates of $M_{23}C_6$ and the formation of Z- and Laves- phase in the heat-affected zone after thousands hours of service.

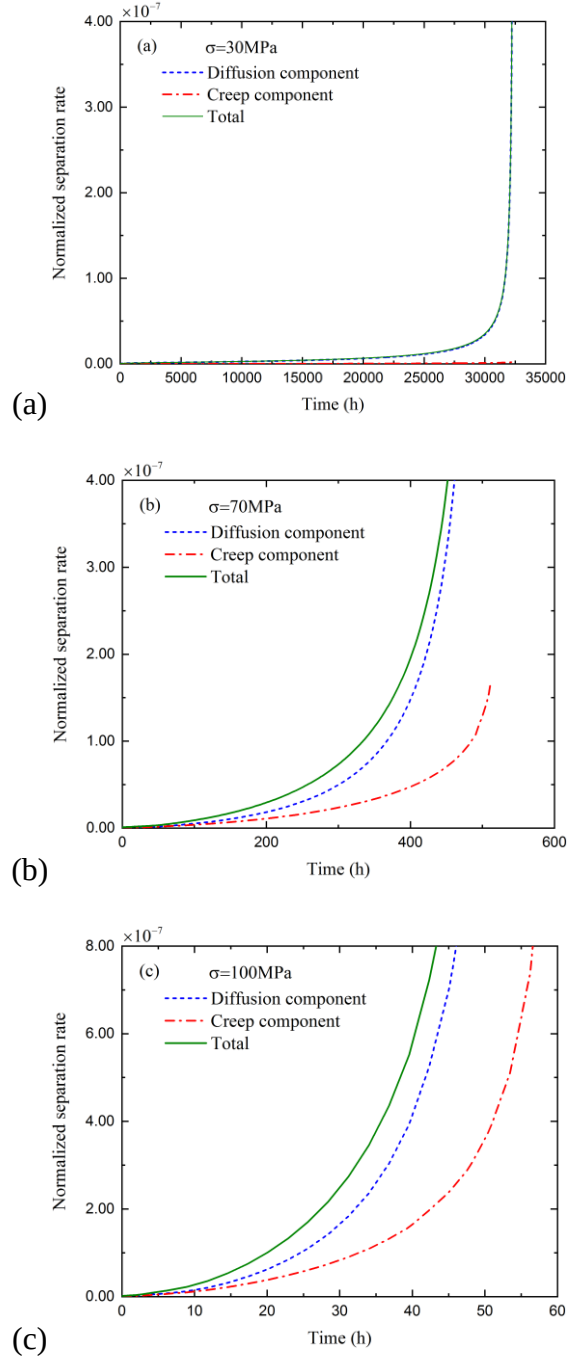


Figure 4.9 The normal separation rate during the creep fracture process for applied stress of (a) 30MPa, (b) 70MPa and 100MPa.

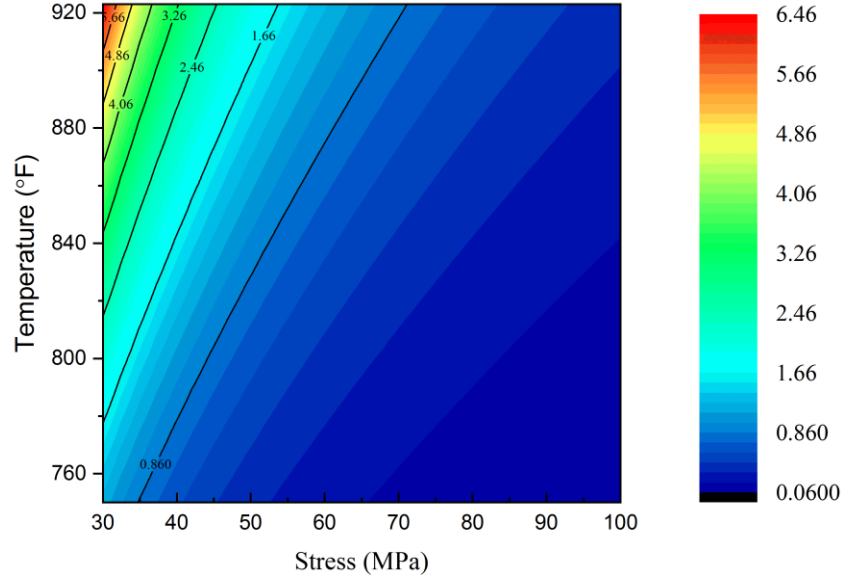


Figure 4.10 Contour plot of the parameter L , which represents the competition of GB diffusion and creep deformation to the cavity growth.

4.5.2 Type IV cracking

The Type IV failure, as shown in Fig 4.11, is successfully simulated by using the micromechanics model. By taking advantage of the microstructure model, we account for the material heterogeneities in the fine-grained HAZ. It should be noted that the deformation is enlarged by 10 times for the ease of visualization. Compared with the base metal and weld metal, the FGHAZ exhibits the most serious damage in the welded joints. This is generally believed to be related with the distribution of precipitated carbides in the FGHAZ. The coarse precipitates such as $M_{23}C_6$ and Laves phases aggregate at grain boundaries in FGHAZ, providing nucleation sites for creep voids. Therefore, $(F_n/N_R)^{HAZ} =$ and $(F_n/N_R)^{BM}$ is employed in the current simulation to represent the difference of cavity nucleation in BM and FGHAZ. In addition, the strength of the FGHAZ is 70% as that of the base material, as measured by the hardness show in Fig. 3.6. The

softened HAZ can result in fast dislocation creep, and it may induce earlier cavity nucleation and contribute more to the cavity growth. Meanwhile, the higher boundary to volume fraction in the FGHAZ also provides a stronger potential for creep cavities on grain boundaries or triple junctions in FGHAZ due to grain boundary sliding. It is observed that most of the small cracks are located on the grain boundaries that are close to the normal of the loading direction. Due to the stress transfer from the crack tip to its neighbor, the stress concentration is observed in the grains around the crack tip. This would promote cavitation and cracking of the neighboring grain boundaries. Finally, the microcracks on the grain boundaries link up and form the macrocrack, which results in the loss of load carrying capability in the fully cavitated grain boundaries.

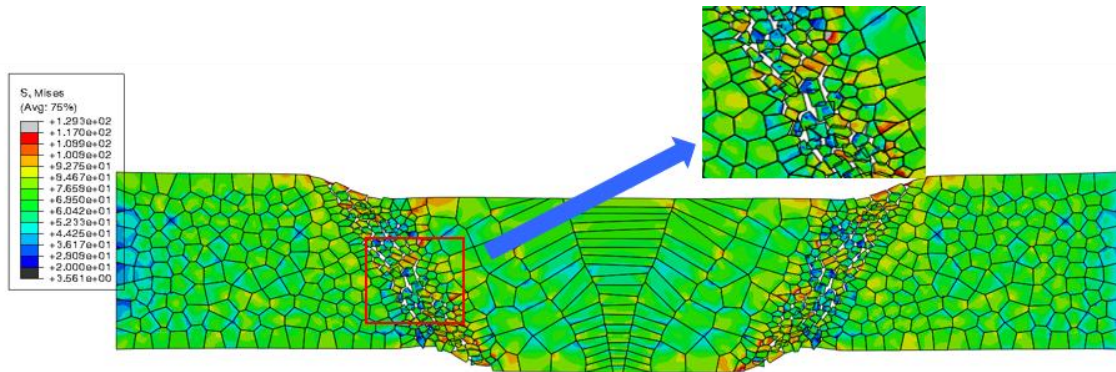


Figure 4.11 Simulation results for Type IV failure. There are extensive small cracks in the fine-grained HAZ.

Type IV cracking could be influenced by the microstructure evolution in the late stage of long-term creep exposure, such as the dynamic recovery, recrystallization, and coarsening of precipitates. In principle it is possible to extend our computations to incorporate the microstructure changes. Though it is difficult to account for general microstructure changes in sharp-interface models, sequentially coupled finite element model and Phase field methods provide feasible ways and efforts to do so are in progress.

4.6 Summary

Creep fracture process of Type IV failure involves cavity nucleation on grain boundaries, their growth, microcracking by coalescence, and the propagation of microcracks to the formation of macrocrack, which leads to the final intergranular creep fracture in the HAZ of welded joints. A microstructure-informed micromechanical model was applied to systematically study the creep cavitation and damage evolution of the Type IV failure. By taking advantage of the microstructure-based model, we can explicitly model the actual microstructure and examine the effects of grain scale material heterogeneities, including grain size and morphology, grain orientation and material heterogeneous properties of different zones, i.e., the base metal, heat-affected zone and weld metal. The numerical results illustrate the creep fracture is a cavity-growth controlled process at low applied stress, while increasing stress it is a coupled cavity-nucleation and cavity-growth process. From the fracture mechanism point of view, the creep fracture is governed by grain boundary diffusion in long-term creep crack with low stress and high temperature loading conditions, and the contribution of creep deformation becomes more important

with increased applied stress or decreased temperature. Moreover, the computational model provides quantitative lifetime prediction for CSEF steel weldments. To this end, this methodology can be used as a powerful tool to evaluate the very-long-term creep and damage behavior of many other alloys and their weldments at high temperatures.

5 INDENTATION SCHMID FACTOR AND INCIPIENT PLASTICITY BY NANOINDENTATION POP-IN TESTS IN HEXAGONAL CLOSE-PACKED SINGLE CRYSTALS

5.1 Introduction

The instrumented nanoindentation technique provides the measurements of indentation load, P , and indentation depth, h , with nanometer resolution [92, 93]. When using a spherical nanoindenter (or sharp indenters with blunt tips), the initial load-displacement response can be described by the elastic Hertzian solution

$$P = \frac{4}{3} E_r \sqrt{R h^3}, \quad (5.1.1)$$

where R is the tip radius, the reduced indentation modulus is $E_r = [(1 - \nu_s^2)/E_s + (1 - \nu_i^2)/E_i]^{-1}$ for elastically isotropic solids, E is the Young's modulus, ν is Poisson's ratio, and subscripts i and s denote indenter and substrate, respectively. The elastic limit is often characterized by a sudden displacement excursion (or called burst, pop-in), which corresponds to the homogeneous dislocation nucleation when the stress volume size is small (usually sub-micrometer) and the pre-existing defect density is low (e.g., fully annealed and then electrochemically polished samples). From the pop-in loads, the maximum shear stress from the isotropic Hertzian solution is found to be $1/30 \sim 1/5$ of the shear modulus, such as a number of face-centered-cubic (FCC) and body-centered-cubic (BCC) single crystals [17, 94], B2-structured NiAl single crystal [95], and HCP single crystals [96, 97].

The Schmid factor in uniaxial tests, defined as the ratio of the maximum resolved shear stress to the uniaxial stress, is frequently used to analyze the possibly activated slip systems in single crystals. It can be easily calculated from geometric relationships, as shown in Fig. 5.1(a) for FCC single crystals with $\{111\}\langle 1\bar{1}0\rangle$ slip systems and in Fig. 5.1(b) for B2 single crystals with $\{110\}\langle 001\rangle$ slip systems. Similarly, the indentation Schmid factor is defined in Li et al. [19] by the ratio of maximum resolved shear stress to the maximum contact pressure,

$$S_{ind}^{(\alpha)} = \frac{1}{p_0} \max\{\tau_{RSS}^{(\alpha)}(x_i)\}, \quad (5.1.2)$$

where $\tau_{RSS}^{(\alpha)}$ is the resolved shear stress of the α -th slip system, and the maximum contact pressure p_0 is given by

$$p_0 = \left(\frac{6PE_r}{\pi^3 R^2} \right)^{1/3}. \quad (5.1.3)$$

The largest indentation Schmid factor among all possible slip systems is given in the inverse pole figure for FCC single crystals in Figs. 5.2(a) and for NiAl single crystal in Fig. 5.2(b). Although the orientation dependence resembles that of uniaxial Schmid factors, the variation with respect to the crystallographic orientation is significantly reduced. While no pop-in tests have been conducted to cover the entire triangle in Fig. 5.1, our previous experiments on NiAl single crystals [95] over the entire triangle are found to agree with the prediction in Fig. 5.2(b), validating the $\{110\}\langle 001\rangle$ slip systems and the use of indentation Schmid factors.

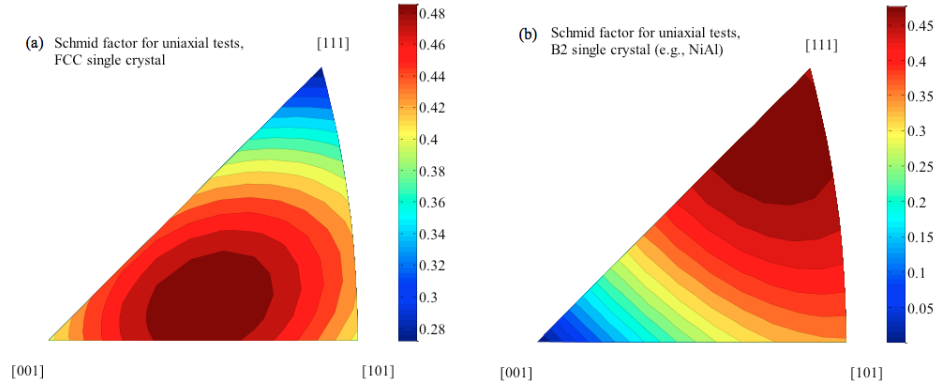


Figure 5.1 Contour plots of the Schmid factors for (a) FCC single crystals with $\{111\}\langle 1\bar{1}0 \rangle$ slip systems, and (b) NiAl single crystal with B2 structure and $\{110\}\langle 001 \rangle$ slip systems under uniaxial test.

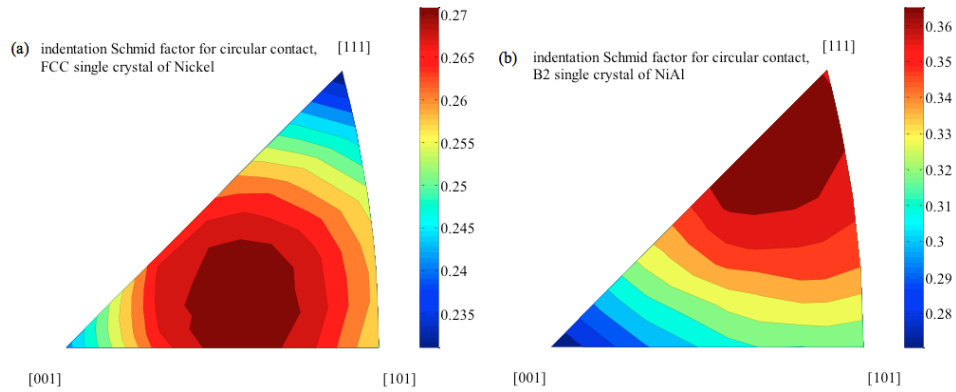


Figure 5.2 Contour plots of the indentation Schmid factors for (a) FCC single crystals with $\{111\}\langle 1\bar{1}0 \rangle$ slip systems, and (b) NiAl single crystal with B2 structure and $\{110\}\langle 001 \rangle$ slip systems under spherical indentation.

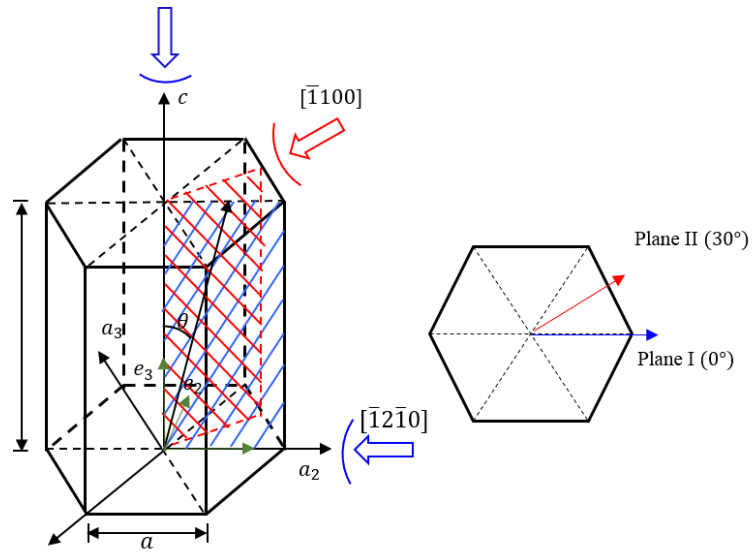
In this study, the pop-in loads required for homogeneous dislocation nucleation in HCP single crystals such as Mg, Hf, and Ti will be investigated as a function of crystallographic orientation and elastic anisotropy, as motivated by the following observations. First, HCP single crystals oftentimes have multiple slip systems in operation, and the macroscopic plastic properties, including critical resolved shear stress (CRSS) and hardening moduli, are very sensitive to the temperature and c/a ratio [98]. The CRSS ratios of various slip systems can be directly measured by uniaxial or other simple tests [18, 19], but can only be indirectly determined from indentation hardness tests [20, 21, 99]. It should be noted that crystalline materials under indentation will generally display indentation size effects, with the CRSS being the asymptote at one end and the pop-in asymptote at the other end. It is thus of crucial importance to examine whether the pop-in loads can be used to determine the ratios of theoretical strengths of various slip systems. Second, microstructural characterizations of deformation behavior at small scales are tedious experiments, such as transmission electron microscopy (TEM) [22-24] and neutron and synchrotron x-ray diffraction technique [100]. Combining nanoindentation and TEM techniques, Kwon et al. [101] found the activation of multiple slip systems in Ti single crystals with various indentation directions. However, the TEM characterization was conducted after multiple successive pop-ins so that the dislocation microstructure upon the incipient plasticity could not be determined. In situ TEM tests of Mg nanowires [102, 103] reveal interesting synergistic activation of multiple slip systems and most interestingly the simultaneous initiation of a large number of twin partials. These experiments suffer the complication of surface dislocation nucleation and are also restricted to certain crystalline

orientations. Third, due to the spatio-temporal limitations, it is more desirable for molecular simulations to compare to experimental measurements at small stressed volumes. For example, Barrett et al. [104] showed the breakdown of Schmid law in homogeneous and heterogeneous dislocation nucleation in Mg single crystals under uniaxial stresses. The evolution of dislocation microstructure in HCP single crystals under nanoindentation has been simulated in Alhafez et al. [105]. As explained earlier, a direct comparison to these simulations works by TEM or other characterization techniques is extremely challenging, as opposed to the relatively convenient pop-in measurements.

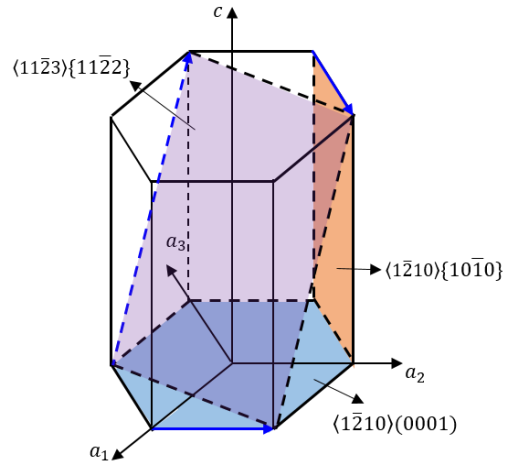
5.2 Pop-in measurements of HCP single crystals

Geometric representation of the HCP lattice is given in Fig. 5.3(a), where θ is the zenith angle formed between the indentation direction and the c -axis. Three types of slip systems are schematically illustrated in Fig. 5.3(b), including basal $\langle a \rangle$, prismatic $\langle a \rangle$, and second pyramidal $\langle c + a \rangle$, slip systems.

Nanoindentation pop-in measurements on Hf single crystals are provided in Fig. 5.4. Because Hf single crystals cannot be grown in the optical floating zone furnace, polycrystalline Hf rods (from Alfa Aesar) were annealed to produce very large grains, which ensured the nanoindentation response reflecting its single crystal behavior. In the disk-shaped specimen of 2 mm in thickness and 6.35 mm in diameter, only 7~8 grains can be observed in the entire surface after annealing at 1600 °C and 25 hours in vacuum. The grain orientations were determined by backscatter Laue diffraction as shown by the indentation directions in the legend of Fig. 5.4. Nanoindentation tests were performed on



(a)



(b)

Figure 5.3 Schematic sketch of (a) HCP crystal structures under indents within the two shaded plane with zenith angle ranging from 0 to $\pi/2$, and (b) three possible slip systems, including basal $\langle a \rangle$, prismatic $\langle a \rangle$ and 2nd pyramidal $\langle c + a \rangle$ slip systems.

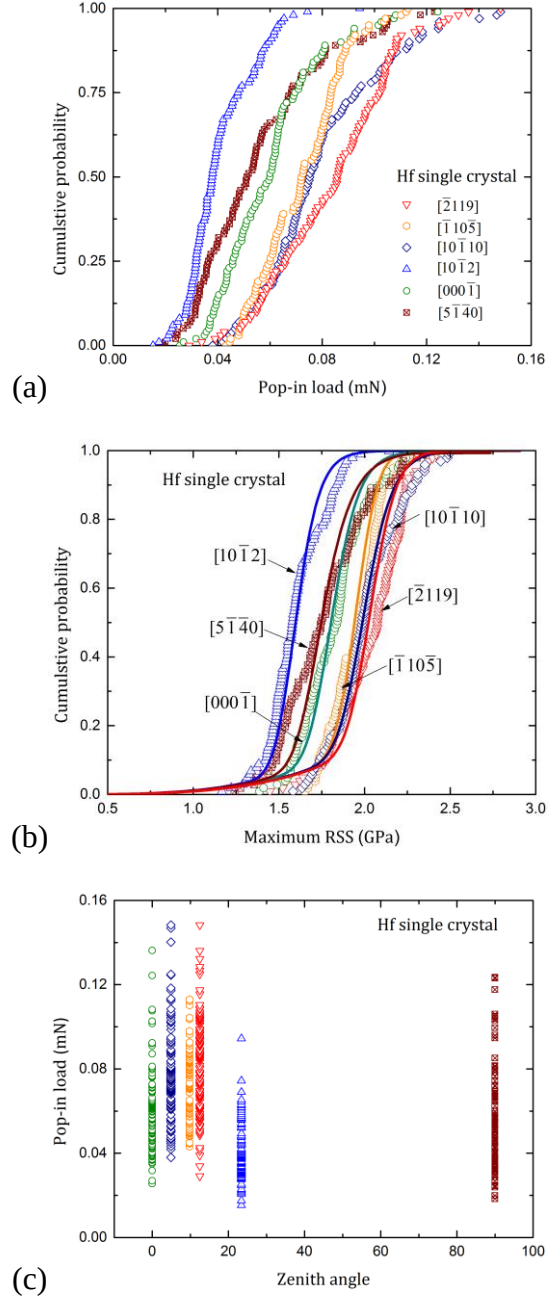


Figure 5.4 (a) Cumulative pop-in probability f as a function of pop-in load, (b) Cumulative pop-in probability f versus maximum resolved shear stress, and (c) pop-in load in variation with zenith angle θ for Hf single crystals under spherical indentation in different directions.

electrochemically polished surfaces of these grains using a Nanoindenter XP (MTS Nano Instruments, Oak Ridge, TN). All the tests were performed in load control, using a constant loading rate of $\dot{P}/P = 0.05s^{-1}$ at room temperature. A spherical nanoindenter with tip radius of 580 nm was used. The area function of the indenter was calculated using the Hertzian contact solution for indentation on an electro-polished tungsten sample which is elastically isotropic, and the tip radius was calibrated using the methodology in Li et al. [106].

Statistical measurements of the pop-in loads can be easily conducted, and the resulting cumulative pop-in probability is given in Fig. 5.4(a). As reviewed in Gao and Bei [14], there are two contributions to the statistical variation of the pop-in loads. When the corresponding resolved shear stress is close to the theoretical strength, the variations arises from the stress-assisted, thermally activation process of homogeneous dislocation nucleation. In this case, decreasing the temperature or increasing the loading rate will make the cumulative probability curve to approach a Heaviside function [107, 108]. The variation of pop-in loads may also result from activating pre-existing defects, and such a heterogeneous dislocation nucleation mechanism involves a length scale, being the spacing of these defects, and a defect strength that is much lower than the theoretical strength. Thus, this stochastic behavior usually leads to long tails at low pop-in loads/stresses, and it is not sensitive to the change of temperature and loading rate. Therefore, when using the statistical measurements to determine the theoretical strengths, we shall not use the mean value of the pop-in loads because of the possible convolution of the above two types of

dislocation nucleation mechanisms, need to ensure the thermal activation regime is probed, and then choose the appropriate upper bound values of the pop-in data.

As will be shown later in Section 5.4, it is not possible to have just one type of slip systems that accounts for all the available orientations in Figs. 5.4 and 5.5. Thus the maximum shear stress from isotropic Hertzian contact is calculated from pop-in loads in Fig. 5.4(a), and the cumulative pop-in probability curves are fitted to a unified model that couples both homogeneous and heterogeneous dislocation nucleation processes as given in Fig. 5.4(b) and Appendix A. Such a treatment does not address the elastic anisotropy and various slip systems, but it proves that most of the pop-in data actually fall into the thermally activated process for homogeneous dislocation nucleation. Therefore, the upper bound values (e.g., 95% of the cumulative probability) in Fig. 5.4(c) will be used for the evaluation of theoretical strengths in Section 5.4.

It should be noted that nanoindentation pop-in tests in HCP single crystals are very scarce in literature. Catoor et al. [109] conducted pop-in tests of Mg single crystals with three indentation directions, as summarized in Fig. 5.5. Similar to observations in Mason et al. [107] and Li et al. [110], the load-displacement curves before the pop-in can be fitted to the elastic Hertzian solution in Eq. (5.1.1). Again the upper bound values in Fig. 5.5(b) will be used to calculate the theoretical strengths.

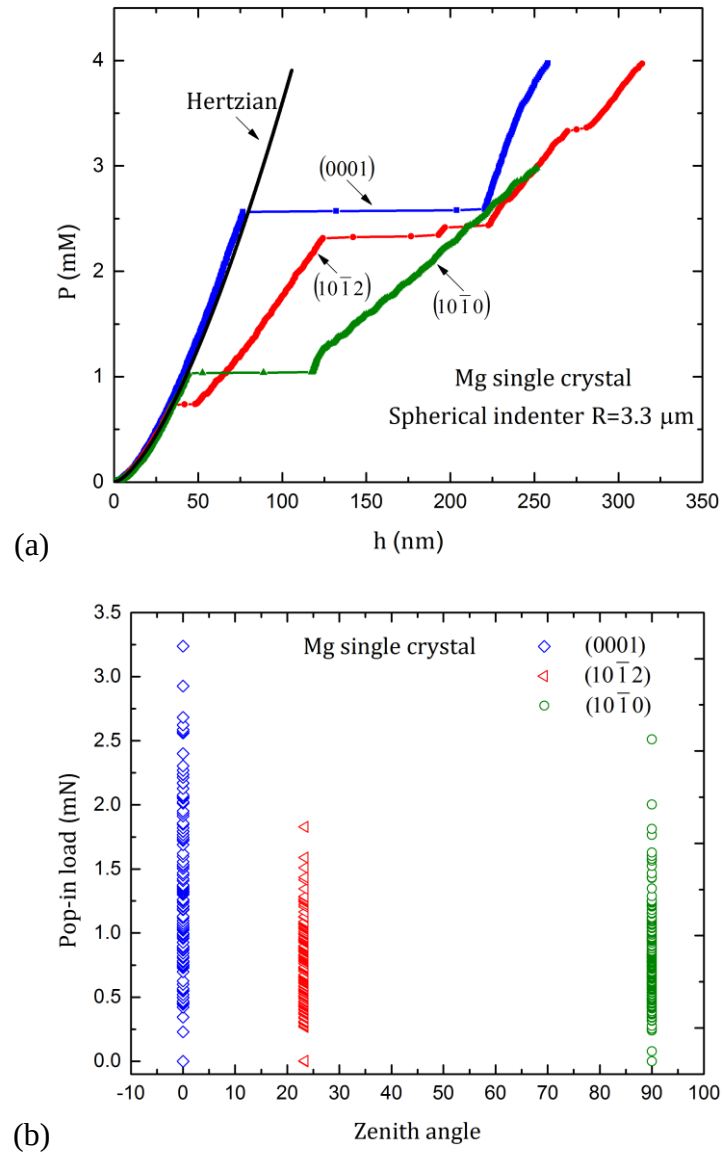


Figure 5.5 Load-displacement curves for Mg single crystal under spherical indentation with a tip radius of $R = 3.3 \mu\text{m}$, and (b) cumulative pop-in probability f versus pop-in load for Mg single crystals.

5.3 Indentation Schmid factor under anisotropic Hertzian contact

Consider an elastically anisotropic half-space under Hertzian contact with a spherical indenter in Fig. 5.6. It has been proved rigorously [95, 111, 112] that the contact area is elliptical and the contact pressure is given by

$$p(x_1, x_2) = p_0 \sqrt{1 - (x_1/a_1)^2 - (x_2/a_2)^2}, \quad (5.3.1)$$

where p_0 is the maximum contact pressure, and a_1 and a_2 are the half axes of the ellipse [111]. For normal materials, it has been found that the degree of ellipticity is negligible, and thus the contact shape can be assumed to be circular (Fig. 5.3). The contact analysis gives the maximum contact pressure as,

$$p_0 = \left(\frac{6PE_r^2}{\pi^3 R^2} \right)^{1/3}, \quad (5.3.2)$$

where the reduced indentation modulus $E_r = [(1 - \nu_s^2)/E_s + (1 - \nu_i^2)/E_i]^{-1}$ for isotropic solids or $E_r = [1/E_{eff} + (1 - \nu_i^2)/E_i]^{-1}$ for anisotropic solids, E_s and ν_s are Young's modulus and Poisson's ratio of the isotropic specimen and E_{eff} is the effective indentation modulus of anisotropic specimen which will be determined later. E_i and ν_i are the Young's modulus and Poisson ratio of the diamond indenter, respectively, 1141 Gpa and 0.07.

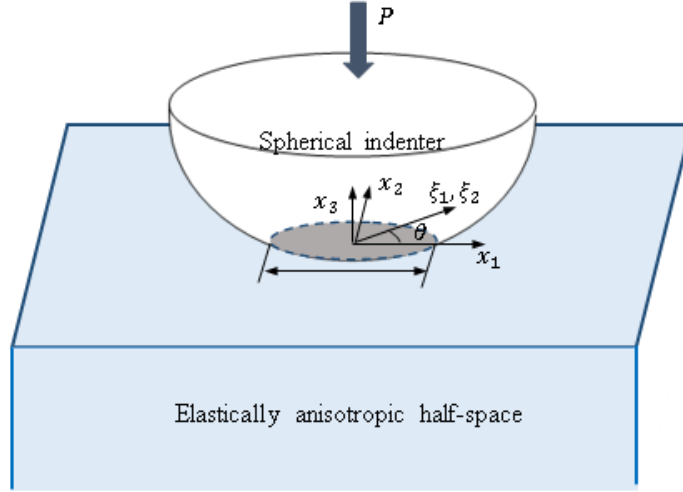


Figure 5.6 Schematic illustration of an elastically anisotropic specimen under spherical indentation. The contact area is assumed to be circular of radius a .

Fig. 5.4a shows schematic sketch of indentation directions with the zenith angle ranging from 0 to $\pi/2$ (Fig. 5.4a), where the zenith angle is the angle between the c-axis and the indentation direction. The three most favorable slip systems of HCP crystal structures, including the basal $\langle a \rangle$ slip $\langle 1\bar{2}10 \rangle (0001)$ prism $\langle a \rangle$ slip $\langle 1\bar{2}10 \rangle \{10\bar{1}0\}$ and 2nd pyramidal $\langle c + a \rangle$ slip $\langle 11\bar{2}3 \rangle \{11\bar{2}2\}$ are sketched in Fig. 5.4b. The resolved shear stress on the α th slip system $\tau_{rss}^{(\alpha)}$ is computed from the indentation stress fields σ_{ij} by

$$\tau_{rss}^{(\alpha)} = \sigma_{ij} s_i^{*(\alpha)} m_j^{*(\alpha)}, \quad (5.3.3)$$

where α ranges from 1 to the total number of the slip systems, and $s_i^{*(\alpha)}$ and $m_j^{*(\alpha)}$ are the slip direction and slip normal of the α th slip mode, with the Latin subscripts ranging from 1 to 3, and the usual summation convention on repeated subscripts is implied. The indentation Schmid factor S under Hertzian contact is defined as the ratio of the maximum shear stress (among all slip systems) to the maximum contact pressure

$$S = \frac{\tau_{rss}^{\max}}{p_0} = \frac{1}{p_0} \max_{\alpha} \{ \tau_{rss}^{(\alpha)}(x_i) \}. \quad (5.3.4)$$

As long as the stress fields $\sigma_{ij}(x_k)$ are known, we can determine the slip system and locations in the specimen where the maximum indentation Schmid factor S is reached.

The Hertzian stress fields can be determined from the stress distribution in Eq. (5.1.1) and the Green tensor. Consider the surface tractions on the half-space

$$\mathbf{t} = \mathbf{t}_0 \sqrt{1 - 1 - (x_1/a_1)^2 - (x_2/a_2)^2}, \quad (5.3.5)$$

with $\mathbf{t}_0 = (t_{01}, t_{02}, t_{03})^T$, the displacement field in the material can be obtained as

$$\mathbf{u}(x_1, x_2, x_3) =$$

$$\iint_S \mathbf{w}(x_1 - x'_1, x_2 - x'_2, x_3) \mathbf{t}_0 \sqrt{1 - 1 - (x'_1/a_1)^2 - (x'_2/a_2)^2} dx'_1 dx'_2 \quad (5.3.6)$$

where the Green tensor $\mathbf{w}(x_1, x_2, x_3)$ is the displacement field in the half-space solid under a unit point load applied at the coordinate origin. To evaluate the stress fields, the Stroh formalism and the two-dimensional Fourier transform are used to derive the analytical stress fields in the elastically anisotropic solids under Hertzian contact [111]. Integrating the Green tensor with a parabolic Hertzian pressure distribution allows one to find the entire stress fields. Based on the results of contact stress fields, an extreme search for the maximum resolved shear stress is conducted by using the Nelder-Mead simplex algorithm, and the maximum indentation Schmid factor is obtained for each slip system according to the definition of indentation Schmid factor in Eq. (5.3.1). The calculated results are based

on Hf lattice constant ratio $c/a = 1.5802$, and elastic constants $c_{11} = 181.1\text{GPa}$, $c_{12} = 77.2\text{GPa}$, $c_{13} = 66.1\text{GPa}$, $c_{33} = 196.9\text{GPa}$ and $c_{44} = 55.7\text{GPa}$ [113]. Parameters for Mg and Ti single crystals can be found in [109] and Kwon et al. [101].

Results in Figs. 5.7-5.9 are also compared to the uniaxial Schmid factors in Figs. 5.10-5.12, respectively, with respect to the zenith angle in the two hatched planes in Fig. 5.3(a). Following the formulation in [114, 115], a given slip system, $\{h\ k\ i\ l\}\langle u\ v\ t\ w\rangle$, corresponds to the slip plane normal

$$\mathbf{m} = \left[2h + k, h + 2k, \frac{3l}{2} \left(\frac{a}{c} \right)^2 \right], \quad (5.3.7)$$

and the slip direction

$$\mathbf{s} = [u - t, v - t, w]. \quad (5.3.8)$$

The Schmid factor is calculated from the cosine functions $\cos \phi$ and $\cos \lambda$,

$$\cos \phi(\lambda) = \frac{u_1 u_2 + v_1 v_2 - \frac{1}{2}(u_1 v_2 + u_2 v_1) + \left(\frac{c}{a} \right)^2 w_1 w_2}{\left[\left(u_1^2 + v_1^2 - u_1 v_1 + \left(\frac{c}{a} \right)^2 w_1^2 \right) \left(u_2^2 + v_2^2 - u_2 v_2 + \left(\frac{c}{a} \right)^2 w_2^2 \right) \right]^{1/2}} \quad (9)$$

where $[u_1\ v_1\ w_1]$ is the slip plane normal or the slip direction in 3-index notation, and $[u_2\ v_2\ w_2]$ represents the 3-index loading direction.

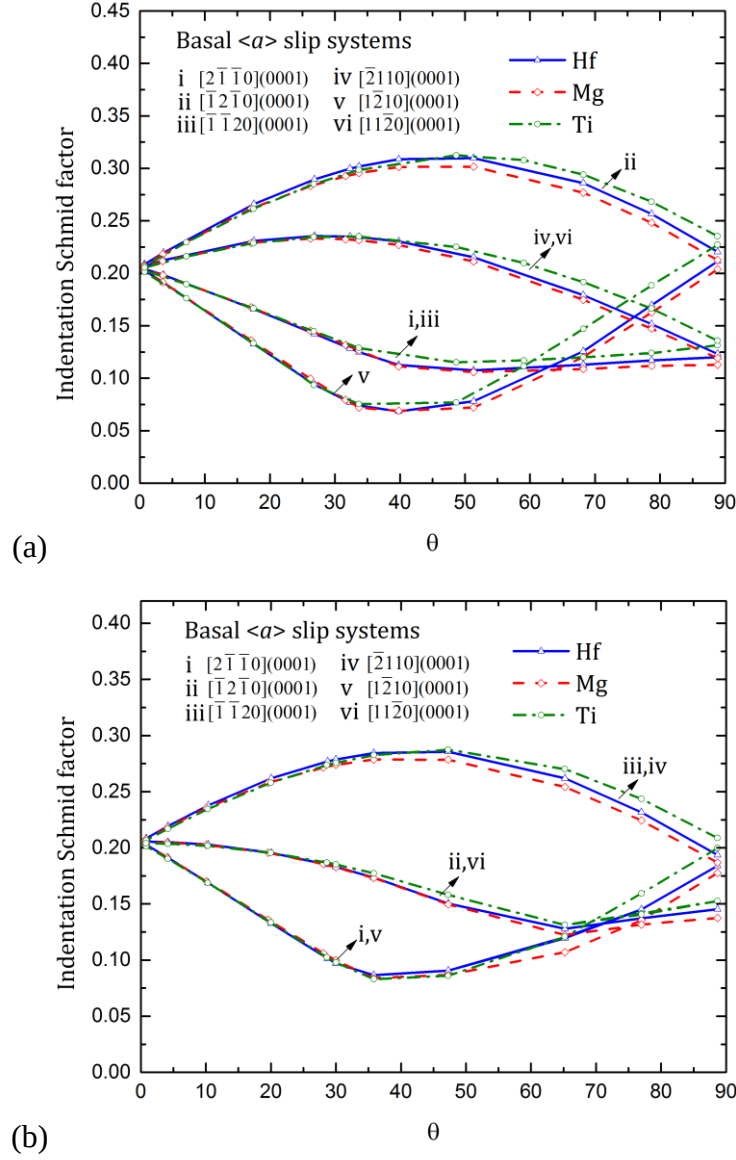


Figure 5.7 The indentation Schmid factor for the basal $\langle a \rangle$ slip systems as a function of the zenith angle θ for Hf, Mg and Ti single crystals with the indentation direction restricted to Plane I in (a) and to Plane II in (b). Refer to Fig. 5.3(a) for these two planes.

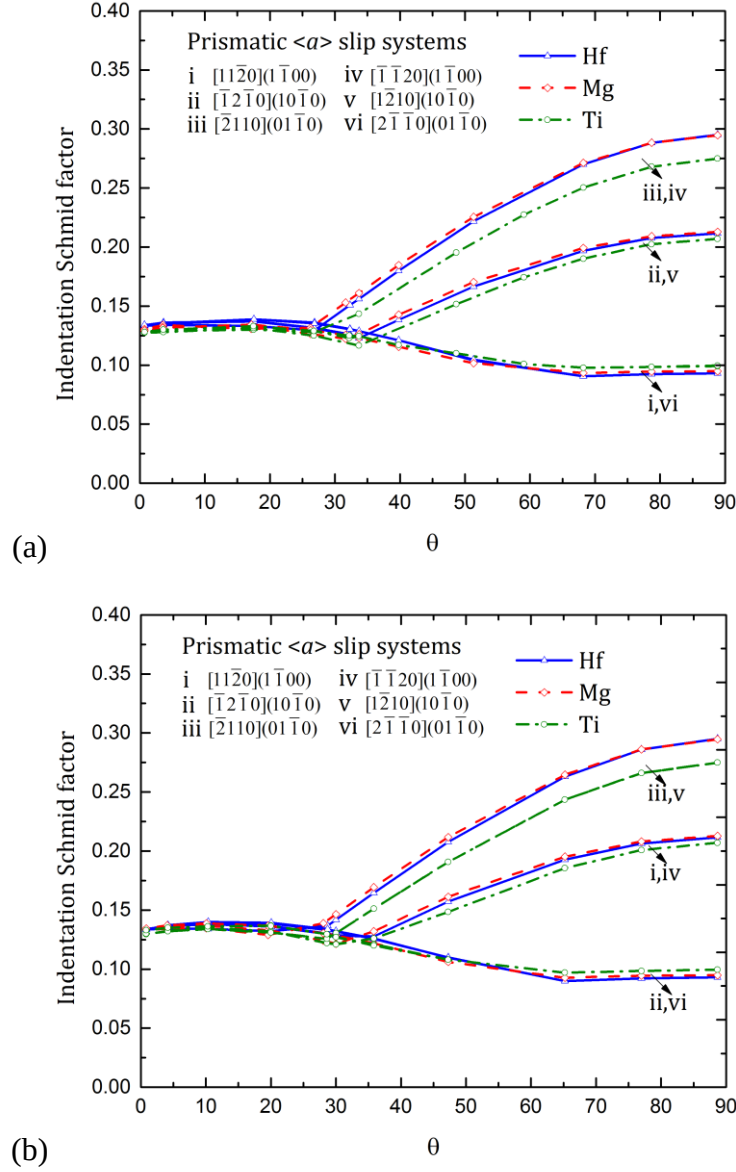
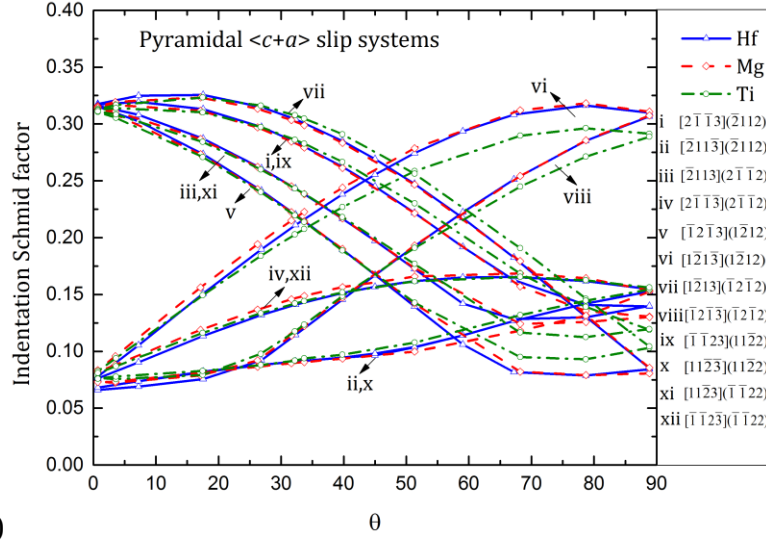
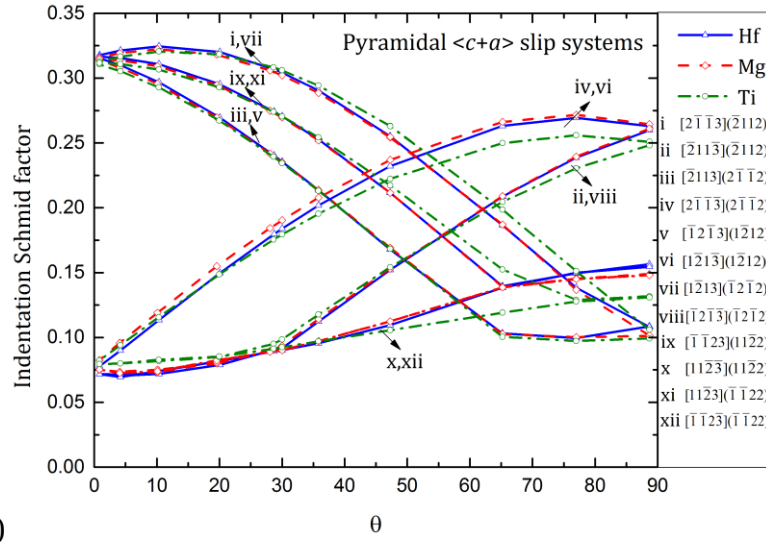


Figure 5.8 The indentation Schmid factor for the prismatic $\langle a \rangle$ slip systems as a function of the zenith angle θ for Hf, Mg and Ti single crystals with the indentation direction restricted to Plane I in (a) and to Plane II in (b). Refer to Fig. 5.3(a) for these two planes.



(a)



(b)

Figure 5.9 The indentation Schmid factor for the second-order pyramidal $\langle c + a \rangle$ slip systems as a function of the zenith angle θ for Hf, Mg and Ti single crystals with the indentation direction restricted to Plane I in (a) and to Plane II in (b). Refer to Fig. 5.3(a) for these two planes.

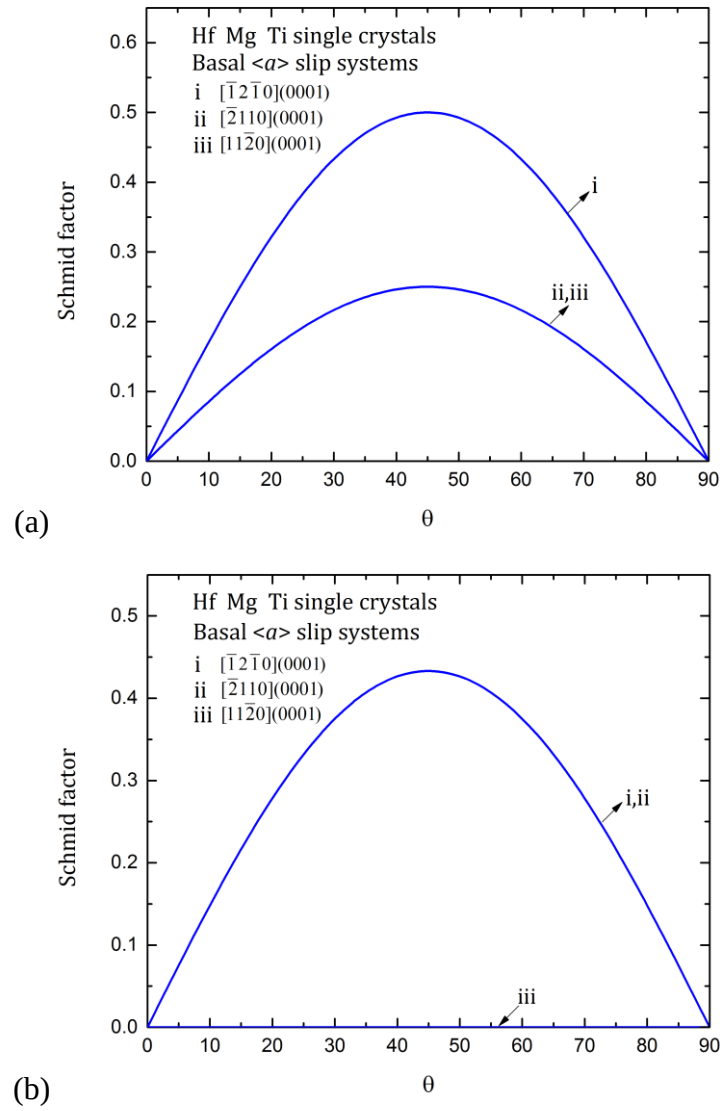


Figure 5.10 The uniaxial Schmid factor for the basal $\langle a \rangle$ slip systems as a function of the zenith angle θ for Hf, Mg and Ti single crystals with the indentation direction restricted to Plane I in (a) and to Plane II in (b). These results can be contrasted to those in Fig. 5.7.

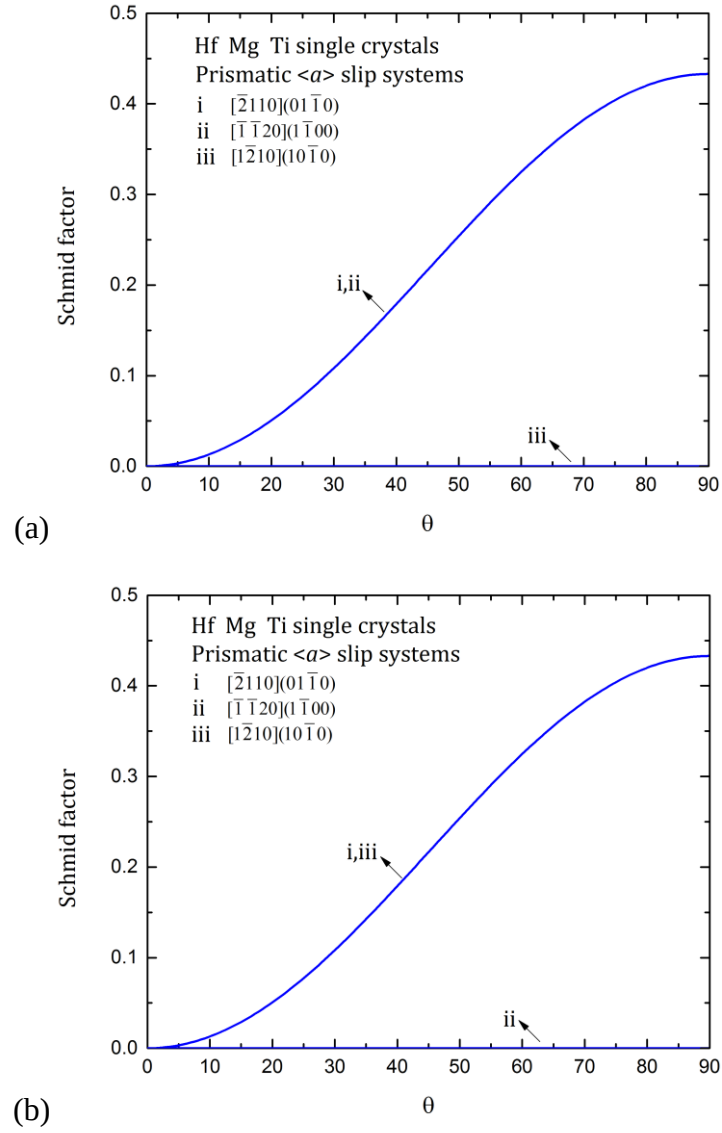


Figure 5.11 The uniaxial Schmid factor for the prismatic $\langle a \rangle$ slip systems as a function of the zenith angle θ for Hf, Mg and Ti single crystals with the indentation direction restricted to Plane I in (a) and to Plane II in (b). These results can be contrasted to those in Fig. 5.8.

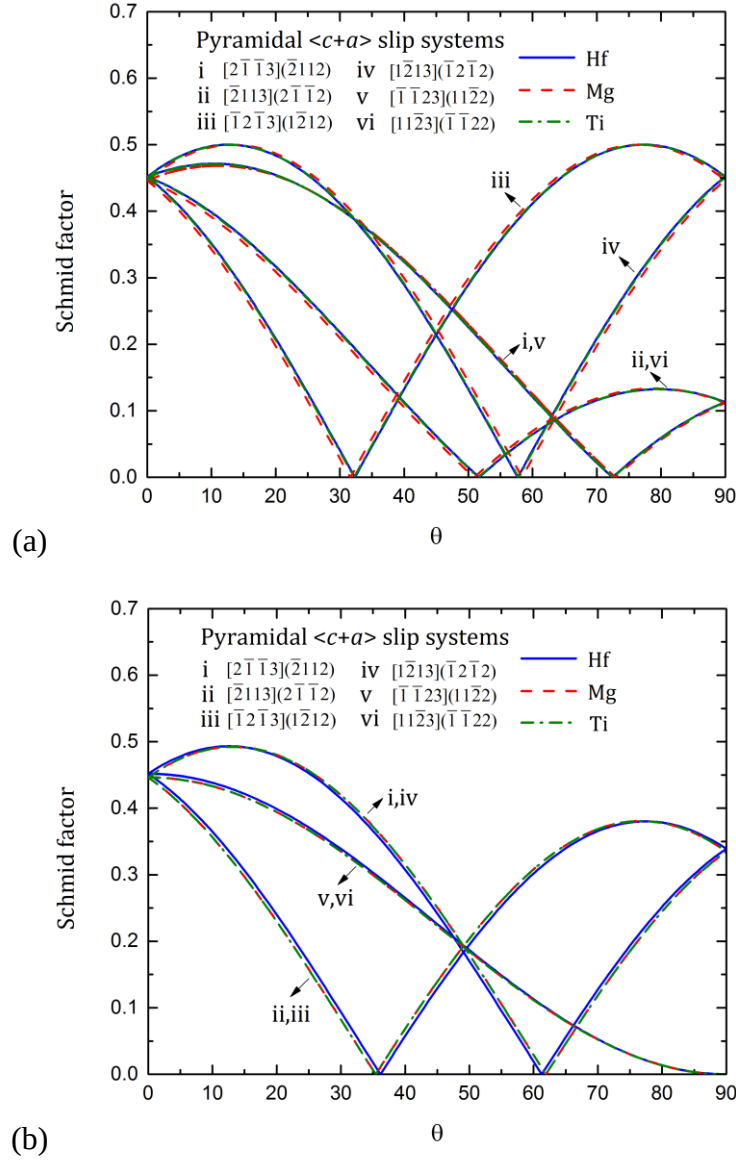
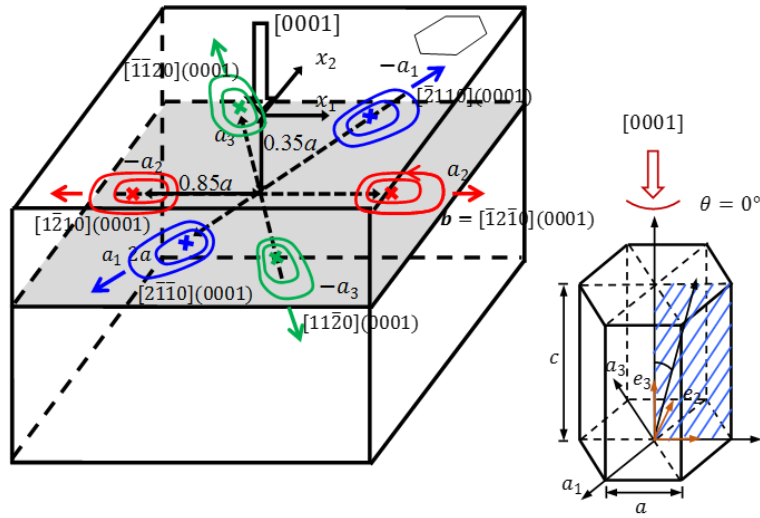


Figure 5.12 The uniaxial Schmid factor for the second-order pyramidal $\langle c + a \rangle$ slip systems as a function of the zenith angle θ for Hf, Mg and Ti single crystals with the indentation direction restricted to Plane I in (a) and to Plane II in (b). These results can be contrasted to those in Fig. 5.9.

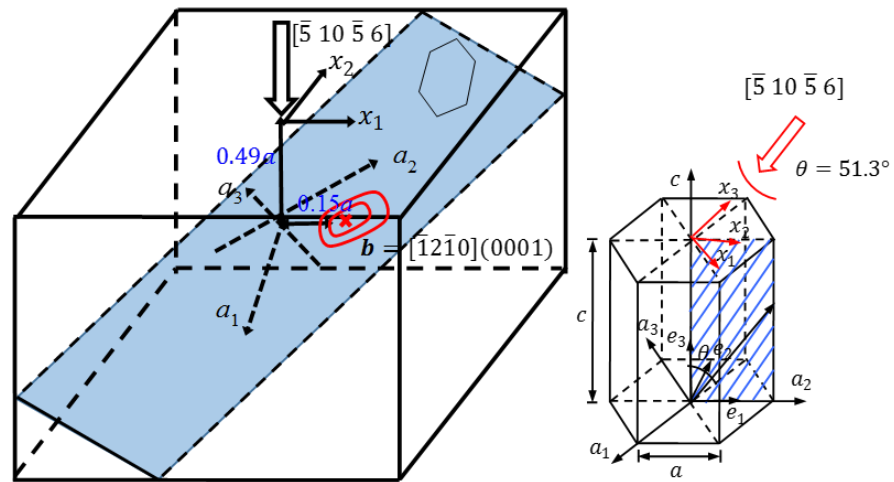
5.3.1 Basal $\langle a \rangle$ slip systems

As shown in Fig. 5.3(a), the variation of the zenith angle θ is restricted to the two high-symmetry planes, $(10\bar{1}0)$ plane and $(11\bar{2}0)$, and the corresponding indentation Schmid factors are given in Figs. 5.7(a) and 5.7(b) respectively. Although there are three independent basal $\langle a \rangle$ slip systems, positive and negative slip directions yield six slip systems to be investigated. Some of them will lead to the same results because of geometric symmetry, for example, slip system i and iii in Fig. 5.7(a). The maximum values of 0.3155 and 0.2857 are reached at $\theta \approx 45^\circ$ for Plane I and Plane II, i.e., Figs. 5.7(a) and 5.7(b), respectively. It should be noted that the uniaxial Schmid factor vanishes when loading along the c -axis and a -axis, as shown in Fig. 5.10, which are the “hard” directions. In contrast, the corresponding indentation Schmid factors are non-zero and about 2/3 of the maximum value with respect to the zenith angle, clearly owing to the complex stress fields under the indentation. The overall dependence of the highest indentation Schmid factor on the zenith angle in Fig. 5.7, on the other hand, is the same as that in Fig. 5.10. That is, hard/soft directions in uniaxial tests are also hard/soft directions in indentation, but to a much lesser degree. These findings can rationalize the presence of basal $\langle a \rangle$ slip systems even when the indenting direction is at $\theta = 0, 90^\circ$. Additionally, different HCP single crystals have no effect in the uniaxial Schmid factor in Fig. 5.10, while the difference among Hf, Mg and Ti becomes noticeable when θ is larger than about 30° . Such a difference arises from both the degree of elastic anisotropy and the c/a ratio.

The locations where the indentation Schmid factors reach maxima are shown schematically in Fig. 5.13 for three representative indentation directions. When indenting along the c -axis, symmetry condition dictates six maxima on the plane below the indenter. Clearly the stress field along the x_3 axis does not permit a shear stress component in the basal plane, so these maxima are located quite off from the contact axis and thus form a rosette pattern in Fig. 5.13(a), as confirmed by experimental observations [24]. When indenting along the $[\bar{5} 10 \bar{5} 6]$ direction in Fig. 5.13(b) and the a -axis in Fig. 5.13(c), only the locations corresponding to the highest S_{ind} are depicted with their corresponding slip systems. From these plots, we can see that when the indenting direction rotates from c -axis to a -axis, the plane with the highest S_{ind} rotates from a horizontal to a vertical one. Results in Fig. 5.13 are for indentations along Plane I in Fig. 5.3(a), and those along Plane II are given in Fig. 5.14. Indentation along c -axis for Plane 2 is obviously the same as that for Plane I in Fig. 5.13(a). Because of symmetry, there are two or four maxima in Figs. 5.14(a) and 5.14(b) for two indentation directions, $[\bar{5}504]$ and $[\bar{1}100]$, and again the planes with the highest S_{ind} rotate as the indentation direction varies. Lastly we note that even though these predictions are based on elastic contact fields, the onset of these dislocations will be followed by dislocation growth and multiplication, so that these maxima can also be used to predict the slip traces in micro-indentation of HCP single crystals.

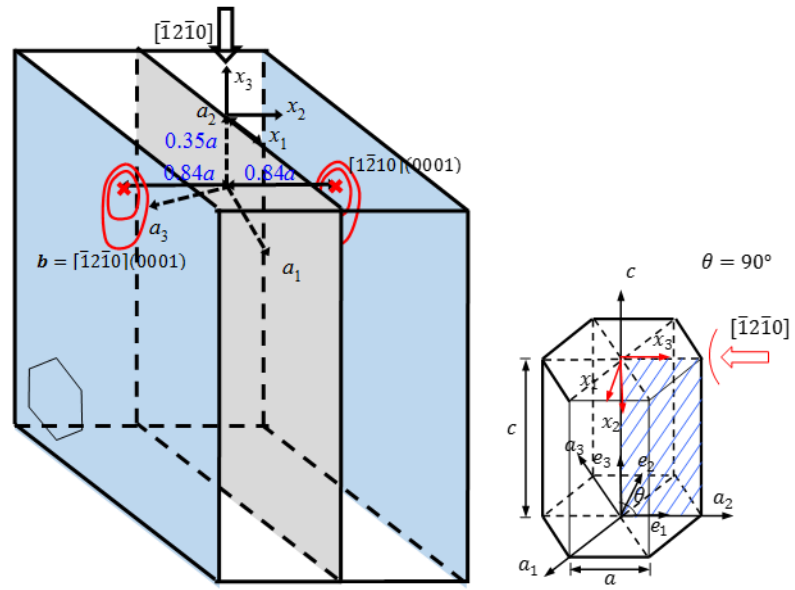


(a)



(b)

Figure 5.13 Predicted locations of the maximum resolved shear stress on the basal $\langle a \rangle$ slip systems (a) under c-axis indentation. (b) under $[\bar{5} 10 \bar{5} 6]$ direction indentation (within plane I). and (c) under a-axis ($[\bar{1}2\bar{1}0]$ direction) indentation (within plane I).



(c)

Figure 5.13 Continued

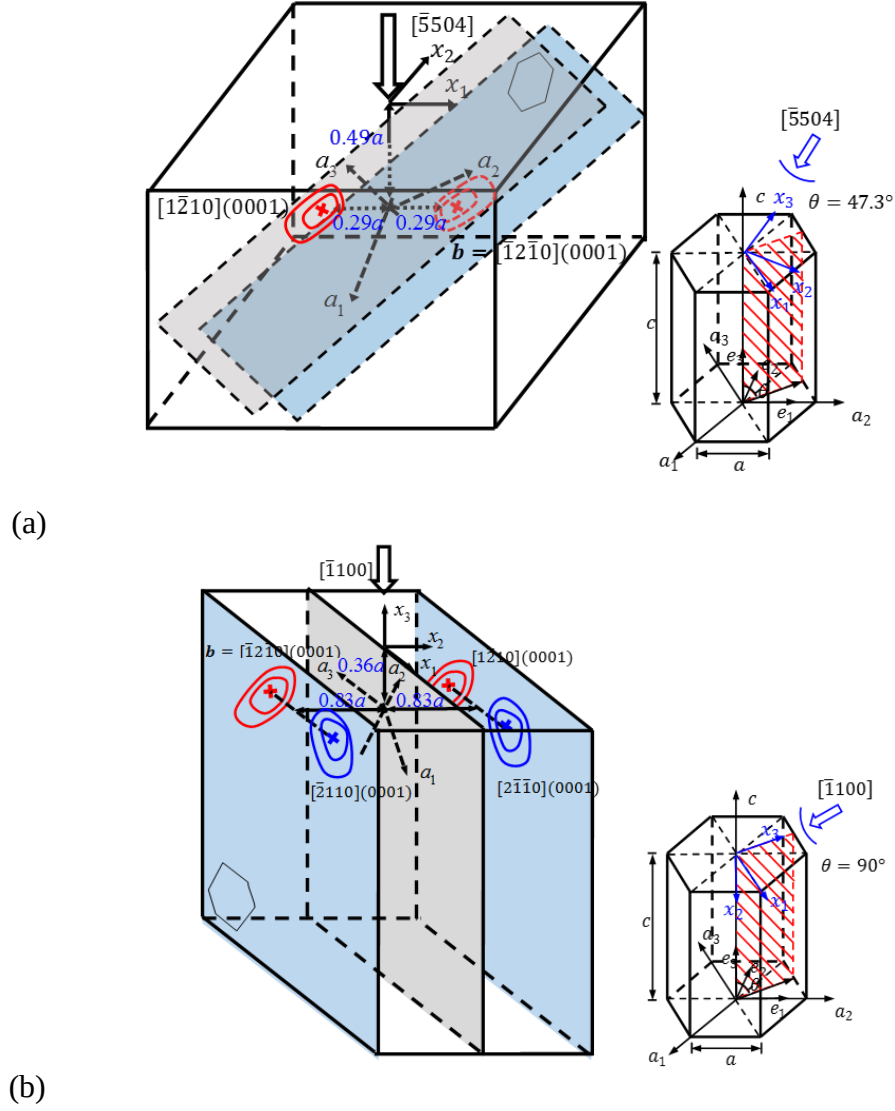


Figure 5.14 Predicted locations of the maximum resolved shear stress on the basal $\langle a \rangle$ slip systems (a) under $[\bar{5}504]$ direction indentation (within plane II). and (b) under $(\bar{1}100)$ direction indentation (within plane II).

Fig. 5.13 description: (a) Because of the highly symmetric indentation direction, there are six equivalent maxima with a value of 0.208, which is located at the plane of depth of $0.36a$ and $0.85a$ away from the contact axis with a being contact radius; (b) The maxima is located at $(0.15a, 0, -0.49a)$ on the $[\bar{1}\bar{2}\bar{1}0](0001)$ slip system, and the maximum value of indentation Schmid factor is $S_{ind} = 0.302$; and (c) For the $[\bar{1}\bar{2}\bar{1}0](0001)$ slip system, the location of maximum resolved shear stress is $(0, -0.84a, -0.35a)$, and $S_{ind} = 0.213$, By symmetry, there is an equivalent maximum resolved shear stress on the $[1\bar{2}10](0001)$ slip systems.

Fig. 5.14 description: (a) For the $[\bar{1}\bar{2}\bar{1}0](0001)$ slip system, the maximum RSS is located at $(0.29a, 0.07a, -0.49a)$, and the maximum indentation Schmid factor is $S_{ind} = 0.279$. Equivalently, the $[1\bar{2}10](0001)$ slip system occurs at a symmetry location; (b) For $[\bar{1}\bar{2}\bar{1}0](0001)$ slip system, the location of maximum RSS is at $(-0.13a, 0.83a, -0.36a)$. The maximum indentation Schmid factor is $S_{ind} = 0.187$. Because of symmetry, there are four possible equivalent maxima, respectively, on $[2\bar{1}\bar{1}0](0001)$, $[\bar{2}110](0001)$, $[\bar{1}\bar{2}\bar{1}0](0001)$ and $[1\bar{2}10](0001)$ slip systems.

5.3.2 Prismatic $\langle a \rangle$ and second-order pyramidal $\langle c + a \rangle$ slip systems

The variation of S_{ind} with respect to θ is shown in Figs. 5.8 and 5.9, and the uniaxial Schmid factor versus θ in Figs. 5.11 and 5.12, for the prismatic $\langle a \rangle$ and the second-order pyramidal $\langle c + a \rangle$ slip systems, respectively. For each slip system, searching the maximum resolved shear stress in the entire space will lead to multiple local extrema. The sudden turns on the curves in Fig. 5.8 correspond to the shift of one extremum to the other extremum being the global maximum. The same maximum value, 0.295, is obtained when indenting perpendicular to the c -axis for the prismatic $\langle c \rangle$ slip system. In Figs. 5.7, 5.8, 5.10, and 5.11, the maximum values are always reached by just one curve, while the maximum ones shift among the set of slip systems in Figs. 5.9 and 5.12. Just as the symmetry argument in Fig. 5.7, results for the two Planes in Fig. 5.9 show different combinations of slip systems that have the same indentation Schmid factor. Similar “butterfly” shapes are observed in Figs. 5.9 and 5.12, but the indentation case has much reduced variation of the magnitudes. The highest values vary in the range of about 0.26~0.32 in Fig. 5.9. For this reason, when stretching along c -axis, one can exclude certain type of slip system, e.g., basal $\langle a \rangle$ and prismatic $\langle a \rangle$ slip systems because their uniaxial Schmid factors vanish. But this conclusion cannot be made for indentation conditions because the corresponding indentation Schmid factors are not zeros and not far different from the highest values.

The CRSS ratios of HCP single crystals are known to be sensitive to the c/a ratio, but the dependence of indentation Schmid factors on this ratio is generally very small, as shown by the comparisons of Mg, Hf, and Ti single crystals in Figs. 5.8 and 5.9.

5.4 Theoretical strengths and experimental comparisons

From discussions on Fig. 5.4 and Fig. 5.5 in Section 5.2, it is believed that the upper bound value of the pop-in loads corresponds to the athermal theoretical strength for homogeneous dislocation nucleation. Combining Eqs. (5.1.2) and (5.1.3) and substituting the theoretical strength τ_{th}^α into the resolved shear stress, the predicted pop-in load for the α -th slip system is given by

$$P_{pop-in}^{(\alpha)} = \left(\frac{\tau_{th}^\alpha}{S_{ind}^\alpha} \right)^3 \frac{\pi^3 R^3}{6E_r^2} = \frac{\pi^3 c_{11} R^3}{6} \left(\frac{\tau_{th}^\alpha}{c_{11}} \right)^3 f^\alpha(\theta), \quad (5.4.1)$$

In the above equation, $f(\theta) = \frac{c_{11}^2}{E_r^2 S^3}$, where the orientation dependence arises from both E_r and S_{ind}^α . Figure 5.15 shows the corresponding results for Mg, Hf, and Ti single crystals, all of which show the same trends. If the deformation is governed by basal $\langle a \rangle$ slip systems, the pop-in load will be high near $\theta=0^\circ$ and 90° , showing roughly the reverse trend of the highest $S_{ind}(\theta)$ in Fig. 5.7. For prismatic $\langle a \rangle$ slip systems, the highest pop-in load takes place in the range of $0^\circ \sim 30^\circ$, corresponding to the low values of indentation Schmid factors in Fig. 5.8. For the second-order pyramidal $\langle c + a \rangle$ slip systems, the highest pop-in load takes place at about 50° .

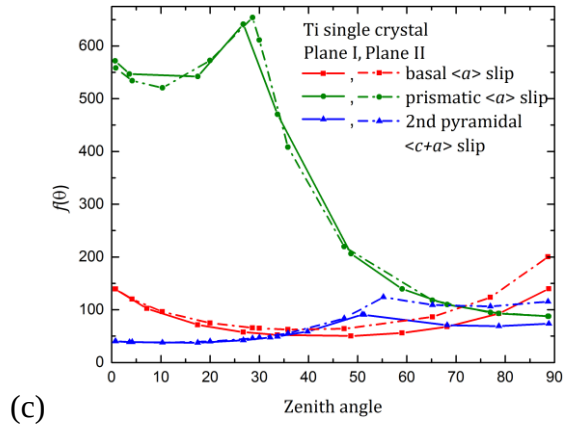
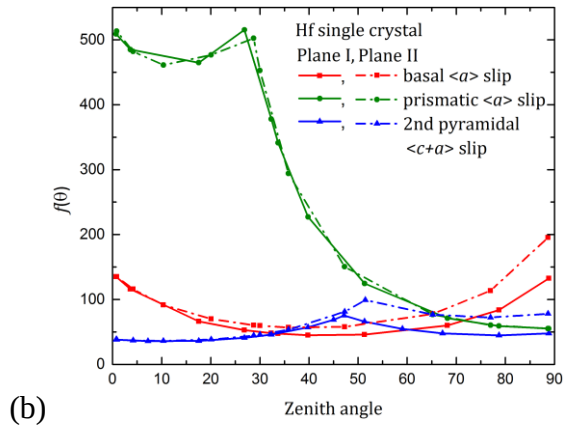
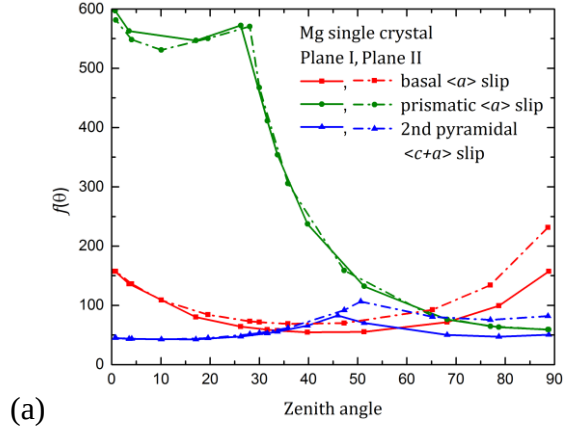


Figure 5.15 The orientation dependence of the pop-in load, as described by $f(\theta)$ in Eq. (5.4.1), is plotted against the zenith angle for the three types of slip systems.

A direct comparison of the three types of slip systems in Fig. 5.15 is not meaningful, because their theoretical strengths may be quite different. From all types of slip systems, we have

$$P_{popin} = \frac{\pi^3 C_{11} R^2}{6} \min \left(\left(\frac{\tau_{th}^{bas}}{C_{11}} \right)^3 f^{bas}(\theta), \left(\frac{\tau_{th}^{pris}}{C_{11}} \right)^3 f^{pris}(\theta), \left(\frac{\tau_{th}^{pyr}}{C_{11}} \right)^3 f^{pyr}(\theta) \right) \quad (5.4.2)$$

Consequently, in order to determine which type of slip systems is activated for the homogeneous dislocation nucleation, we aim to see if a certain choice of $(\tau_{th}^{bas}, \tau_{th}^{pris}, \tau_{th}^{pyr})$ can lead to the same dependence on the zenith angle in experimental results in Fig. 5.4 and Fig. 5.5.

For Hf single crystals, the macroscopic mechanical tests, slip trace analysis, and microstructural characterizations suggest the activation of prismatic $\langle a \rangle$ (more common) and basal $\langle a \rangle$ (less common) slip systems at room temperatures [113]. However, these measurements give the critical resolved shear stress, τ_{CRSS} , which is a measure of the resistance of dislocation gliding rather than the strength required for dislocation nucleation. The comparison between Figs. 5.4 and 5.15 shows that no individual type of slip systems, and in fact no choice of $(\tau_{th}^{bas}, \tau_{th}^{pris}, \tau_{th}^{pyr})$ in Eq. (5.4.2), can explain the observed trend in Fig. 5.4(c) for the entire range of zenith angle. The variation of pop-in loads in the θ -range of about $0^\circ \sim 30^\circ$ resemble the prismatic $\langle a \rangle$ slip system in Fig. 5.15(b), but this type of slip systems predicts a very low pop-in load near 90° that disagrees with the experiments. This

observation of Hf single crystals is in sharp contrast to previous study of NiAl single crystals, where the indentation Schmid factor and the formulation in Eq. (5.4.1) are valid for all the indentation directions that span the inverse pole figure in Fig. 5.2(b). It is thus anticipated that a combination of various types of slip systems, or stress components other than the resolved shear stress, may dictate the incipient plasticity. If an indentation Schmid factor of 0.31 is used by ignoring elastic and slip anisotropy, a theoretical value of about 2.4 GPa from Fig. 5.4(b) is obtained, which is 0.043 times the shear modulus c_{44} , or $c_{44}/23.2$.

The overall trend in Fig. 5.5(b) for Mg single crystals appears to agree with that of basal $\langle a \rangle$ slip systems in Fig. 5.15(a). However, TEM studies in [109] showed dominance of other types of slip systems for indentations towards the $[10\bar{1}2]$ plane. The CRSS ratios of various types of slip systems may be quite large, such as basal:prismatic:pyramidal = 4:10:11 [116] or 1:8:6 [18] for Mg single crystals. However, the theoretical strength ratios may not deviate significantly from unity. For example, from ab initio calculations [117], the theoretical strengths are 2.57 GPa for basal, 1.99 GPa for prismatic, and 2.62 GPa for pyramidal slip systems for Mg single crystals. Although we cannot determine the activated slip system in Fig. 5.5(b), using 90% pop-in loads gives a theoretical strength of 1~1.5 GPa. Barrett et al. [25] suggested that in certain orientation range, the dominant mechanism for homogeneous dislocation nucleation is governed by some certain slip systems, which however cannot be confirmed by Fig. 5.5(b) due to very limited number of orientations and also due to TEM observations of dislocation microstructures that are different from their predictions.

No pop-in tests were systematically conducted in Kwon et al. [24], but they employed focused ion beam milling and TEM technique to investigate the dislocation microstructure in Ti single crystals under spherical nanoindentation. Again almost all types of slip systems contribute to the observed dislocation microstructure. Note that the CRSS values for Ti singles are 209 MPa, 181 MPa, and 474 MPa for basal, prismatic, and pyramidal slip systems [19].

5.5 Summary

The indentation Schmid factor has been found to be a useful parameter to determine the theoretical strength in NiAl single crystals. This concept is employed in this work for the study of incipient plasticity and nanoindentation pop-in tests in HCP single crystals. The variation of indentation Schmid factor with respect to the indentation direction is calculated from the anisotropic elastic Hertzian contact solutions for three types of slip systems. Their dependence on the zenith angle resembles that of the uniaxial Schmid factor, but the indentation Schmid factor never vanishes and actually varies within at most 50% of the highest value. Comparing the predicted and measured pop-loads, it is concluded that the homogeneous dislocation nucleation under nanoindentation cannot be governed by any individual type of slip systems. Instead, either a combination of basal $\langle a \rangle$, prismatic $\langle a \rangle$, and second-order pyramidal $\langle c + a \rangle$ slip systems with variable weights with respect to the zenith angle, or stress components other than the resolved shear stress, governs the incipient plasticity. Additionally, the locations where the resolved shear stresses reach maxima can be used to predict the dislocation patterns under indentation.

6 CHAPTER 6 CONCLUSIONS

As concluding remarks, the objective of this dissertation work is to understand the deformation and damage mechanisms of structural materials by using computational methods at different length scales. To achieve this goal, a series of microstructure-based mechanisms-based finite element models have been developed to investigate the deformation and damage behavior of advanced alloy and welded joints. The summary of the thesis work is as follows,

- (a) We have developed a microstructure-informed mechanisms-based finite-element model to numerically study the high temperature creep behavior of CSEF steel weldments. A mechanism-based constitutive model which accounts for the dislocation creep and Coble creep (diffusional creep) is used for the grain interior plasticity, and a Newtonian viscous model is employed to describe grain boundary sliding. The numerical results of strain field distribution show encouraging quantitative agreement with DIC measurement, particularly illustrating the effect of pre-welding tempering on the evolution of strain localization in HAZ of ferritic steel weldments. We found that the thermally activated dislocation creep, diffusional creep as well as grain boundary sliding all contribute to the high temperature deformation of ferritic steel weldments, and their relative significance to the total strain accumulation in the fine grained HAZ is quantified. The effects of weldment heterogeneities, including the large grain size gradients in the microstructure and the variation of material hardness,

on the high temperature creep deformation are numerically studied. The computational simulations provide valuable insights of the micromechanical and microstructural origins for the strain localization in fine-grained HAZ of CSEF steel weldments.

(b) A microstructure-informed micromechanical model was applied to systematically study the creep cavitation and damage evolution of the Type IV failure in CSEF steel weldments. The physical fracture mechanisms at different length scales, including cavity nucleation on grain boundaries, their growth, microcracking by coalescence, and the propagation of microcracks to the formation of macrocrack, are all involved. By taking advantage of the microstructure-based model, we can explicitly model the actual microstructure and examine the effects of grain scale material heterogeneities, including grain size and morphology, grain orientation and material heterogeneous properties of different zones (BM, WM and HAZ). The computational simulations illustrate the creep fracture is a cavity growth-controlled process at low applied stress, while increasing stress it is a coupled cavity nucleation-controlled and cavity growth-controlled process. From the fracture mechanism point of view, the creep fracture is governed by grain boundary diffusion in long-term creep failure at low stress and high temperature loading conditions, and the contribution of creep deformation becomes more important with increased applied stress or decreased temperature. Moreover, the computational model provides quantitative lifetime prediction for CSEF steel weldments, and it can

be used as a powerful computational tool to predict very-long-term creep fracture behavior of many other high temperature materials and their weldments.

- (c) The indentation Schmid factor has been employed for the study of incipient plasticity and nanoindentation pop-in tests in HCP single crystals (Ti, Mg and Hf). Their dependence on the zenith angle resembles that of the uniaxial Schmid factor, but the indentation Schmid factor never vanishes and actually varies within at most 50% of the highest value. Comparing the predicted and measured pop-loads, it is concluded that the homogeneous dislocation nucleation under nanoindentation cannot be governed by any individual type of slip systems. Instead, either a combination of basal $\langle a \rangle$, prismatic $\langle a \rangle$, and second-order pyramidal $\langle c + a \rangle$ slip systems with variable weights with respect to the zenith angle, or stress components other than the resolved shear stress, governs the incipient plasticity. Additionally, the locations where the resolved shear stresses reach maxima can be used to predict the dislocation patterns under indentation.

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