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# **Imparted benefits on mechanical properties by achieving grain boundary migration across voids**

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# Thermal cracking: clarifying the effects of phases, voids and grains through characterisation and crystal plasticity modelling

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## Abstract

Thermally-induced cracking typically occurs during the cooling stage of various manufacturing processes, and is commonly seen in multiphase or the joints of dissimilar materials due to mismatch in their thermo-mechanical properties, such as thermal expansion, elastic-plastic deformation and, in some cases, phase transformation. However, the underlying cracking mechanism associated with local microstructure is still elusive. To improve the mechanistic understanding of thermal cracking, this work uses the diffusion-bonded 9Cr-1Mo steel as an example to study the key microstructural variables, such as interfacial phases, voids, grain boundary migration and crystallographic orientations. Meanwhile, a temperature-dependent crystal plasticity model, coupled with a cohesive zone model, is developed to provide more insights into the thermal-induced stress distribution at the grain scale. It is found that the stress at the void-free boundary of martensite and ferrite is dominated by shear, and its magnitude is insufficient to nucleate cracks. Whereas voids at phase boundaries can induce significant tensile stress, resulting in cracking at the phase boundaries as well as diffusion-bonded interfaces. Also, the occurrence of interfacial grain boundary migration plays an important role in local stress distribution. These microstructural features and their evolution are experimentally investigated, and newly developed crystal plasticity model is used to verify the experimental data. These findings enhance the understanding of the influence of microstructure features on thermal cracking and provide a guide to designing and fabricating the microstructure with improved thermal crack resistance in various manufacturing processes.

**Keywords:** Thermal crack; Void; Grain boundary; Martensite; Crystal plasticity; Diffusion Bonding

## 1. Introduction

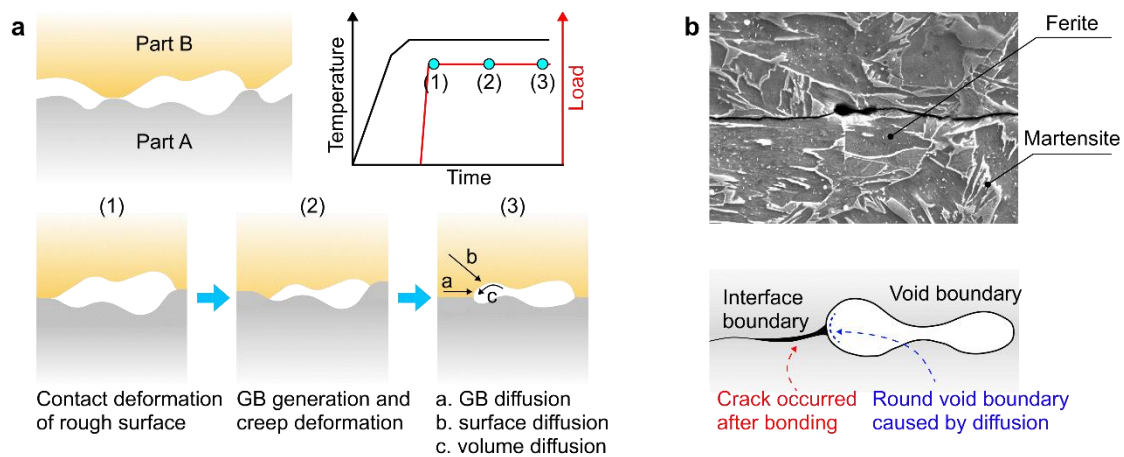
Welding (bonding) multi-phase or dissimilar materials could provide superior mechanical and/or multi-functional properties compared to a metallic, single-phase material [1]. Manufactured multiphase or dissimilar metallic components have great potential in extremely demanding environments. For example, martensite and ferrite dual-phase steel exhibits high ultimate tensile strength and excellent formability, resulting in efficient sheet-forming processes for producing automotive components cost-effectively [2]. Also, in the nuclear fusion industry, multi-materials, such as CuCrZr alloy, W and SS316L are welded to withstand the electromagnetic loads and neutron irradiation while providing strength and geometrical stability [3]. However, the two phases or metals often exhibit significantly different thermal and/or mechanical properties. As a result, the interfaces are often subjected to severe thermally-induced stresses [4], often leading to cracking and premature failure of components [5].

9Cr-1Mo steel is a commonly used martensite-ferrite dual-phase steel in the nuclear industry because of its excellent resistance to irradiation and creep damage [6]. High-quality welding joints satisfying the critical specifications applied in the nuclear industry have been demonstrated using advanced joining methods [7-10]. Among these, diffusion bonding [11] can obtain an optimal uniform microstructure and indistinguishable interfacial properties to the base material [12].

After diffusion bonding at elevated temperatures, the bonded parts must be cooled to room temperature, which is a complex thermal-metallurgical-mechanical process, increasing thermal stress concentration at the joint boundary due to the mismatch in their coefficients of thermal expansion (CTE). In addition to thermal expansion, the cooling process of some multiphase steels, e.g., diffusion bonded 9Cr-1Mo steel, is usually accompanied by the martensite transformation [13]. Phase transformation from austenite to martensite is driven by a diffusion-less process [14]. Due to martensite transformation during cooling, volume expansion occurs, resulting in an opposite volumetric change of another phase in the steel [15], e.g., retained austenite or ferrite. Such anomalous plastic flow is so-called transformation plasticity, contributing to internal stresses at the grain level and local cracking [16].

Although the mismatch in CTE, opposite volumetric change and transformation plasticity are the main reasons that induce local stresses, the existence of voids would further complicate the local stress state. Voids, as local defects acting as precursors of various failures, are commonly seen in advanced fabrications, including additive manufacturing [17, 18], diffusion bonding [19, 20] and sintering [21]; however, the role that voids play under thermal loading is unclear, particularly when interacting with thermal cracks (e.g. in this work, thermal cracks were found crossing voids in a diffusion bonded 9Cr-1Mo steel sample). To distinguish the un-bonded interface and thermal cracks,

the mechanism of diffusion bonding and the associated microstructure evolution described in [22] are summarised in Fig. 1a. It is noted that the void tip is sharp in the initial stage (2) when the surface asperities come into contact. As atomic diffusion continues, the void closes. The void tips become more circular by continued diffusion, as shown in Fig. 1. The proposed cracking mechanism in Fig.1a is consistent with the sharp crack seen in Fig. 1b which was generated by thermal cracking during the cooling process of the diffusion bonded sample.



**Fig. 1 Mechanism of voids closure and interfacial grain boundary cracking:** (a) voids closure process and (b) evidence to show that the thermal cracking occurs after the diffusion bonding process.

In prior modelling of the thermally-induced stresses in weldments were simplified by only considering the macroscopic level response without accounting for any microscopic crystallographic orientations, phases or voids due to the lack of appropriate mechanism models [4, 23]. For example, Yaghi et al. [24] simulated the stress evolution during the welding of P91 steel pipe, in which the phase transformation was considered by equivalent volumetric change and yield strength of phases. Finite element modelling did not take in account the responses from individual phases. More specifically, the localised deformation at grain/phase boundaries/voids and their interactions under thermal loading were ignored, which has been proved critical for microcrack initiation [4].

The crystal plasticity finite element (CPFE) method is widely used to capture grain-level mechanical responses. It can also depict the phase discrepancy by considering individual phase crystal structures and their thermal-mechanical properties [25]. CPFE has been extensively used in crack initiation where stresses are generated all or in part by temperature change [25-27]. Moreover, the stress-strain response induced by thermal mismatch and grain level elastic anisotropy was examined [28]. Nonetheless, CPFE modelling of thermal cracking and grain/phase boundary damage, like the example in Fig. 1b, is scarce, probably due to the requirement of a specific modelling method for phase boundary behaviours [29]. Cohesive zone model (CZM) with traction-separation law is attractive, because of its capability on simulating microcrack initiation and failure of the phase/grain

boundary, which has been combined with CPFE to examine the overall failure process from stress/stain concentration to fracture [30, 31].

Thus, this study aims to establish a temperature-dependent CPFE coupled with CZM to provide insights into the thermal-stress-induced damage initiation, evolution and cracking in dual-phase steel, as well as investigate how underlying microstructure features, such as voids, phases and GBs, may affect the cracking behaviours. The proposed model and results are validated and supported by experimental characterisations of the samples fabricated by diffusion bonding. The effects of interfacial voids and their size, GB migration and grain orientation will be quantitatively analysed and compared. The experimental and modelling results enhance the understanding of the thermal crack formation and provide guidelines on improving thermal crack resistance in manufacturing.

## **2. Experimental method**

### **2.1 Diffusion bonding process**

The as-received material is commercial 9Cr-1Mo steel. The samples were first prepared by a diffusion bonding process. To obtain comparable results, the bonding surfaces of all samples were mechanically polished by SiC papers (up to P1200) and rinsed in propanolol before applying a load. The diffusion bonding was conducted in vacuum with a pressure just below  $5 \times 10^{-4}$  mbar. The heating rate and cooling rates were pre-set to be 1 °C/s. The bonding temperature was 900 °C with a compressive pressure of 15 MPa throughout the bonding cycle. The bonding temperature and pressure were maintained for 20 mins, 40 mins and 60 mins to reveal the effects of dwell time on the microstructure evolution.

The thermal cycle of diffusion bonding affects the microstructure evolution and phase transformation, since the phase transformation temperature (austenitisation process),  $A_1$  (820°C) 9Cr-1Mo steel [24] is lower than the bonding temperature (900°C). When the temperature is held at 900°C, a dual-phase microstructure comprising the ferrite and austenite phases is formed. The austenite phase was subsequently transformed into martensite during the cooling, according to Ref. [24], the martensite transformation starts at 375°C and ends at 200°C.

### **2.2 Microstructure characterization**

The microstructure at the bonding interface was characterised by scanning electron microscopy (SEM) and electron backscatter diffraction (EBSD). SEM analyses were performed in a TESCAN CLARA scanning electron microscope. EBSD was performed using the Oxford Instruments EBSD system. All samples were sectioned by electrical discharge machining (EDM) and metallographically ground by a series of SiC papers (up to P4000). To reveal the phase morphology, the samples were



then electropolished for 30 seconds in a solution of 10 vol% perchloric acids in glacial acetic acid at room temperature at the voltage of 25 V. For EBSD analysis, the samples were electropolished for 60 seconds in the same solution at the voltage of 15 V. The SEM accelerating voltage for EBSD mapping was selected to be 30 V, and the EBSD scanning step size was 0.15  $\mu\text{m}$ .

Fig. 2 shows the interface microstructure of the as-bonded samples under three bonding conditions. Figs. 2a and 2b are the EBSD-IPF (inverse pole figure) map and BC (band contrast) map acquired from the sample after 20mins bonding. The fine martensite with dark colour in the BC map can be seen due to the high density of lattice defects within the martensite phase. The coarser ferrite grains were also identified with relatively bright colour. The microstructure evolution as a function of bonding time is shown in Fig. 2c-h. After 20mins bonding, the bonding area shows a high fraction of connected interfacial grain boundary (IGB) cracks (see Fig. 2c and 2d), generating a long decohesion of bonding interface. As the bonding time increases, the fraction of IGB cracks decreases. In addition to IGB cracks, voids closure and IGB migration are two main microstructural evolution processes. As summarised in Fig. 3, the voids gradually close; meanwhile, IGBs migrate across the original bonding line. Whether the IGB migration and void closure are beneficial in resisting interfacial cracks during cooling is unknown. To clarify this question and reveal the associated underlying mechanism, the integrated CPFPE-microstructure characterisation systematically studied. .

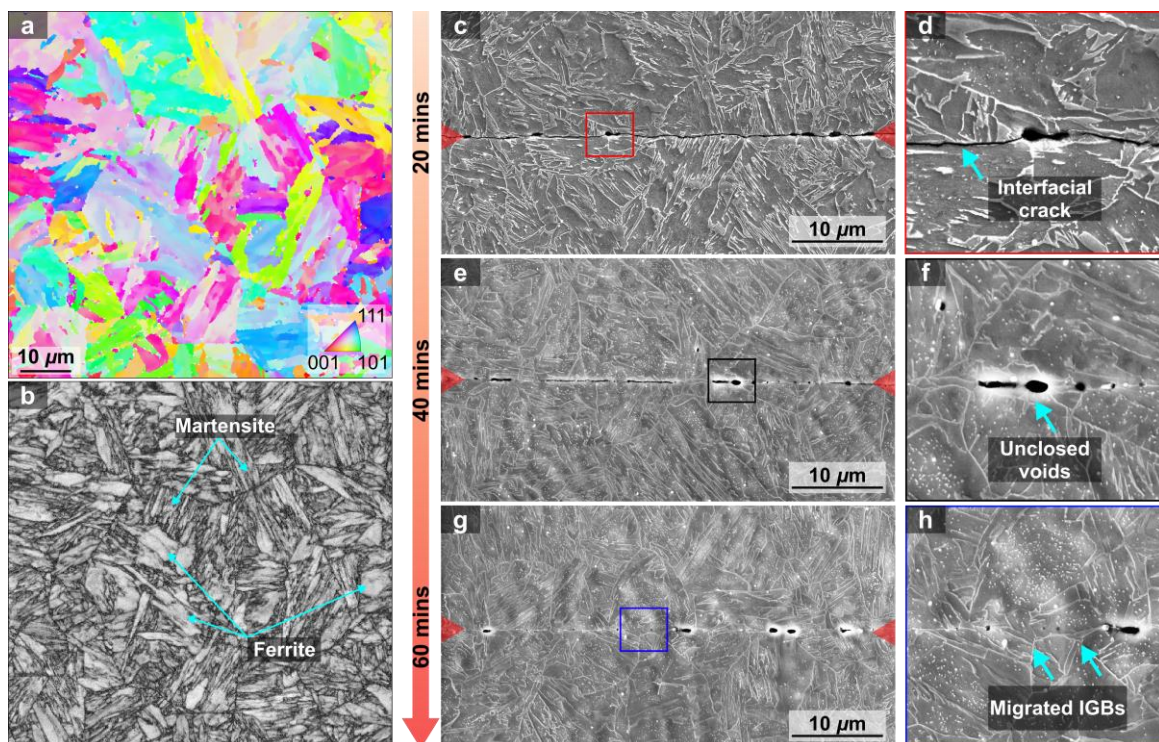


Fig. 2 Microstructure details of as-bonded 9Cr-1Mo steel after diffusion bonding at 900°C: (a) EBSD-IPF map after 20mins bonding, (b) EBSD-BC map after 20mins bonding, (c) and (d) SEM images after 20mins bonding, (e) and (f) SEM images after 40mins bonding, (g) and (h) SEM images after 60mins bonding

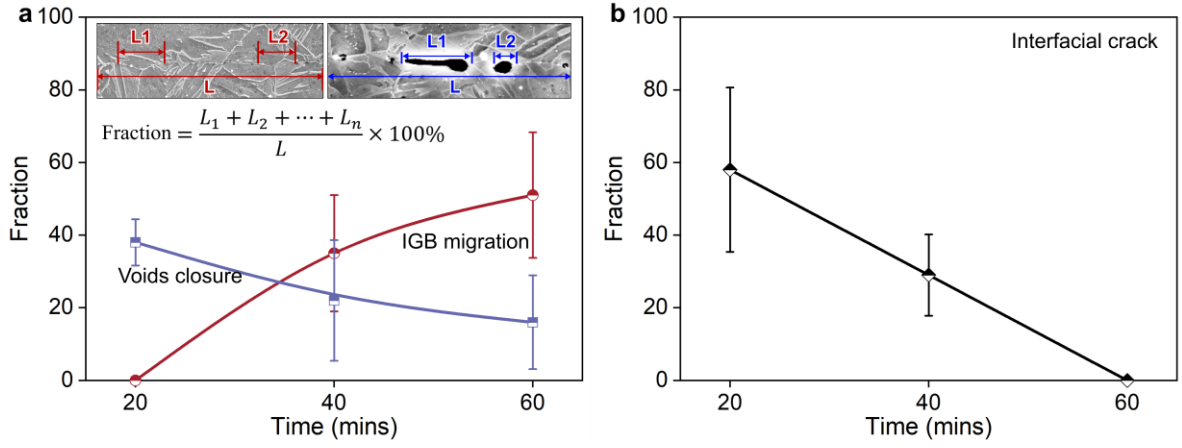


Fig. 3 Evolution of microstructure features with bonding time increase: (a) IGB migration and voids closure, and (b) interfacial crack

### 3. Modelling strategy

#### 3.1 Crystal plasticity-based microstructural model

A temperature-dependent crystal plasticity model was used to capture the stress-strain response during cooling. This model has been developed to reveal the anisotropic elasticity and plasticity by considering an individual phase's elasticity modulus, crystal slip systems and thermal expansion coefficient. In the work a dual-phase 9Cr-1Mo steel model comprising the martensite phase and ferrite phases was established.

The total deformation gradient  $\mathbf{F}$  of both martensite and ferrite phases multiplicatively decomposed into the elastic  $\mathbf{F}^*$ , plastic  $\mathbf{F}^P$  and thermal deformation  $\mathbf{F}^\theta$  gradients.

$$\mathbf{F} = \mathbf{F}^* \cdot \mathbf{F}^P \cdot \mathbf{F}^\theta \quad (1)$$

The lattice deformation due to temperature change is described by

$$\dot{\mathbf{F}}^\theta = \dot{T} \alpha_{th} \mathbf{F}^\theta \quad (2)$$

where  $T$  is the temperature and  $\alpha_{th}$  is the isotropic coefficient of thermal expansion (CTE).

The plastic velocity gradient  $\mathbf{L}^P$  in the ferrite phase is determined by the shear slip rates  $\dot{\gamma}^\alpha$  from all activated slip systems  $\alpha$ .

$$\mathbf{L}^P = \sum_{\alpha=1}^N \dot{\gamma}^\alpha \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha \quad (3)$$

where  $\mathbf{s}^\alpha$  represents slip direction and  $\mathbf{m}^\alpha$  is normal to the slip plane for the slip system  $\alpha$ ;  $N$  represents the total number of slip systems.

Following the approach of Voothaluru [32], the contribution of martensite phase transformation is taken into account as an additional term in  $\mathbf{L}^P$ :

$$\mathbf{L}^P = \sum_{\alpha=1}^N \dot{\gamma}^{\alpha} \mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha} + \sum_{x=1}^N \dot{\gamma}^x \mathbf{s}_{tr}^x \otimes \mathbf{m}_{tr}^x \quad (4)$$

where  $\mathbf{s}_{tr}^x$  and  $\mathbf{m}_{tr}^x$  are the transformation and habit vectors on the transformation system  $x$ . The shearing rate for each transformation system  $x$  is denoted by:

$$\dot{\gamma}^x = \gamma_{rt} \dot{f}^x \quad (5)$$

where  $\gamma_{rt}$  is a characteristic shear for transformation and  $\dot{f}^x$  is the volume fraction of martensite.

The relationship between the slip rate  $\dot{\gamma}^{\alpha}$  and the movement of dislocations is described by a dislocation-based Orowan equation [33], such that the slip rate on an individual slip system  $\alpha$  is determined by

$$\dot{\gamma}^{\alpha} = \rho_M b v^{\alpha} \quad (6)$$

where  $\rho_M$  is the mobile dislocation density,  $b$  is the magnitude of the Burgers vector,  $v^{\alpha}$  is the velocity of dislocations, which is determined by thermally activated dislocation escape from obstacles such as lattice defects [34]. The slip rate  $\dot{\gamma}^{\alpha}$  along the  $\alpha$  slip system can be further expressed as

$$\dot{\gamma}^{\alpha} = \rho_M b^2 v_0 \exp\left(-\frac{\Delta F}{k_B T}\right) \sinh\left(\frac{\Delta V}{k_B T} (|\tau^{\alpha}| - \tau_c^{\alpha})\right) \quad (7)$$

where  $T$  is the loading temperature,  $k_B$  is the Boltzmann constant,  $v_0$  is the jump frequency for dislocation escape,  $\Delta F$  is the activation energy,  $\Delta V$  is the activation volume,  $\tau^{\alpha}$  is the resolved shear stress and  $\tau_c^{\alpha}$  is the critical resolved shear stress.

A Taylor slip hardening rule is used for the evolution of critical resolved shear stress  $\tau_c^{\alpha}$  on the  $\alpha$  slip system [35]

$$\tau_c^{\alpha} = \tau_{c0} + \mu G b \sqrt{\rho_{SSD} + \rho_{GND}} \quad (8)$$

where  $G$  is the shear modulus of the material,  $\tau_{c0}$  is the initial critical resolved shear stress without dislocation density hardening,  $\mu$  is a dimensionless material-specific constant;  $\rho_{GND}$  is the density of geometrically necessary dislocations (GND);  $\rho_{SSD}$  is the density of statistically stored dislocations (SSD) determined by an equation using effective plastic strain as [36]

$$\dot{\rho}_{SSD} = \lambda \cdot \dot{p} \quad (9)$$

$$\dot{p} = \left(\frac{2}{3} \mathbf{D}^P : \mathbf{D}^P\right)^{1/2} \quad (10)$$

where  $\lambda$  is the hardening coefficient and  $\mathbf{D}^P$  is calculated from  $\mathbf{D}^P = \text{sym}(\mathbf{L}^P)$ .

The density of GND is calculated based on the Nye tensor, in which local plastic strain gradients supporting the lattice curvature are used

$$\mathbf{\Lambda} = \tilde{\mathbf{N}} \times \mathbf{F}^p = \sum_{i=1}^N \rho_{Gs}^{\alpha} \mathbf{b}^{\alpha} \otimes \mathbf{s}^{\alpha} + \rho_{Get}^{\alpha} \mathbf{b}^{\alpha} \otimes \mathbf{t}^{\alpha} + \rho_{Gen}^{\alpha} \mathbf{b}^{\alpha} \otimes \mathbf{m}^{\alpha} \quad (11)$$

where  $\rho_{Gen}^i$  is the normal component of the edge dislocation density,  $\rho_{Get}^i$  denotes the tangential component of the edge dislocation density, and  $\rho_{Gs}^i$  is screw dislocation component. Eq. (11) can be recast as

$$\mathbf{A}\rho_G = \bar{\mathbf{\Lambda}} \quad (12)$$

where  $\bar{\mathbf{\Lambda}}$  is the vectorized Nye's tensor and  $\mathbf{A}$  is a linear tensor. Because the Eqn. (12) cannot be uniquely solved, the L2 norm method is used according to Ref. [37-39]

$$\rho_{GND} = \sqrt{\sum_{i=1}^N (\rho_{Gs}^{\alpha})^2 + (\rho_{Get}^{\alpha})^2 + (\rho_{Gen}^{\alpha})^2} \quad (13)$$

The body centred cubic (BCC) crystal structure was used to describe the lattice structure of the martensite phase, which exhibits behaviour approximately similar to that of the BCT martensite [32].  $\langle 111 \rangle \{110\}$  and  $\langle 111 \rangle \{211\}$  24 slip systems in total are considered for both the martensite phase and ferrite phase. 24 transformation systems for martensite transformation are considered [40]. The dislocation-based crystal plasticity constitutive law was implemented as a UMAT subroutine of a finite element code in ABAQUS [34].

In order to calibrate the material properties of the two phases, the CPFE model was first used to simulate a simple uniaxial tensile condition. The virtual microstructures of the martensite and ferrite phases were defined by Neper [41]. Based on the characterisation results shown in Fig. 2, the average grain size of ferrite is set to  $30\mu\text{m}$ . The martensite phase exhibits a hierarchical microstructure in the EBSD map (Fig. 2a), in which three typical microstructure features corresponding to different length scales can be seen, namely the prior austenite grain boundary (PAGB), packets with polygonal shapes and strip-like blocks distributed in parallel. According to EBSD and SEM characterisation, the size of PAG was set to  $30\mu\text{m}$  with three packets in each grain, and the block's width is  $0.7\mu\text{m}$  in each packet. The quasi-3D CPFE model subject to plane stress condition was used [42] as shown in Fig. 4, in which the left, bottom and front surfaces are constrained by  $U_x=0$ ,  $U_y=0$  and  $U_z=0$ , respectively, while the front surface is free of any constraint. The material properties at room temperature are listed in Table 1. The tensile behaviour of the two phases are in good agreement with that in Ref. [43] for 9Cr-1Mo steel.

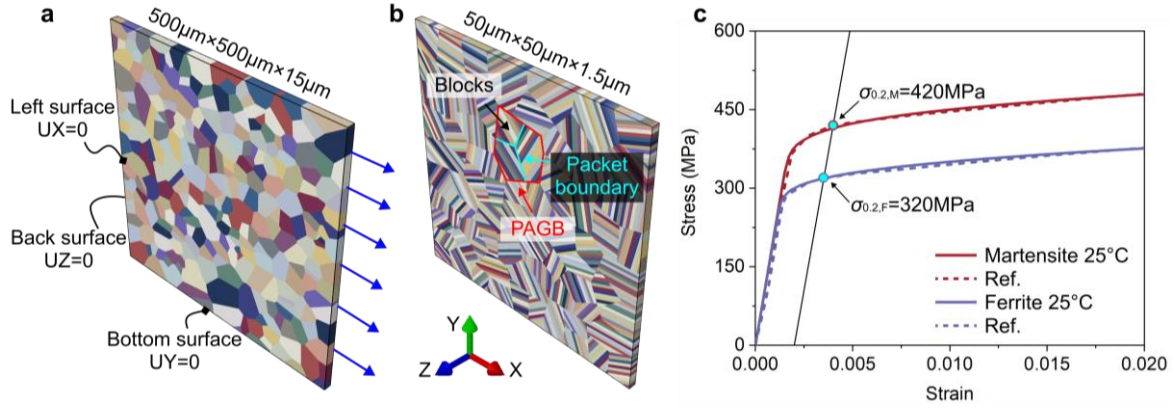


Fig. 4 CPFE model validation: (a) ferrite phase with plane stress boundary conditions, (b) martensite phase and (c) comparison of room temperature tensile behaviours with reference

Table 1 Material properties at room temperature used in CPFE

Phase	E (GPa)	G (GPa)	$\mu$	$\Delta V$ $\mu\text{m}^3$	$\Delta F$ (J)	$k_B$ (JK <sup>-1</sup> )	$\lambda$ ( $\mu\text{m}^{-2}$ )	$\tau_c^\alpha$ (MPa)	$b$ ( $\mu\text{m}$ )	$\rho_M$ ( $\mu\text{m}^{-2}$ )
Martensite	205.5 [4]	79	0.1	$40 \times b^3$	$2.60 \times 10^{-20}$	$1.38 \times 10^{-23}$	60	168.1	$2.5 \times 10^{-4}$	$1 \times 10^{-2}$
Ferrite	201.6 [4]	77.5	0.37	$40 \times b^3$ [44]	$2.60 \times 10^{-20}$ [44]	$1.38 \times 10^{-23}$	175	128.1 [44]	$2.5 \times 10^{-4}$ [44]	$1 \times 10^{-2}$ [44]

The temperature dependant CPFE material properties for 9Cr-1Mo steel were then determined. The temperature dependant Young's modulus of ferrite and martensite follows the linear equation according to Ref. [4]

$$E_F = \left(-\frac{8T}{95^\circ\text{C}} + \frac{3870}{19}\right)\text{GPa} \quad (14)$$

$$E_M = \left(-\frac{9T}{95^\circ\text{C}} + \frac{3950}{19}\right)\text{GPa} \quad (15)$$

Shear modulus was obtained based on  $E$  from  $G = E/(2(1 + \nu))$ , where  $\nu=0.3$ . The critical shear strength was first obtained according to the stress-strain curve in [43], and then set to be linearly dependent on temperature according to

$$\tau_{c,M}^\alpha = (-0.1T + 170.6)\text{MPa} \quad (16)$$

$$\tau_{c,F}^\alpha = (-0.09T + 130.3)\text{MPa} \quad (17)$$

The martensite phase transformation and associated discrepancy in thermal expansion between martensite and ferrite are the main reasons for internal stress. Given the  $M_s$  and  $M_f$  temperatures of the selected steel are  $375^\circ\text{C}$  and  $200^\circ\text{C}$ , respectively, the calculation domain in this work focuses on the temperature range from  $375^\circ\text{C}$  to room temperature ( $25^\circ\text{C}$ ) [4]. The representative finite element volume with martensite and ferrite phases is shown in Fig. 5. The volume consists of a

hierarchical martensite matrix as described in Fig. 4b. The interfacial void with 3 $\mu\text{m}$  length and 1 $\mu\text{m}$  width was located at IGB in the region of interest (ROI). To compare the effects of individual microstructure features on local cracking behaviour, three cases were defined as depicted in Fig. 5c: the case without a void, Type A where one side of the IGB is ferrite and Type B where both sides of IGB are ferrite. The individual martensite blocks and ferrite grains orientations were assigned by three Euler angles. No global texture was considered in the model, as we focus on the local behaviour around the IGB. However, to obtain comparable results, the grains at the triple junction of the IGB or void boundary are controlled with the same orientations in all cases. The “soft-hard” grain pair was artificially induced, as depicted in Fig. 5d. The maximum Schmid factor ( $SF_{\text{max}}$ ) of soft and hard grains were 5.0 and 3.5, respectively. It is noted that the finite element method was unable to illustrate the changes in grain morphology due to martensite phase transformation. Hence, the martensite phase in Fig. 5b is assumed to have hierarchical microstructure with BCC crystal structure from the beginning of the calculation (375°C).

During the temperature change in the calculation domain, the total strain is comprised of elastic deformation, plastic deformation, thermal expansion, volumetric change due to phase transformation and phase transformation plasticity [24]. The thermal expansion can be described by  $\alpha_{th}$  in Eqn. (2). For the martensite phase, the thermal expansion and volumetric change due to phase transformation can be combined mathematically to obtain the overall effective thermal coefficient  $\alpha_{th,M}$ ; this method has been successfully used in models of dual-phase steels [45-48]. The volumetric change of 9Cr-1Mo steel has been reported as  $3.75 \times 10^{-3}$  [45]. Thus, for the martensite phase, the strain rate induced by thermal expansion  $\dot{\epsilon}_T$  and volumetric change due to phase transformation  $\dot{\epsilon}_{VOL}$  can be expressed as

$$\dot{\epsilon}_T + \dot{\epsilon}_{VOL} = \alpha_{th} \dot{T} + 3.75 \times 10^{-3} \dot{f}^x \quad (M_f \leq T \leq M_s) \quad (18)$$

where  $f^x$  ranges from 0 to 1, linearly with temperature. Thus, the overall CTE of martensite  $\alpha_{th,M}$  is  $-0.84 \times 10^{-5}$  ( $M_f \leq T \leq M_s$ ) and  $1.3 \times 10^{-5}$  ( $T \leq M_f$ ) [49]. CTE of the ferrite phase  $\alpha_{th,F}$  is set to be  $1.4 \times 10^{-5} \text{ K}^{-1}$  throughout the calculated domain [49]. The phase transformation induced plasticity of the martensite phase is captured by Eqn. (4).



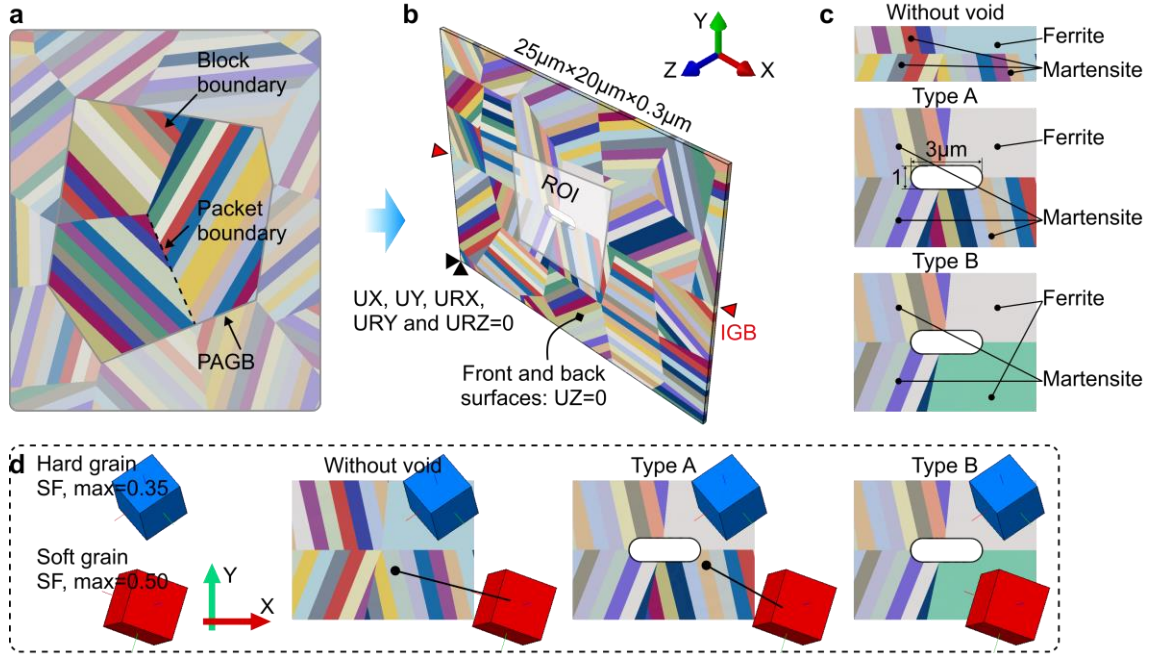


Fig. 5 Details of representative volume: (a) hierarchical structure of martensite, (b) boundary conditions and ROI, (c) three cases with different local microstructure in ROI, (d) orientation control in three cases.

### 3.2 Interfacial grain boundary damage model

Thermal cracking behaviour at the diffusion bonding interface were modelled by a cohesive zone model (CZM). The method is often used to model boundary cracks in metallic materials, such as nickel-based superalloy [31], twinning-induced plasticity steel [29] as well as 9Cr-1Mo steel [50, 51]. CZM can describe normal and shear stress localisation around the interface. The material interface will enter the damage stage when the local stress reaches the threshold, eventually initiating a crack. In this work, interfacial grain boundaries were assumed to follow a bi-linear traction-separation law (TSL), as shown in Fig. 6a. The GB was defined to be purely elastic with stiffness  $K_i$  until damage begins. When the traction force reaches the predefined threshold  $\tau_i^m$ , based on a damage initiation criterion, the GB will enter the damage stage during which the stiffness of the grain boundary reduces with increasing separation  $\delta_i$ . The IGB cracks will eventually initiate when the separation  $\delta_i$  reaches the threshold value  $\delta_i^f$ .

According to the TSL, the evolution of stress due to damage can be written as:

$$\tau_i = (1 - d_i)K_i\delta_i \quad (19)$$

where  $i = n$  and  $s$  represents the normal and shear direction;  $d_i$  is the stiffness damage factor, which is defined based on the energy criterion in the damage stage

$$d_i = \frac{\delta_i^f(\delta_i^{max} - \delta_i^0)}{\delta_i^{max}(\delta_i^f - \delta_i^0)} \quad (20)$$

where the  $\delta_i^f$  is a critical separation when cracking occurs,  $\delta_i^{max}$  refers to the maximum value of the effective separation achieved during the loading history, and  $\delta_i^0$  is the separation when the damage initiates. The relationship between  $\delta_i^f$  and cohesive energy  $G_i^C$  can be described as

$$\delta_i^f = 2G_i^C / \tau_i^m \quad (21)$$

Considering the complex stress state near the interface especially when microvoids exist, the TSL for the mixed-mode loading is illustrated in Fig. 6b. The maximum stress values  $\tau_n^m$  and  $\tau_s^m$  are the threshold stress for damage initiation, and the critical cohesive energy  $G_n^C$  and  $G_s^C$  are the threshold for cracks in the normal and shear directions, respectively. The quadratic nominal stress criterion (QUADS) considering the contribution from both normal and shear is

$$\left\{ \frac{\tau_n}{\tau_n^0} \right\}^2 + \left\{ \frac{\tau_s}{\tau_s^0} \right\}^2 = 1 \quad (22)$$

where the Macaulay bracket guarantees that the normal stress  $\tau_n$  is positive, while compression does not initiate damage. QUADS=1 represents damage initiation and GB softening. The damage variable (SDAG) evolution during softening is described by a power law as

$$\left\{ \frac{G_n}{G_n^C} \right\}^\lambda + \left\{ \frac{G_s}{G_s^C} \right\}^\lambda = 1 \quad (23)$$

where  $\lambda$  is an exponent that is set to unity according to Ref. [29].  $G_n^C$  and  $G_s^C$  are the cohesive energy under normal and shear loading modes.

Damage initiation is defined by QUADS, following Eqn. (22). Considering that the elastic stiffness of the IGB should be higher than that of the grain interior, the elastic stiffness of IGB at room temperature is thus defined by  $K_n = 210\text{GPa}$ ,  $K_s = K_n / (2(1 + \nu))$  [52]. The temperature-dependent  $K_i$  follow the same trend of martensite phase shown in Eqn. (15),  $K_n = (-\frac{9T}{95^\circ\text{C}} + \frac{4035}{19})\text{GPa}$ . The threshold of stress for damage initiation is normally defined as 1 to 4 times of yield strength [53]. Therefore, in the current work  $\tau_n = 546\text{MPa} \approx 1.3\sigma_{0.2,M}$  (Recall Fig. 4c), and  $\tau_s = 0.33\tau_n$ . The cohesive energy  $G_i$  is estimated by [31]

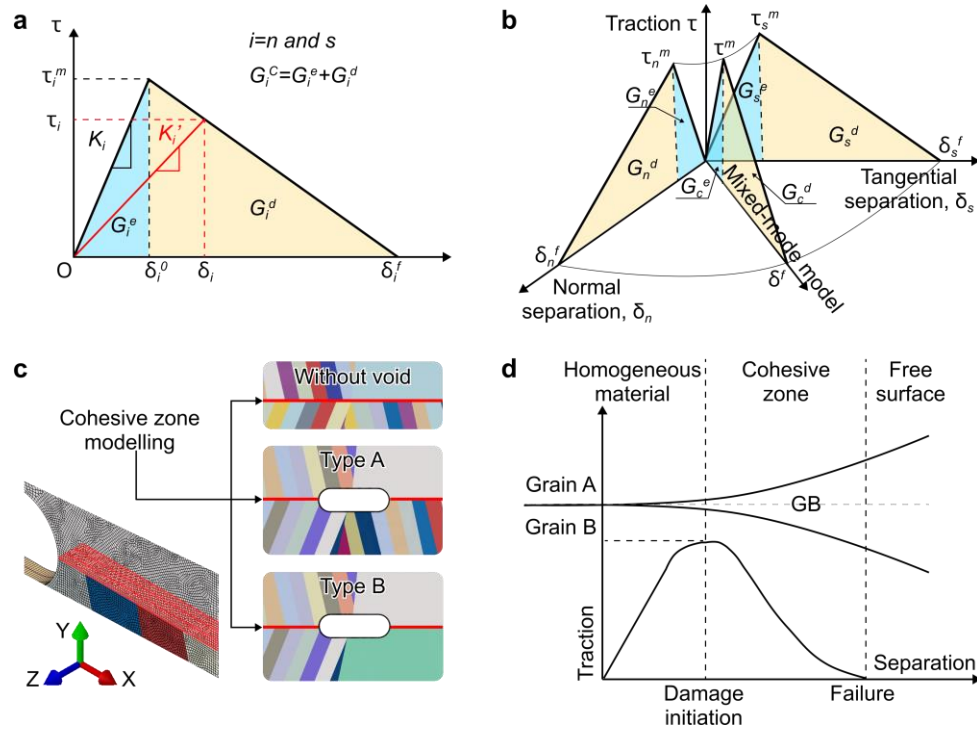
$$G_i = \frac{K_c^2(1-\nu^2)}{E} \quad (24)$$

Where  $K_c$  is the stress intensity factor, which is set to be  $24\text{MPa} \cdot \sqrt{\text{m}}$  according to the range reported in [54] for 9Cr-1Mo steel.

The integrated CPFE-CZM model can describe the deformation behaviours of both grain interior and GB. Specifically, the temperature-dependent CPFE can capture stress and strain localisation and slip activation under thermal loading. At the same time, CZM determines the damage of GB and updates the stress state with CPFE. By adopting this computational framework, the CPFE-CZM model for



three defined cases is shown in Fig. 6c. Fig. 6d illustrates the damage principle from initiation to propagation to final cracking in a specific IGB.



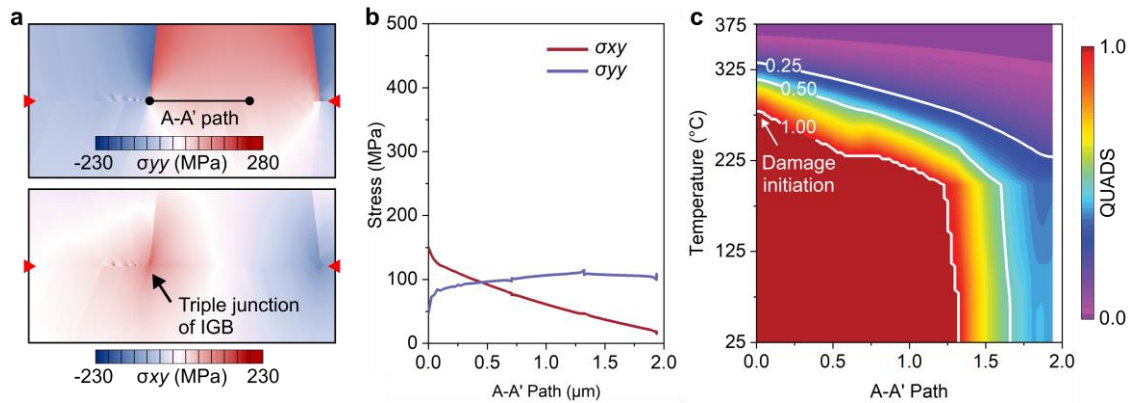
**Fig. 6 Details of CZM:** (a) bi-linear traction separation law and the nomenclature, (b) traction separation law for a normal load, shear load and mixed mode load, (c) setting of the integrated CPF-E-CZM model and (d) IGB damage principle.

## 4. Results and discussion

### 4.1 Interfacial grain boundary behaviours

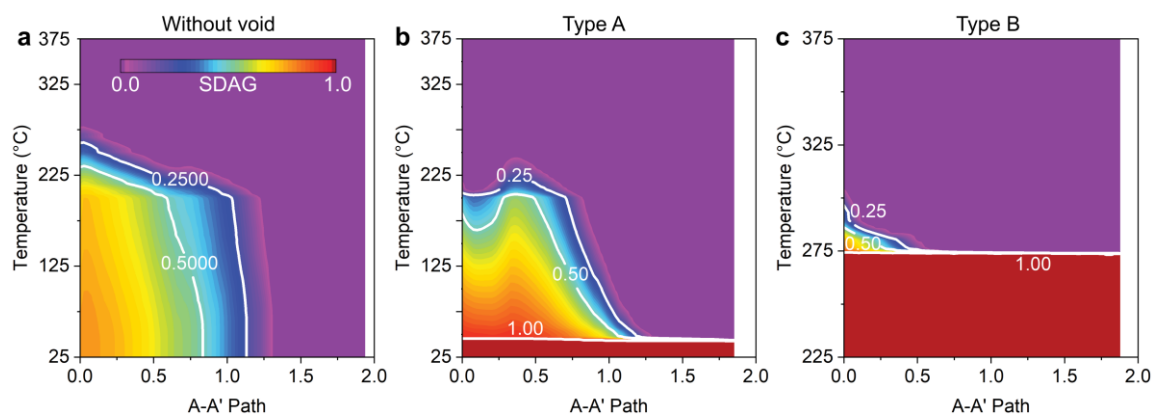
Fig. 7 shows the interfacial behaviour in absence of any interfacial voids. The distributions of normal  $\sigma_{yy}$  and shear stress  $\sigma_{xy}$  in Fig. 7a are obtained at the temperature where damage initiates, as indicated in Fig. 7c. Both normal  $\sigma_{yy}$  and shear stress  $\sigma_{xy}$  concentrate at the triple junction of the IGB. This site involves different phases adjacent to each other (phase boundary), where the mismatch of thermal expansion and the crystallographic misorientation are the main causes of the elevated stresses. Fig. 7b gives the stress profiles on path A-A', which clearly shows that the shear stress component  $\sigma_{xy}$  reaches its the maximum of 150 MPa at the triple junction and reduces as the distance from the triple junction increases. In comparison, the normal stress  $\sigma_{yy}$  at the triple junction is 50MPa, far less than the shear stress. Its magnitude gradually increases with distance, eventually reaching a plateau of about 100MPa. Considering the stress field along the A-A' path shown in Fig. 7a and b, Fig. 7c show the damage value (QUADS) along the A-A' path as a function of temperature. The damage initiates at the triple junction when the temperature reduced to about 280°C. The

length of damaged IGB gradually increases as the cooling continues and stops at  $1.32\mu\text{m}$  at the room temperature ( $25^\circ\text{C}$ ).



**Fig. 7 IGB behaviours in the case without void:** (a) normal  $\sigma_{yy}$  and shear stress  $\sigma_{xy}$  at the temperature where damage initiates, (b) line results of normal  $\sigma_{yy}$  and shear stress  $\sigma_{xy}$  at the same temperature of (a), (c) QUADS distribution along with IGB with the change of temperature

The damage processes and the cracking behaviours of all three cases (without void, Type A and Type B with voids) are presented in Fig. 8. First, the crack doesn't initiate in the case without the void, and the maximum SDAG is only about 0.8 at the triple junction (Fig. 8a), implying that the IGB would be safe if no voids or other defects exist. In contrast, thermal cracking occurs in both Type A and B (Fig. 8b and c) containing a micro-void, implying the adverse effects of interfacial voids on IGB damage. Recall that the grain on one side of IGB is martensite and another side is ferrite in Type A, unlike Type B where grains on both sides are ferrite. Even though the results shown in Fig. 8b and c indicate thermal cracks in both Type A and B regardless of the phase state around the void, the cracking behaviours of these two types are different, which is discussed in the following sections.

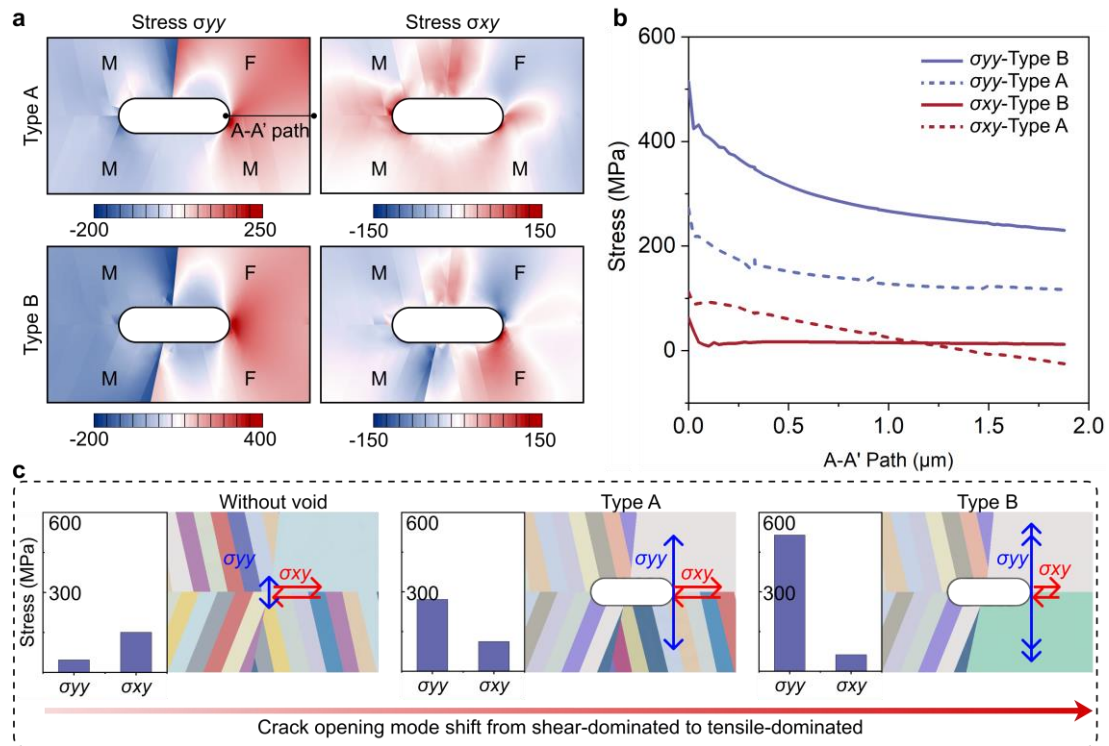


**Fig. 8 damage processes and the cracking behaviours of three cases corresponding to Fig. 6c:** (a) without void, (b) Type A and (c) Type B.

The stress localisations in Type A and B interfaces were further analysed to reveal the underlying cracking mechanism induced by the void. Fig. 9a illustrates the stress distributions of Type A and Type B interfaces. Both  $\sigma_{yy}$  and  $\sigma_{xy}$  are concentrated at the void boundary in Type A. Different from

the case without the void, the concentration of  $\sigma_{yy}$  in Type A is more pronounced than that of the  $\sigma_{xy}$ , as illustrated in Fig. 9b. The maximum  $\sigma_{yy}$  is about 280MPa at the void boundary. In contrast, the maximum  $\sigma_{xy}$  is about 100MPa and both reduce with distance away from the void boundary. Compared with the case without void, the shear stress  $\sigma_{xy}$  induced by the phase boundary still exists in Type A. In addition, the void introduces a high magnitude of  $\sigma_{yy}$  at IGB. In Type B, the grain on the two sides of IGB is set to be ferrite. Without the phase boundary at the IGB, the shear stress  $\sigma_{xy}$  is rather negligible. However, the normal stress  $\sigma_{yy}$  is found to be more severe, reaching about twice that in Type A interface (Fig. 9b).

From the results shown in Figs. 7, 8 and 9, the stress state at the IGB during cooling with and without considering the interfacial voids is revealed: First, the existence of the phase boundary induces a shear stress concentration, but the magnitude is not enough to open a crack under the calculated condition. Second, the interfacial voids trigger severe normal stress  $\sigma_{yy}$  at the void boundary in both Type A and Type B interfaces, which is the main cause of IGB thermal cracking. The stress state for IGB thermal crack opening is summarised and presented in Fig. 9c.



**Fig. 9 Stress state at IGB during cooling:** (a) distributions of  $\sigma_{yy}$  and  $\sigma_{xy}$  in Type A and B at 280°C, (b) line results in path A-A' according to Fig. 9a, (c) summary of stress opening mode for the cases without void and Types A and B with voids.

The stress evolution in Type A and B reveals the relationship between the stress components and IGB thermal cracking behaviours. Figs. 10a and 10d show the QUADS in Types A and B. Considering that the crystallographic orientations of grains in two types are the same, the thermal-induced IGB

damage is due to the different stress states in the two types. The evolutions of normal stress  $\sigma_{yy}$ , overlaid with the contour lines of QUADS=1, are shown in Fig. 10b and e. The damage initiation along with the IGB (refer to the contour lines of QUADS=1) shows good agreements with the maximum value of  $\sigma_{yy}$ , which provides compelling evidence of the dominant role played by  $\sigma_{yy}$  in thermal-induced IGB crack initiation and evolution in both Type A and B.

From the results in Fig. 8, the IGBs of both types are expected to be damaged and eventually cracked before cooling to room temperature. However, the damage or crack initiation and propagation in the two types are very different. The damage initiates at 242°C in Type A (Fig. 10a), introducing IGB thermal cracking at 45°C (Fig. 8b). In contrast, for Type B, the temperatures for damage initiation and cracking are 303°C (Fig. 10d) and 275°C (Fig. 8c), suggesting that in Type B, IGB has less damage resistance than Type A. The different cracking behaviours caused by the phase state between Type A and B are explained below. First, the magnitude of  $\sigma_{yy}$  in Type B is much higher than that in Type A, especially near the void boundary (also see Fig. 9b). Second, the morphology of martensite and ferrite is different. As shown in Fig. 10c and f, the  $\sigma_{yy}$  concentrates more in a local area near the void boundary in the single ferrite grain in Type B at three typical moments (QUADS=0.25, 0.5 and 1), while  $\sigma_{yy}$  in Type A shows a less concentrated distribution with continued cooling because of the interactions between martensite blocks (black arrow in Fig. 10c). The maximum value of  $\sigma_{yy}$  has moved to the position 0.45  $\mu\text{m}$  away from the void boundary at 251°C (Fig. 10b).

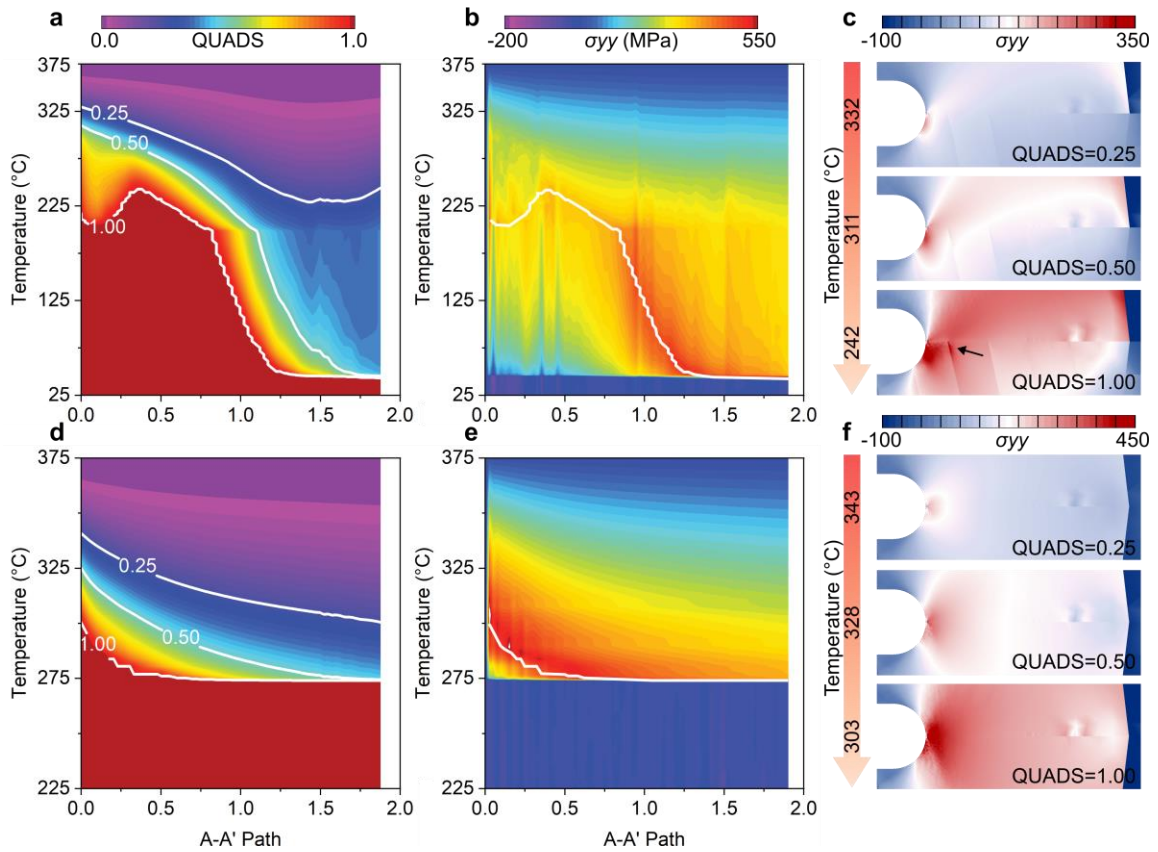


Fig. 10 Relationship between IGB damage behaviours and stress: (a) and (d) show evolutions of QUADS; (b) and (e) are evolutions of  $\sigma_{yy}$ , (c) and (f) are distributions of  $\sigma_{yy}$  at three typical moments. (a), (b) and (c) are results of Type A; (d), (e) and (f) are results of Type B.

## 4.2 Effects of Interfacial grain boundary migration

The effects of IGB migration on interfacial thermal cracks are studied in this section. The statistical results in Fig. 3a show that as the dwell time increases, the fraction of IGB migration increases while the fraction of interfacial cracks decreases. This implies the potential correlation between IGB migration and the reduction in thermal cracking. Fig. 11 provides more intuitive and evident traits which support the above-mentioned correlation. In Fig. 11a, the IGB migration occurs with the martensite phase within the grain. The martensite blocks are parallel but tilt toward the IGB plane. It is readily seen that the IGB thermal cracks stopped when it encountered migrated IGB (martensite phase). However, Fig. 11c shows that the crack first encountered the ferrite phase in the grain with migrated IGB. The crack passes through the ferrite phase but stops in front of the martensite phase, as shown in the enlarged figure in Fig. 11c. Another feature induced by IGB migration is that the crack path changes and follows the substructure boundary of the migrated grain, as shown in Fig. 11e. The schematic diagrams in Fig. 11 illustrate proposed crack propagation mechanism.



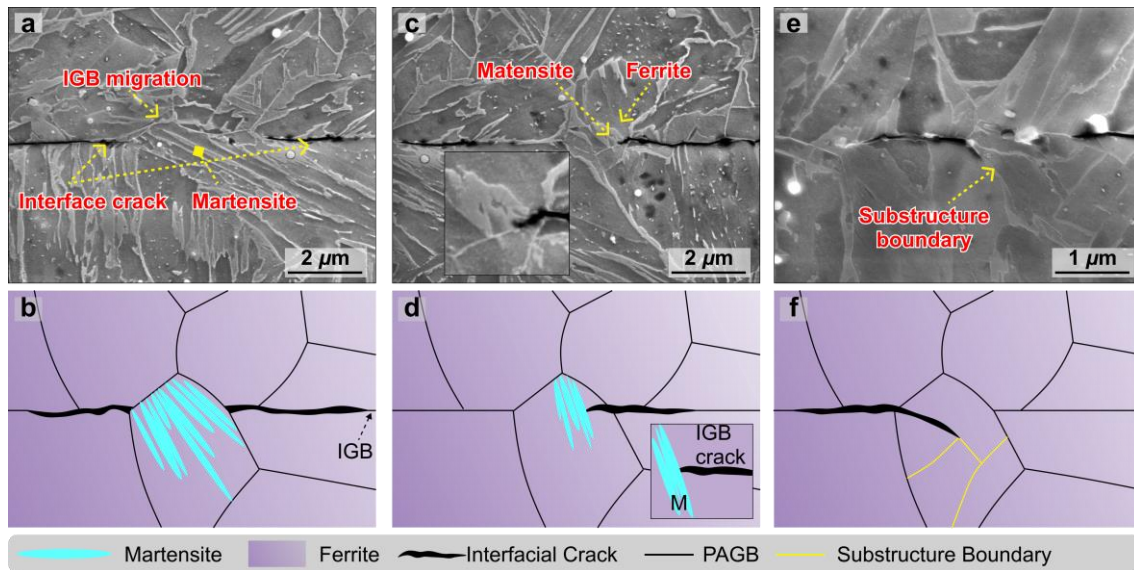
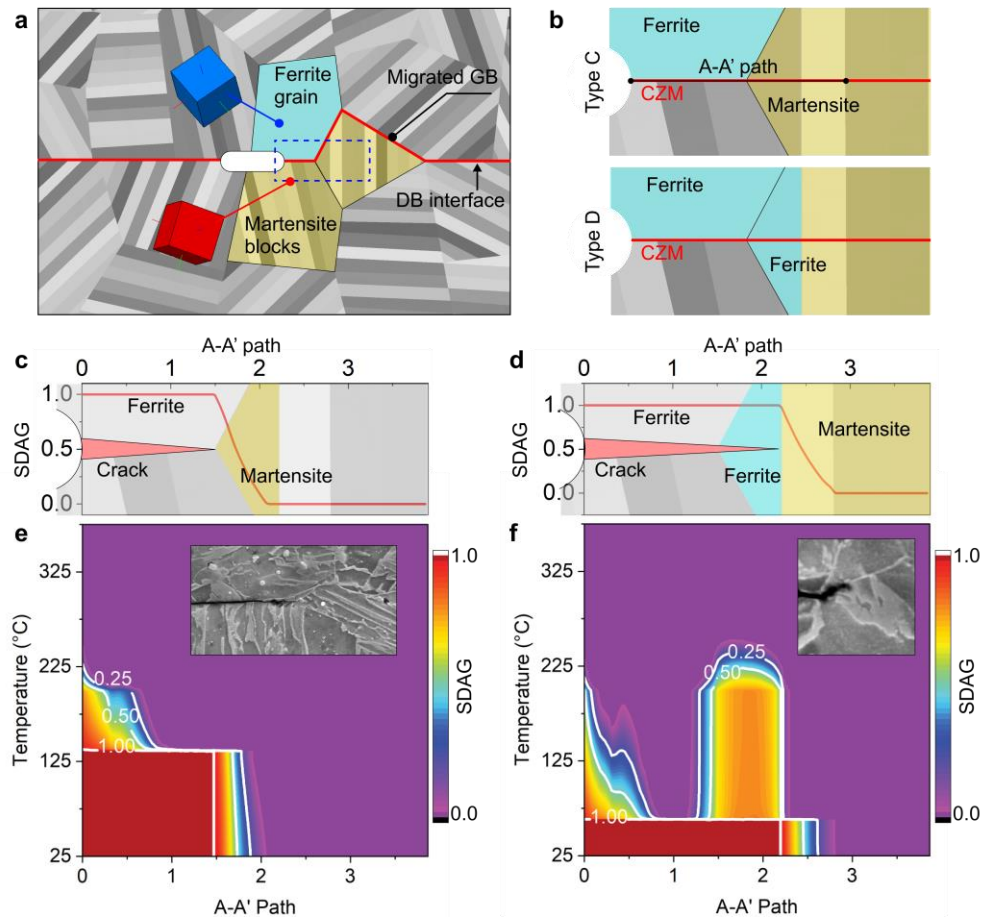


Fig. 11. Three microstructure features with respect to the effects of IGB migration on interfacial cracking: (a) and (b) show crack propagation stopping when it encountered a migrated IGB with martensite, (c) and (d) show the crack path through the ferrite but stopping in front of the martensite, (e) and (f) shows the crack following the substructure boundary of migrated grain.

To further understand the IGB migration and thermal cracking correlations shown in Fig. 11, the CPFE-CZM model was used accordingly. As shown in Fig. 12a, based on the grain morphology in Fig. 5b, the migrated IGB is initiated on the right side of the void. The grain orientations of ferrite and martensite blocks at the void boundary were controlled to be a “hard-soft” grain pair, the same as with Type A in Fig. 5. The migrated grain was subdivided into martensite blocks, which are perpendicular to the IGB plane. Two types were considered according to the experimental observation shown in Fig. 11a and c, named Type C and Type D. In Type C, the phase of the migrated grain is full martensite blocks corresponding to the phase distribution in Fig. 11a. In Type D, the first block on the left side of migrated grain is set to be the ferrite phase, which the IGB crack will first encounter during cooling according to the phase distribution in Fig. 11c. It should be noted that to consider both IGB and intragranular thermal cracking, the CZM is used in both IGB and martensite/ferrite interiors, as shown in Fig. 12b. The damage and crack criteria are the same for both IGB and grain interior throughout the whole CZM model. Once the stress in the bulk of the grain reaches the critical value, intragranular failure occurs and final macroscopic cracks can be observed. The differences in crack resistance of GB and grain interior are not considered in Type C and Type D, but comparable results can be obtained based on the model, which allows us to correlate the IGB migration-phase state to stress state-cracking behaviours.

Fig. 12c shows the damage variation along the A-A' path of Type C after cooling to room temperature. The phase map is overlaid to show crack behaviours with different phases. Results indicate that the crack (where SDAG=1) stops when it encounters the migrated IGB with the martensite phase. The SDAG gradually decreases through the martensite interior and eventually drops to zero. On the

contrary, the crack propagates through the ferrite phase (SDAG=1) in the migrated grain in Type D (Fig. 12d), but it is hindered by the martensite phase with the decreases in SDAG. Results in Fig. 12c and d show good agreements for each selected phase distribution to the experimental observations obtained in Fig. 11. Moreover, the IGB damage evolutions in Type C and D captured by the model are shown in Fig. 12e and f. The damage initiates at about 225°C in both types, which is not influenced by the phase distribution.



**Fig. 12 Model details and cracking behaviours considering the IGB migration:** (a) grain morphology, (b) two types with different phase distribution, (c) SDAG of Type C after cooling with phase distribution overlaid, (d) SDAG of Type D after cooling, (e) SDAG evolution of Type C, (f) SDAG evolution of Type D

The IGB cracking behaviours shown above are strongly influenced by the IGB migration and predominantly because of their phase distribution in the migrated grain. The intrinsic effects of IGB migration and associated phase distribution on the stress state are further discussed in Fig. 13. The evolution of normal  $\sigma_{yy}$  and shear stress  $\sigma_{xy}$  in Type C at IGB (refer to F/M interface in Fig. 13) follow the same rule as described in Section 4.1 and the damage initiation is dominated by the normal component  $\sigma_{yy}$ . However, the normal stress diminishes sharply at the triple junction of migrated GB, and then explicitly exhibits lower or negative  $\sigma_{yy}$  in the martensite blocks, which would contribute less to crack opening. The shear component  $\sigma_{xy}$  at the martensite phase is relatively higher due to

the thermal expansion mismatch induced by the phase boundary, but the  $\sigma_{xy}$  alone at the interface is insufficient to open a crack, as discussed in Section 4.1. Fig. 13c explicitly shows stress components and QUADS variation along the A-A' path at 325°C. The predicted stress histories in Type D are shown in Fig. 13d, e and f. The ferrite interior exhibits considerable  $\sigma_{yy}$  at the beginning of the damage initiation (Fig. 13d). This is because thermal expansion and phase transformation of the martensite phase would induce the internal loading expected to be accommodated by the relatively soft ferrite phase. Consequently, the internal stress for both normal  $\sigma_{yy}$  and shear  $\sigma_{xy}$  components are high in the ferrite grain, as depicted in Fig. 13d and e, which further generates grain damage (Fig. 13f) and a crack path for IGB cracking.

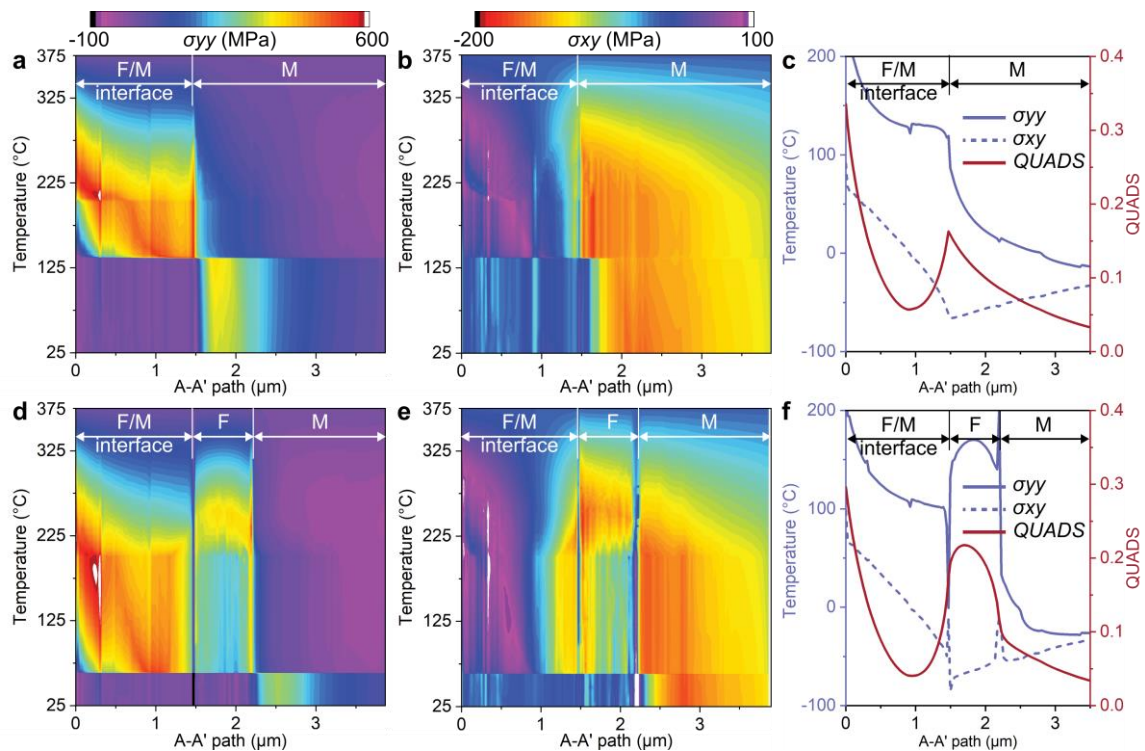


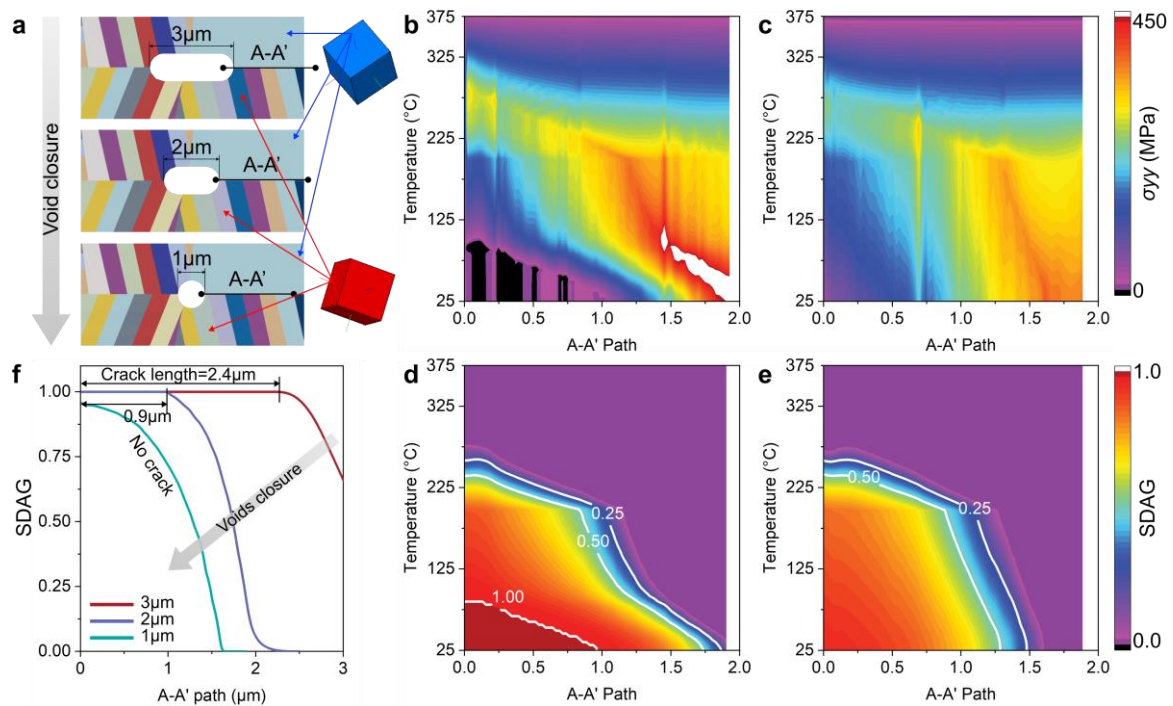
Fig. 13 Evolution of stress components and IGB damage with respect to the effects of IGB migration: (a) and (b)  $\sigma_{yy}$  and  $\sigma_{xy}$  in Type C, (c) line results of  $\sigma_{yy}$ ,  $\sigma_{xy}$  and QUADS in Type C, (d) and (e)  $\sigma_{yy}$  and  $\sigma_{xy}$  in Type D, (f) line results of  $\sigma_{yy}$ ,  $\sigma_{xy}$  and QUADS in Type D

### 4.3 Effects of void closure

The effects of voids closure on thermal cracking are presented in Fig. 14. The models with three sizes of void (3μm, 2μm and 1μm) are established based on the grain morphology of Type A shown in Fig. 5b. To obtain comparable results, the orientations of the ferrite grains and martensite blocks on the right side of the void are kept the same as shown in Fig. 14a. The thermal cracking behaviour seems to correlate with the existence of voids, due to the highly concentrated normal stress  $\sigma_{yy}$  on the void boundary. The evolution of  $\sigma_{yy}$  in the cases with 1μm and 2μm void is thus shown in Fig. 14 b and c.



Compared with the 2 $\mu\text{m}$  void, the 1 $\mu\text{m}$  void introduces a moderate  $\sigma_{yy}$  at the void boundary from the beginning of the damage initiation (about 275°C in Fig. 14b). Consequently, the case with 1 $\mu\text{m}$  void shows a short length of IGB that suffers damage (1.6 $\mu\text{m}$ ) compared to the 4.1 $\mu\text{m}$  (which passed through the whole ferrite/martensite interface) in 3 $\mu\text{m}$  void case. More importantly, as summarised in Fig. 14f, the length of the crack reduces with voids closure. The length of the crack is 0.9 $\mu\text{m}$  in the 2 $\mu\text{m}$  void case, which is three times shorter than that of the 3 $\mu\text{m}$  void case. No crack occurs in the case with a void that shrinks to 1 $\mu\text{m}$ , which gives a huge optimisation potential to improve the joint mechanical properties.



**Fig. 14** Effects of void closure on IGB cracking: (a) models with three sizes of voids, (b) evolution of  $\sigma_{yy}$  with 2 $\mu\text{m}$  void, (c) evolution of  $\sigma_{yy}$  with 1 $\mu\text{m}$  void, (d) evolution of SDAG with 2 $\mu\text{m}$  void, (e) evolution of  $\sigma_{yy}$  with 1 $\mu\text{m}$  void, (f) comparison of SDAG obtained after the cooling process among three models

#### 4.4 Effects of crystallographic orientation

The results in Section 4.1 suggest a strong correlation between the phase distribution and thermal crack initiation, which could eventually lead to IGB thermal cracks. The intrinsic reason behind this is the change in the stress field, which stems from the combination of different phases on the two sides of the IGB so as to affect IGB damage. The stress field in the local area around voids is in the length scale of the grain size; the micromechanical response from that scale is sensitive to the crystallographic orientation. This section thus further examines the crystallographic sensitivity of IGB damage. Fig. 15a indicates the grain orientations in Type A and Type E. Based on the orientations in Type A, the ferrite grain in Type E is set to be the same as the martensite block, with the 'soft'

orientation along the  $y$  direction. It was found that the change in orientation of ferrite grain activates different slip systems in the adjacent martensite blocks. Fig. 15b illustrates the primary and secondary slip field of the martensite block at about 280°C in both types, results from which show that the primary and secondary activated slip systems in Type A are different from those in Type E. It is notable that the slip fields in Type A generate a large plastic zone where the activated slip systems promote long-range dislocation slip, from the void boundary to the boundary between Block A and Block B (white arrow in Fig. 15b). Hence, the IGB damage in Type E is obviously different from Type A (Fig. 10a), as shown in Fig. 16a. The evolutions of  $\sigma_{yy}$  are shown in Fig. 16b. In Type A, the maximum value of  $\sigma_{yy}$  along the IGB gradually moves to the boundary of Block A/B due to the pile-up of long slide dislocations. However, the activated slip systems in Type E generate a highly concentrated  $\sigma_{yy}$  at the void boundary, adversely damaging the IGB so as to generate the crack in the early stage of cooling (Fig. 16a). The damage initiation behaviours at the void boundary and boundary of Block A/B are shown in Fig. 16c. The damage induced by thermal loading is sustained by a long IGB in Type A, which thus show a better crack resistance.

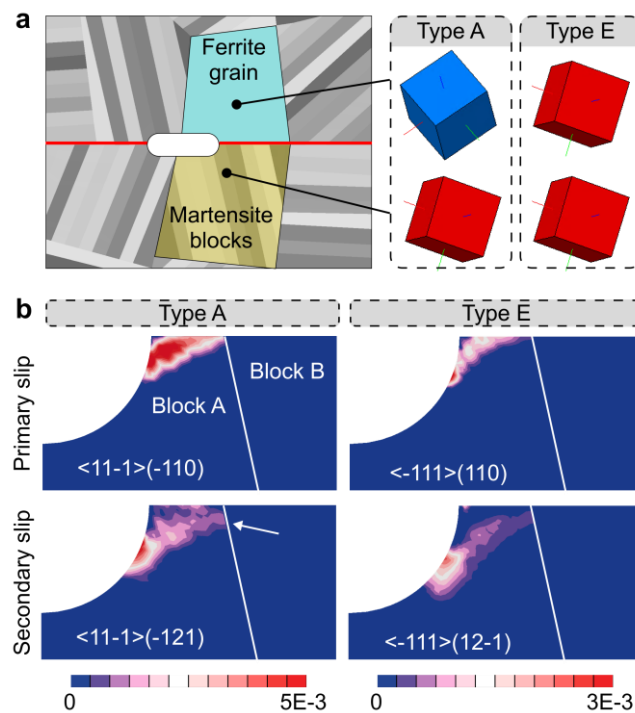


Fig. 15 Model details in discussing crystallographic effects: (a) grain orientations in Type A and Type E, (b) primary and secondary slip field in Type A and Type E

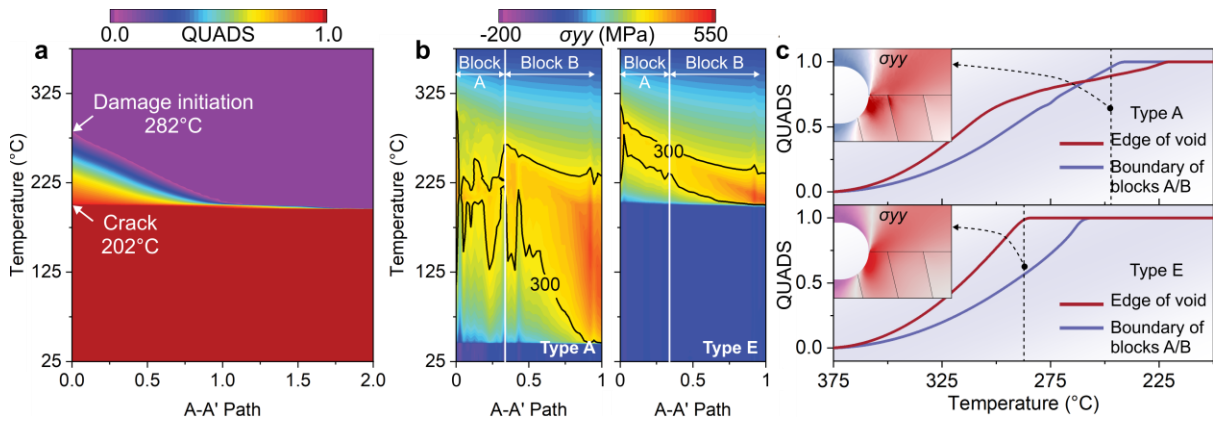


Fig. 16 Comparison of IGB damage behaviour in Type A and Type E: (a) QUADS in Type E, (b)  $\sigma_{yy}$  in Type A and Type E, (c) QUADS at void boundary and boundary of Block A/B

In addition to Type A and Type E, the grain pairs with different misorientations of IGB have been examined. The misorientation of the tested IGBs covers the full range of misorientation in BCC crystal structure, ranging from  $10^\circ$  to  $60^\circ$ . To reduce the indeterminacy, the orientation of Grain C is fixed. The Euler angles and misorientation used are summarized in Table 2. As shown in Fig. 17, no direct relationship was found between the observed IGB damage process/cracking behaviours and grain boundary angle. Nonetheless, the IGB in all 8 cases suffers cracking, and the average cracking moment is when the temperature drops to about  $143^\circ\text{C}$ , with a standard deviation of  $59^\circ\text{C}$ .

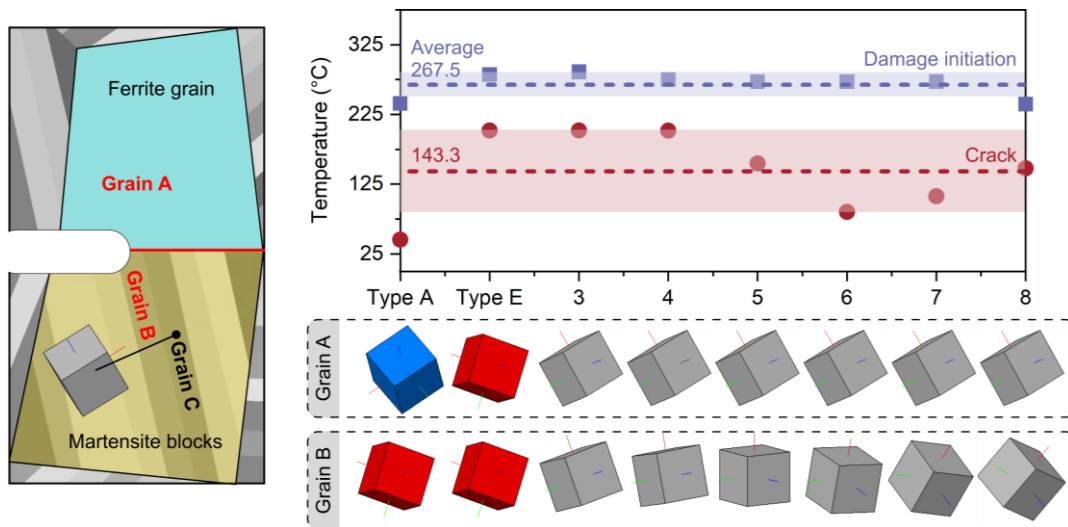


Fig. 17 Crystallographic sensitivity of IGB damaging and cracking.

Table 2 Euler angle and misorientation

	Type A	Type E	3	4	5	6	7	8
Grain A	195.6, 33.9, 21.5	104.9, 19.7, 56.9			113, 32, 7			
Grain B	104.9, 19.7, 56.9	104.9, 19.7, 56.9	104, 30, 6	97, 29, 3.5	75, 34, 18	56, 38,30	36, 50, 35	40, 53, 16
Misorientation			$10^\circ$	$20^\circ$	$30^\circ$	$40^\circ$	$50^\circ$	$60^\circ$

The quantitative results of microstructure effects on IGB cracking are summarized in Table 3 based on all selected cases. It is seen that the void has the most pronounced effects as it directly determines whether cracking occurs. The second important feature is the phase state, as it determines the local stress state so as to influence the damage behaviours of IGB (recall Fig. 10). The crystallographic orientation is estimated to be the less important feature.

**Table 3 Effects of microstructure features on IGB cracking**

	Size of void	Phase state	Grain orientation
Length of crack-best case	No crack (Fig. 7)	2.7 $\mu\text{m}$ (Type A)	2.7 $\mu\text{m}$ (Type A)
Temperature of cracking-best case	No crack (Fig. 7)	45°C (Type A)	45°C (Type A)
Length of crack-worst case	2.7 $\mu\text{m}$ (Type A)	4.1 $\mu\text{m}$ (Type B)	2.9 (Type E)
Temperature of cracking-worst case	45°C (Type A)	275°C (Type B)	202°C (Type E)

## 5. Conclusions

A CPFE-CZM coupled model is developed to provide fundamental insights into thermal cracking in diffusion bonded 9Cr-1Mo steel. The CPFE-CZM is a micromechanical model reflecting the effects of microstructural variables, such as voids, phases and GBs, on thermal cracking. By examining the 9Cr-1Mo steel fabricated through diffusion bonding, the damage initiation and cracking of the IGB were simulated; effects of an interfacial void and its size, GB migration and grain orientation were quantitatively analysed and compared. The main conclusions are summarised below:

1. The stress at void-free IGB between martensite and ferrite is dominated by the shear stress, the magnitude of which is too small to initiate a crack. The existence of voids at IGB induces considerably higher normal stress, which is the main cause of Interfacial Grain Boundary (IGB) cracking.
2. Characterisation results show that the presence of martensite in the migrated grains can stop the interfacial cracking, while the ferrite grains are more susceptible to cracking. The computational results reproduced this phenomenon and point out that high normal tensile stresses are developed inside ferrite grains during cooling, which may pave the way for cracking and eventual fracture. On the contrary, limited normal tensile stress was developed in martensite, which thus shows high cracking resistance.
3. The void size has a significant effect on damage initiation and cracking. Under the selected conditions, in the 2 $\mu\text{m}$  void case, the length of the crack is 0.9 $\mu\text{m}$ , three times shorter than that around the 3 $\mu\text{m}$  void. No cracking occurs if a void is less than 1 $\mu\text{m}$ . The new finding could be used as a criterion to ensure the material's full performance.

4. Based on the quantitative analysis, the void has the most pronounced effects on thermal cracking, followed by phase state, while the crystallographic orientation is the less important parameter.

## 6. Acknowledgements

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