

Slip system-resolved GNDs and SEDs: A multi-scale framework for predicting crack nucleation in single-crystal metals

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ABSTRACT

Scalar forms of geometrically necessary dislocation (GND) and stored energy density (SED) are commonly used to capture localized strain gradients and damage in metals. However, these scalar approaches fail to provide detailed information at individual slip systems, thereby diminishing the slip system-dependent features critical to understanding plasticity and damage behavior. Here, we develop methods to resolve GNDs and SEDs onto individual slip systems through experimental techniques including multi-scale digital image correlation (DIC) and electron backscatter diffraction (EBSD), together with multi-scale simulation approaches including crystal plasticity finite element (CPFE) and discrete dislocation plasticity (DDP). These methods are applied to single-crystal (SX) plates with a circular hole, eliminating the interference from grain boundaries. In contrast to the scalar GNDs, the resolved GNDs show pronounced slip system-dependent and asymmetric distributions around the hole circumference. In addition, the resolved GNDs migrate along with the extension of slip band boundaries, with the growth rate accelerating in the later stages of deformation. Furthermore, under the CPFE framework, the GNDs-mediated SEDs successfully capture the asymmetric cracking behavior and crystallographic planes of crack nucleation observed in the in-situ DIC tests, which cannot be reflected in conventional scalar SEDs. Moreover, compared with micro-DIC (μ DIC) results, the resolved SEDs in the DDP framework accurately capture the slip trace-induced crack nucleation at the micro-scale. The GND-mediated resolved SEDs demonstrate strong potential as a universal damage indicator for metallic materials, enabling accurate prediction of crack nucleation at the micro-scale.

1. Introduction

Dislocations in metallic materials are known as the important carriers of plastic deformation, which play a dominant role in the fracture failure of materials [1–3]. The dislocations are categorized into statistically stored dislocations (SSDs) associated with homogeneous plastic deformation, and geometrically necessary dislocations (GNDs) induced by the gradients of plastic slip [4,5]. Among these, GNDs play a crucial role in causing extra strengthening of the metals with heterogeneous or

gradient microstructures, which significantly enhance the macroscopic performance [6–9]. Mediated by GND, the stored energy density (SED) is widely recognized as a microstructure-sensitive damage indicator [10, 11], which drives microcrack nucleation and propagation [12,13]. In previous studies, the scalar representations of GND and SED were commonly used to capture the strain gradients and damage [14]. By definition, GND is inherently a vector with components specific to individual slip systems, and SED similarly exhibits dependence on individual slip systems [4,10]. However, the scalar forms of GND and SED

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neglect critical physical information at higher dimensions, leading to incomplete or inaccurate characterization of strain gradients and damage.

Some experimental approaches have been developed to map the GND density within metallic materials. Based on the crystallographic orientation distribution characterized using electron backscatter diffraction (EBSD), the Nye tensor was derived from the lattice curvature tensor defined as the spatial derivatives of the misorientation matrix [15]. The scalar GND in EBSD analysis was further calculated through the norm of the Nye tensor [16]. Based on the assumption that GNDs at individual slip systems exist in the configuration with the lowest total energy, some energy minimization algorithms were developed to estimate the resolved GND densities [17–20]. Nevertheless, due to the lack of comparisons with other characterization methods, the EBSD-based algorithm for resolving GNDs onto individual slip systems has not been comprehensively assessed and validated. Furthermore, the digital image correlation (DIC) technique offers opportunities to map the in-plane deformation fields at multi-scales [21–23]. By constructing the fields of plastic deformation gradients using DIC, the scalar GND density was experimentally determined based on the norm of the spatial derivatives of plastic deformation gradients [11,12]. Nevertheless, this DIC-based algorithm is inconsistent with the original slip system-dependent definition of GND densities, as the GNDs are physically defined as the gradients of resolved shear strain along the slip direction [4]. The number of slip system-dependent GNDs to be determined (18 independent components for FCC [15], including 12 edge and 6 screw components) significantly exceeds the constraints provided by the Nye tensor, which has only 9 components [24]. As a result, conventional DIC-based algorithms are limited to determining the scalar form of GND, restricting their applicability in analyzing the distributions of GNDs resolved across individual slip systems.

Additionally, some simulation approaches have been developed to determine the GND density and its derived SED. By incorporating crystallographic slip, the crystal plasticity finite element (CPFE) method effectively captures the anisotropic mechanical response of individual grains at the meso-scale [25–27]. Under the CPFE framework, the scalar GND is commonly used to capture the strain gradient strengthening, which is calculated using the norm of Nye tensor derived from the simulated plastic strain gradient [11,25,28]. As a result, due to the absence of slip system-dependent GNDs, the SED as an important damage indicator was only expressed in its scalar form, which fails to capture the physics of damage distributed across slip systems in CPFE simulation. On the other hand, the discrete dislocation plasticity (DDP) method has been extensively used to investigate plastic deformation at the micro-scale [29,30]. Featured by modeling the activities of individual dislocations at specific slip systems, the DDP simulation framework captures the discrete nature of dislocation patterns and thereby explicitly determines the local dislocation density. Net Burger's vector is employed to find the homogenized scalar GND density in the DDP framework [31], and it serves as a prerequisite to spontaneously calculate the slip system-dependent configuration energy density (CED) and SED [32,33]. Therefore, it is essential to develop GND-mediated resolved SEDs within multi-scale simulation frameworks and employ CPFE and DDP to validate the resolved SEDs against in-situ observations across different scales.

In previous studies, the GND densities at individual slip systems were resolved in some polycrystalline metals, including Al-Mg / Mg alloys (FCC) [34,35], Zr alloys (HCP) [36], and pure Ti (HCP) [37]. For instance, in Al-Mg polycrystals [34], the distribution patterns and evolution of resolved GNDs were analyzed across approximately 8 grains.

The intragranular localized GNDs along sub-grain boundaries (GBs) and slip bands were revealed with a good contrast. However, affected by the initial distribution of Euler angles in polycrystals, the initial misorientations, stress/strain localizations, and slip transfer at GBs introduce unnecessary factors that complicate the interpretation of slip system-dependent GNDs. These complexities in polycrystals also pose challenges to the validation of algorithms for resolving GNDs. Therefore, it is more appropriate to employ single crystals (SXs) to investigate the resolved GNDs and GNDs-mediated SEDs at individual slip systems.

Here, we present a comprehensive study focused on resolving GNDs and SEDs at individual slip systems through a combination of experimental techniques (DIC and EBSD) and simulation methods (CPFE and DDP). The proposed methods are applied to SX plates with a circular hole. A multi-scale DIC technique is developed to capture resolved GNDs at both submillimeter-scale and micro-scale, enabling quantitative comparisons with GNDs resolved using EBSD, CPFE, and DDP. Finally, the crystallographic planes of crack nucleation and cracking locations observed through multi-scale DIC are compared against the predictions from resolved SEDs and conventional scalar SED, highlighting the advances presented by GNDs-mediated resolved SEDs in accurately capturing crack initiation.

2. Methods

2.1. DIC and EBSD characterization

An as-cast Ni-based SX superalloy (Fig. 1a) with an FCC lattice is selected for in-situ tensile tests combined with DIC and EBSD analyses. This material is widely used in the turbine blades of advanced aero-engines [38]. The detailed chemical compositions and heat-treatment procedure can be found in the reference, and there are no initial dislocations in the as-received SXs [39]. The plate-like specimens with a central circular hole are used in the in-situ tensile tests (Fig. 1b2), which represent the geometric features of film cooling holes in advanced turbine blades [40]. These circular holes are fabricated using the electrochemical jet drilling technique, which minimizes geometric deviation, and prevents the formation of re-cast layers and oxidation/corrosion layers [41]. The in-situ tensile tests combined with DIC are performed under a scanning electron microscope (SEM) (EVO18, Carl Zeiss, Germany), using a mini tensile tester (SEMTesler, MTI Instrument, USA) with a displacement rate of 0.5 mm/s (Fig. 1b1). Additionally, two orientations are chosen for the tests (Fig. 1b3), where the x-axis roughly aligns with $\langle 001 \rangle$ for both, and the y-axis approximately aligns with $\langle 100 \rangle$ and $\langle 110 \rangle$ for #1 and #2, respectively.

A multi-scale DIC technique is developed in this work (Fig. 1c). Two parallel lines with a spacing of 3 mm are drawn on the surface of specimens using laser machining, which are employed to measure the global strain within the gauge length. A ZrO₂ powder-based speckle pattern is applied to the DIC 1 region to capture deformation at the submillimeter-scale with a step size of 2 μm , which is subsequently compared with the CPFE results. After the chemical etching [39], the microstructures of γ/γ' phases are utilized as the deformation carriers within the region of DIC 2 at the micro-scale (step size = 0.19 μm). The micro-DIC (μDIC) results are utilized to justify subsequent DDP simulations. For the regions of DIC 1 and 2, the random errors are evaluated as detailed in **Supplementary Materials S1**. The DIC processing is performed under an open-source platform called Ncorr [43]. Additionally, the EBSD (OXFORD Symmetry2, UK) analysis for the fractured specimens is performed around the circular hole using a step size of 1.2 μm (Fig. 1c4).

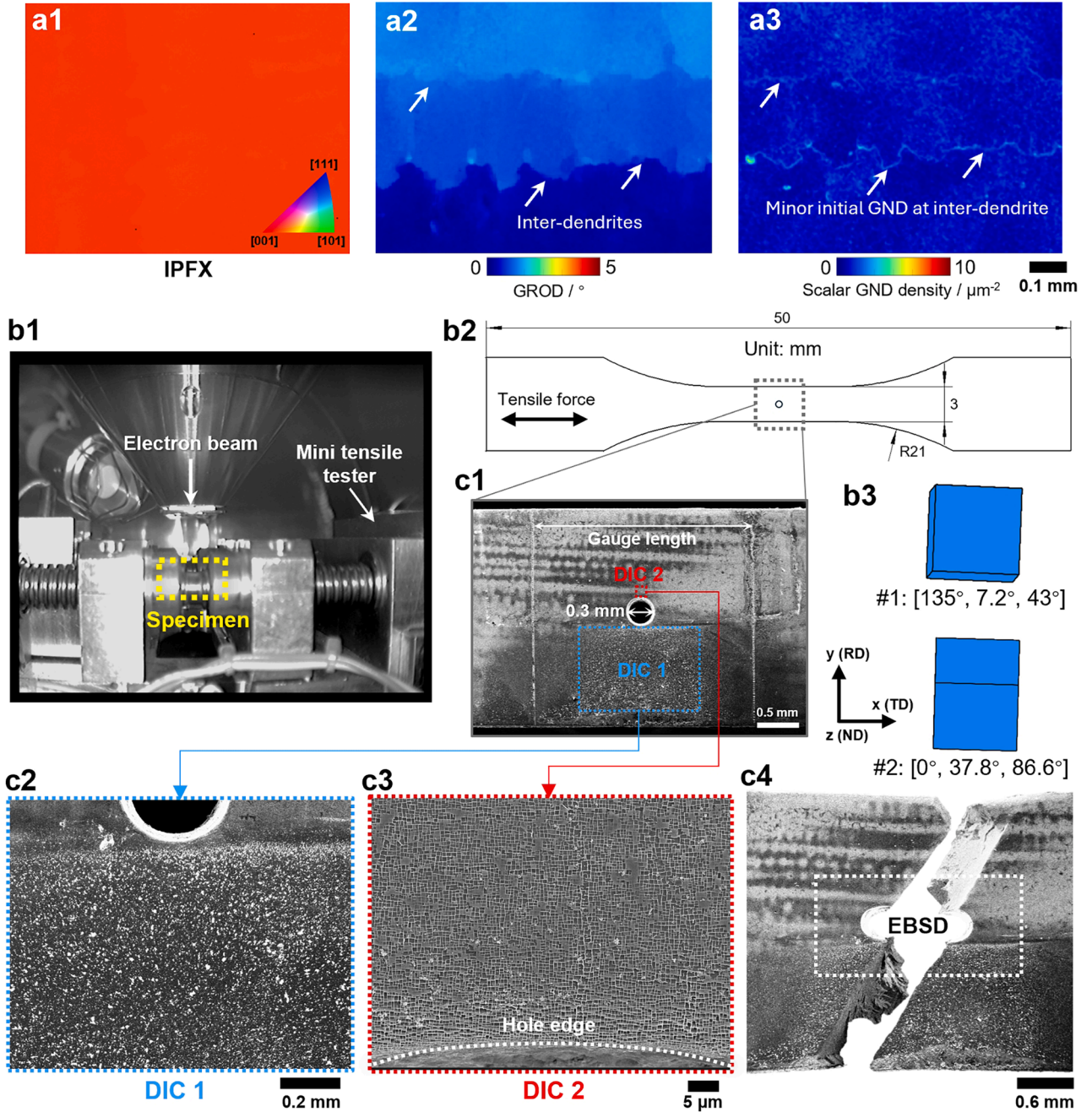


Fig. 1. Experimental setup for SX samples subjected to tensile loading. (a) Initial microstructural characteristics: (a1) IPFX map demonstrating the absence of GBs within the gauge length, (a2) orientation deviation $< 0.5^\circ$ between the adjacent dendrites, as characterized using grain reference orientation deviation (GROD), and (a3) minimal pre-existing GNDs observed at the inter-dendrite regions where orientation changes are minor. (b) In-situ tensile test system: (b1) setup of the in-situ tensile test system integrated within an SEM, and (b2) geometry of the SX specimens, featuring a circular hole and a thickness of 0.7 mm. (b3) Two crystallographic orientations used in the experiments, with Euler angles defined based on the Bunge convention [42]. (c) Multi-scale DIC analysis: (c1)-(c3) speckle patterns as the deformation carriers around the hole at submillimeter- and micro-scales, and (c4) EBSD analysis area for the fractured specimens.

Notably, the strain gradients across γ and γ' phases lead to the formation of GNDs at γ/γ' phase boundaries. According to our statistical analysis [39], the average width of γ channel is 45 nm, indicating that phase boundary-induced GNDs are distributed at the nano-scale. In this paper, to ensure the consistency in the resolutions between DIC and EBSD techniques and CPFЕ and DDP simulations, we focus on analyzing GNDs distributed at the submillimeter and micro-scales, which arise from the strain gradients induced by the structure of circular hole. Besides, in subsequent simulation approaches, the GNDs distributed across γ/γ' phases are implicitly considered in slip resistance using a

homogenized approach. Therefore, the GNDs focused in this paper are specified as structure-induced GNDs, excluding phase boundary-induced GNDs which occur at a much smaller nano-scale.

To solve the GNDs at individual slip systems using DIC and EBSD, we start from the relationship between the Nye tensor α (re-shaped as 9×1 column vector) and slip system-resolved ρ_{GND} ($N \times 1$ column vector, where N denotes the number of GND type) [18]:

$$\alpha = A \rho_{\text{GND}} \quad (1)$$

where A is a linear operator:

$$\mathbf{A} = \begin{bmatrix} b_1^1 l_1^1 & b_1^2 l_1^2 & b_1^3 l_1^3 & \dots & b_1^n l_1^n \\ b_1^1 l_2^1 & b_1^2 l_2^2 & b_1^3 l_2^3 & \dots & b_1^n l_2^n \\ b_1^1 l_3^1 & b_1^2 l_3^2 & b_1^3 l_3^3 & \dots & b_1^n l_3^n \\ b_2^1 l_1^1 & b_2^2 l_1^2 & b_2^3 l_1^3 & \dots & b_2^n l_1^n \\ b_2^1 l_2^1 & b_2^2 l_2^2 & b_2^3 l_2^3 & \dots & b_2^n l_2^n \\ b_2^1 l_3^1 & b_2^2 l_3^2 & b_2^3 l_3^3 & \dots & b_2^n l_3^n \\ b_3^1 l_1^1 & b_3^2 l_1^2 & b_3^3 l_1^3 & \dots & b_3^n l_1^n \\ b_3^1 l_2^1 & b_3^2 l_2^2 & b_3^3 l_2^3 & \dots & b_3^n l_2^n \\ b_3^1 l_3^1 & b_3^2 l_3^2 & b_3^3 l_3^3 & \dots & b_3^n l_3^n \end{bmatrix} \quad (2)$$

where $\mathbf{b}^n$ and $\mathbf{l}^n$ are the Burgers vector and unit vector of the dislocation line in the global coordinate system for the GND type n . For FCC metals, there are 12 independent components of edge GNDs distributed across 12 slip systems. As the Burgers vector is parallel to the line direction of screw GNDs, according to Eqs. (1)–(2), the slip systems with the same slip direction on different slip planes share the same values of screw GND densities. For instance, the screw GND densities at (111)[01–1] and (–111)[01–1] slip systems are identical. Therefore, the number of independent screw GNDs is 6 for the FCC lattice, and the N in Eq. (1) equals 18.

Next, we present how to determine the α using DIC and EBSD, respectively. In DIC analysis, the α is derived from plastic displacement gradient β^p under small deformation condition [15]:

$$\alpha \cong \begin{bmatrix} \frac{\partial \beta_{13}^p}{\partial x_2} - \frac{\partial \beta_{12}^p}{\partial x_3} & \frac{\partial \beta_{11}^p}{\partial x_3} - \frac{\partial \beta_{13}^p}{\partial x_1} & \frac{\partial \beta_{12}^p}{\partial x_1} - \frac{\partial \beta_{11}^p}{\partial x_2} \\ \frac{\partial \beta_{23}^p}{\partial x_2} - \frac{\partial \beta_{22}^p}{\partial x_3} & \frac{\partial \beta_{21}^p}{\partial x_3} - \frac{\partial \beta_{23}^p}{\partial x_1} & \frac{\partial \beta_{22}^p}{\partial x_1} - \frac{\partial \beta_{21}^p}{\partial x_2} \\ \frac{\partial \beta_{33}^p}{\partial x_2} - \frac{\partial \beta_{32}^p}{\partial x_3} & \frac{\partial \beta_{31}^p}{\partial x_3} - \frac{\partial \beta_{33}^p}{\partial x_1} & \frac{\partial \beta_{32}^p}{\partial x_1} - \frac{\partial \beta_{31}^p}{\partial x_2} \end{bmatrix} \quad (3)$$

where $\mathbf{x}$ is the position vector. The β^p can be expressed by plastic deformation gradient $\mathbf{F}^p$ [15]:

$$\beta^p = \mathbf{F}^p - \mathbf{I} \quad (4)$$

To simplify the GND calculation in DIC analysis, Eq. (4) is established under the small deformation condition [44], in which the higher-order small quantities are neglected. Meanwhile, under the small deformation condition, the strain tensor in DIC analysis can be directly represented by β^p [45]. The DIC-based displacement gradients, strains, and Nye tensor are defined in the reference configuration. Subsequently, $\mathbf{F}^p$ can be further estimated using the total deformation gradient $\mathbf{F}$, particularly in the later stages of deformation where the contribution of plasticity is dominant. As demonstrated in Figure S. 3 in Supplementary Materials S3, the incorporation of elastic deformation in the DIC-based algorithm introduces only 2 % and 1.2 % relative errors in scalar and resolved GNDs, respectively.

Then, $\mathbf{F}$ can be expressed by the in-plane displacement fields u and v as mapped in DIC:

$$\mathbf{F} = \begin{bmatrix} \beta_{11} + 1 & \beta_{12} \\ \beta_{21} & \beta_{22} + 1 \end{bmatrix} = \begin{bmatrix} \frac{\partial u}{\partial x_1} + 1 & \frac{\partial u}{\partial x_2} \\ \frac{\partial v}{\partial x_1} & \frac{\partial v}{\partial x_2} + 1 \end{bmatrix} \quad (5)$$

Where the asymmetric portion (lattice rotation) is used in the curl operation of Eq. (3). Hence, in Eq. (3), components α_{13} and α_{23} are accessible when using DIC to determine the Nye tensor.

Additionally, to determine the Nye tensor using EBSD data, α can be expressed by the local lattice curvature tensor κ under small deformation condition [17]:

$$\alpha_{ik} = \kappa_{ki} - \delta_{ki} \kappa_{mm} - v_{klj} \frac{\partial \epsilon_{ij}^{\text{el}}}{\partial x_l} \quad (6)$$

$$\kappa_{ij} = \frac{\partial \phi_i}{\partial x_j}$$

where ϕ_i is the misorientation angle regarding i axis, $\epsilon_{ij}^{\text{el}}$ is the elastic strain, v_{klj} is the Levi–Civita permutation symbol. In Eq. (6), the elastic strain gradients are neglected, as the plastic deformation is dominated when fracture happens at >3.5 % global strain (Fig. 1 c4). As demonstrated in Supplementary Materials S3, the elastic strain gradient term neglected in Eq. (6) is more than an order of magnitude smaller than the other terms. There are 5 accessible components in the Nye tensor when using EBSD data as an input [17]: $\alpha_{12} = \kappa_{21}$, $\alpha_{13} = \kappa_{31}$, $\alpha_{21} = \kappa_{12}$, $\alpha_{23} = \kappa_{32}$, $\alpha_{33} = -\kappa_{11} - \kappa_{22}$.

So far, the components in the Nye tensor can be partially determined using both EBSD and DIC. For FCC metals, there are 18 types of GNDs (12 edge, 6 screw) that need to be solved. In our case, as tabulated in Table S. 3 in Supplementary Materials, there are 4 slip systems with Schmid factors near 0 for the orientation #1 and #2 in Fig. 1 b3, respectively. These slip systems should not be activated when loading along the x -axis. Hence, the number of GNDs to be solved can be further simplified from 18 to 12. Nevertheless, based on Eq. (1), there are only 5 effective constraints for EBSD, and 2 effective constraints for DIC, which are fewer than the 12 unsolved GNDs. Therefore, we introduce an energy minimization algorithm to determine all the GND components, which physically implies that GNDs exist in the configuration with the lowest total energy [19]:

$$\sum_{n=1}^N w^n \rho_{\text{GND}}^n = \min \quad (7)$$

where w^n is the weight associated with the line energy of dislocations, and n is the GND type. It should be noted that $w^n = 1$ for edge GNDs, and $(1-\mu)$ for screw ones [17,34], where μ is the Poisson ratio. Notably, the screw GNDs solved by the above algorithm need to be halved, to account for the simplification of independent screw GNDs from 12 to 6 components.

2.2. CPFE and DDP modeling

In CPFE simulation, the plastic velocity gradient tensor $\mathbf{L}^p$ is derived from the slip shear rates across all the slip systems [46]:

$$\mathbf{L}^p = \dot{\mathbf{F}}^p (\mathbf{F}^p)^{-1} = \sum_{s=1}^{12} \dot{\gamma}^s \mathbf{s}^s \otimes \mathbf{n}^s \quad (8)$$

where $\mathbf{F}^p$ is the plastic deformation gradient tensor, the vectors $\mathbf{s}^s$ and $\mathbf{n}^s$ represent the slip direction and the slip plane normal, respectively. It should be noted that the strain in CPFE simulation is defined as the Green–Lagrange strain in the reference configuration, under finite deformation conditions [47]. For the FCC lattice, the total number of slip systems is 12. The slip shear rate for the s -th slip system is calculated as follows [48]:

$$\dot{\gamma}^s = \rho_{\text{ISSD}} v_D b^2 \exp \left(-\frac{\Delta H}{k_B T} \right) \sinh \left(\frac{\Delta V}{k_B T} |\tau^s - \tau_c^s| \right) \quad (9)$$

where ρ_{ISSD} is the initial density of mobile SSDs, v_D is the attempted frequency of dislocation to overcome obstacles, b is the magnitude of Burgers vector, ΔH and ΔV are the activation energy and activation volume for dislocation slip, respectively; k_B is the Boltzmann constant, T is the absolute temperature, τ^s is the resolved shear stress on the s -th slip system. The slip resistance, also known as the critical resolved shear stress (CRSS), is defined as:

$$\tau_c^s = \tau_0 + \mu b \sqrt{\rho_{\text{GND}}^s + \rho_{\text{SSD}}^s} \quad (10)$$

where τ_0 is the initial slip resistance capturing the effects of lattice friction, solid solution strengthening, and γ' precipitation strengthening. Besides, μ is the shear modulus, ρ_{GND}^s and ρ_{SSD}^s denote the densities of GNDs and immobile SSDs on the s -th slip system, respectively. The ρ_{GND}^s at individual slip system is calculated as the sum of edge ρ_{GNDe}^s and screw ρ_{GNDs}^s components. The evolution of the SSD density accounts for both dislocation multiplication and annihilation processes [49,50]:

$$\dot{\rho}_{\text{SSD}}^s = (K\sqrt{\rho_{\text{SSD}}^s + \rho_{\text{GND}}^s} - 2d_{\text{anni}}\rho_{\text{SSD}}^s) \frac{|\dot{\gamma}^s|}{b} \quad (11)$$

where K governs the rate of dislocation accumulation, and d_{anni} is the minimum annihilation distance for two dislocations with opposite signs [4].

In contrast to DIC and EBSD in 2D conditions, the 3D CPFE framework enables the determination of all components in Nye tensor through the curl operation on $\mathbf{F}^p$ [51]:

$$\boldsymbol{\alpha} = -(\nabla \times \mathbf{F}^p)^T \quad (12)$$

Consequently, based on the solved Nye tensor, we can establish the 9 constraints for GNDs at individual slip systems (see Eq. (1)). Based on the similar energy minimization algorithm described in 2.1 Section, the GNDs at individual slip systems can be further resolved in CPFE simulation. The Nye tensors in CPFE are calculated based on slip and normal directions in the current configuration. We note that the maximum strain levels (of about 10 %) in the following analysis are not sufficiently large such that rigid body rotations are expected to be small. Thus, the differences between small (DIC) and finite (CPFE) deformation analyses are expected to be minimal.

SED as a universal damage indicator, has been proven to be a reliable and microstructure-sensitive quantity for identifying crack nucleation sites [12,25]. It captures the damage caused by dislocation slips and interactions within the local dislocation structures where the energy is stored within materials. From its original physics-based definition [10], the SED is inherently a slip system-dependent quantity, representing the energy stored within the dislocation structures at individual slip

systems:

$$G^s = \int \frac{\xi |\tau^s| \cdot |d\gamma^s|}{\sqrt{\rho_{\text{SSD}}^s + \rho_{\text{GND}}^s}} \quad (13)$$

Additionally, the conventional scalar SED is incorporated for comparisons [52,53]:

$$G = \int \frac{\xi \boldsymbol{\sigma} : d\boldsymbol{\epsilon}_p}{\sqrt{|\rho_{\text{SSD}}| + |\rho_{\text{GND}}|}} \quad (14)$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\epsilon}_p$ are the stress and plastic strain tensors, $|\rho_{\text{SSD}}|$ and $|\rho_{\text{GND}}|$ are the scalar SSD and GND in 1st norm, respectively. All the scalar GNDs presented in this work have the same definition as that in Eq. (14).

The crystal plasticity model described above is implemented in a user-defined material subroutine (UMAT) within the ABAQUS standard analysis framework. A full-scale finite element model is constructed, incorporating appropriate boundary conditions, as shown in Fig. 2b. The geometric model is discretized into 196,215 C3D20R elements. To ensure compatibility with the resolution for the region of DIC 1 (Fig. 1 c2), the region surrounding the hole is meshed with elements having a minimum size of 10 μm . A gradient mesh is generated near the hole to reduce the total number of elements and computational cost. Boundary constraints are applied to the left and back surfaces along the x -axis and z -axis to prevent rigid body displacement during loading, while a single vertex is constrained along the y -axis. A displacement-controlled load is applied to the right surface, achieving the engineering strains for the specimens with #1 and #2 orientations. The simulated strain-stress curve agrees well with the experimental data (Supplementary Materials S5), confirming the validity of the calibrated constitutive parameters, which are summarized in Table S. 1 in Supplementary Materials.

We adopt the 2D DDP method that was proposed in [29] with the calculation of slip system-independent CED in [33], and hence only the equations on calculating the slip system-dependent GND densities and associated SEDs are given below. The GND density at the s -th slip system, as inspired by [32], is given by

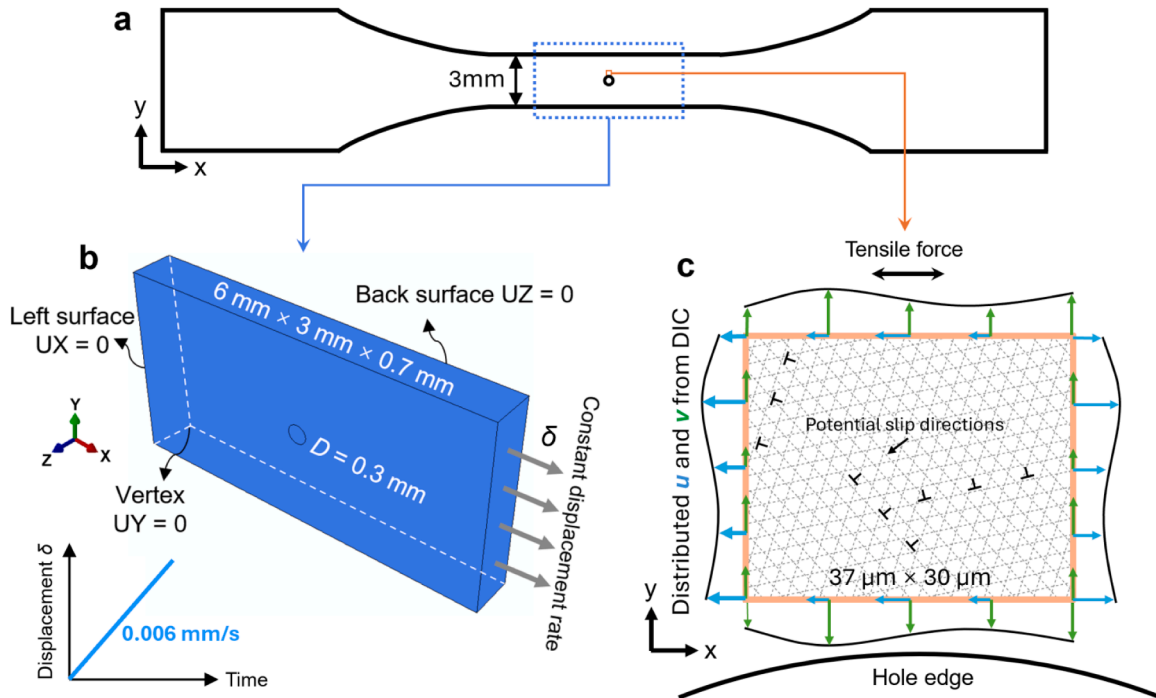


Fig. 2. CPFE and DDP modeling of SX plates with a circular hole. (a) Geometry of the SX specimens with a circular hole used in tensile testing. (b) Computational setup for CPFE simulations, including the specimen geometry, applied boundary conditions, and the loading history. (c) DDP simulation domain with the DIC-based boundary conditions.

$$\rho_{\text{GND}}^s = |\rho_+^s - \rho_-^s| = \frac{1}{\Delta x \Delta y} |N_{\text{dis}+}^s - N_{\text{dis}-}^s| \quad (15)$$

where Δx and Δy are the grid sizes, $N_{\text{dis}+}^s$ and $N_{\text{dis}-}^s$ are the number of dislocations with positive and negative signs with the grid at the s -th slip system. The slip-system dependent SED within the DDP framework, inspired by [11], is given as:

$$G_{\text{SED}}^s = \int \frac{\xi \tau^s d\Gamma^s}{(\rho_{\text{dis}}^s)^{1/2}} \quad (16)$$

where ξ is the fraction of plastic work stored in a dislocation structure and estimated as 0.05 [54], Γ^s and ρ_{dis}^s denotes the crystallographic slip and total dislocation density along the s -th slip system, respective, the

latter of which is calculated as:

$$\rho_{\text{dis}}^s = \rho_+^s + \rho_-^s = \frac{1}{\Delta x \Delta y} (N_{\text{dis}+}^s + N_{\text{dis}-}^s) \quad (17)$$

The region of interest (ROI) modeled in the DDP framework corresponds to the region on the top of hole where the μ DIC is performed at the region of DIC 2 (Fig. 1c3). The dimensions of the DDP ROI are chosen to be identical to the μ DIC region i.e. $37 \mu\text{m} \times 30 \mu\text{m}$, and the crystallographic orientations #1 and #2 in DDP correspond to the ones characterized using EBSD (Fig. 1b3). Potential slip systems are placed with the ROI with the slip spacing as $100b$ to spatially resolve the dislocation activities. Dislocation nucleation sources and obstacles are randomly distributed along the slip systems, with their densities and nucleation strength values calibrated to match experimental tensile results. The

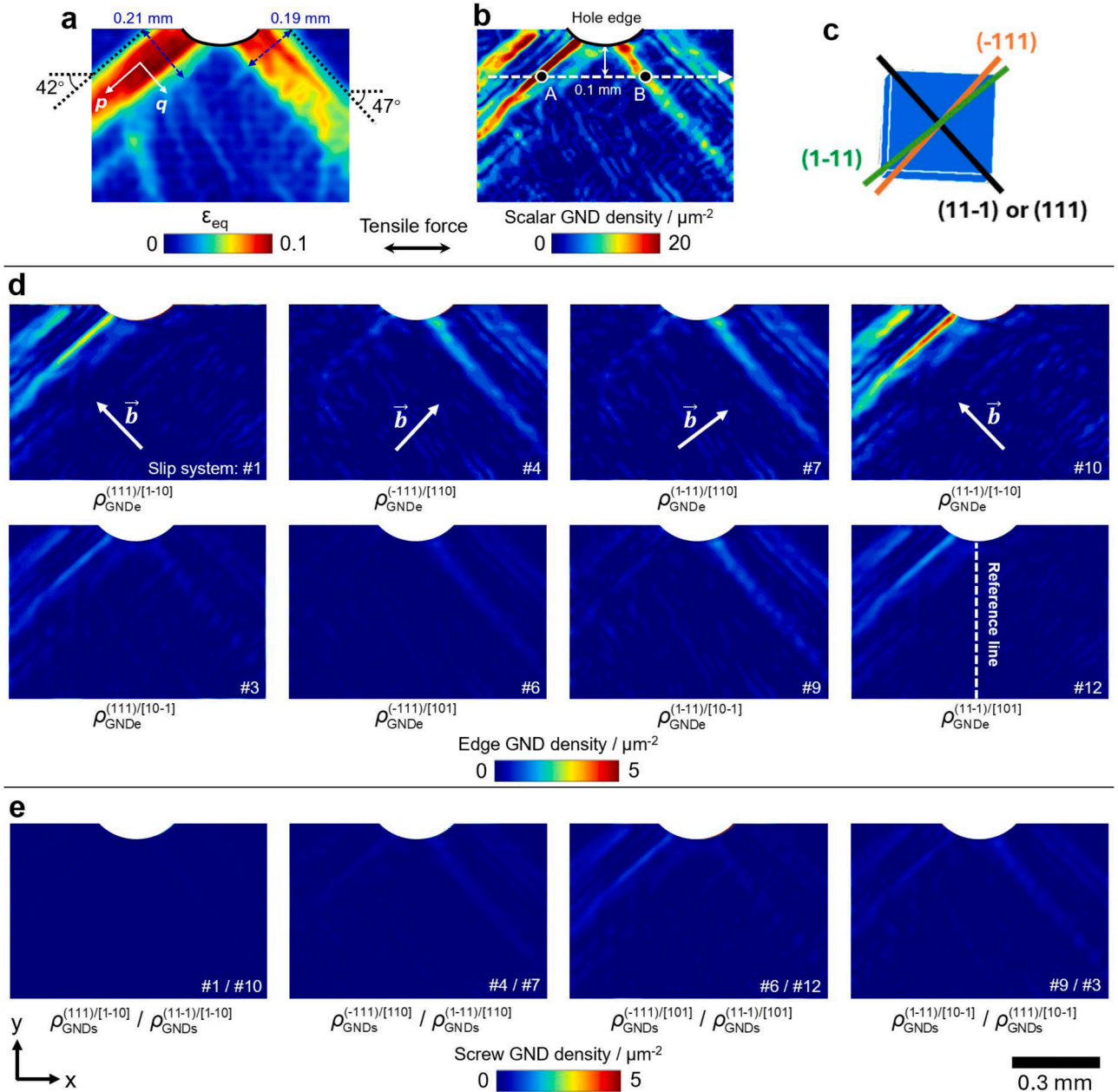


Fig. 3. DIC-based strains and resolved GNDs for orientation #1 specimen ($\sim 3.5\%$ global strain). (a) Equivalent strain pattern within DIC 1 region (Fig. 1 c2). (b) Scalar GND distribution across the analyzed region, with points A and B identified for quantitative comparisons to subsequent CPFE results. (c) The unit cell of SX and potential directions of slip bands. (d)-(e) Patterns of resolved edge and screw GNDs on individual slip systems, demonstrating localization of GNDs at the boundaries of slip bands where large deformation gradients exist. The slip system indices correspond to Table S. 3. Burgers vectors labeled in (d) are approximately in-plane for qualitative analyses, whereas the Burgers vectors of other slip systems in (d) are predominantly out-of-plane.

stress-strain response of the DDP model with the calibrated parameters is shown in **Supplementary Materials S5**. The full-set of displacement data (i.e. including both displacement along x - and y -direction) from the μ DIC analysis is imposed on the four boundaries. This setup ensures that the loading conditions applied on the SX specimens best reflect the experimental scenarios, and hence the deformation and damage are faithfully predicted.

3. Results

3.1. DIC-based resolved GNDs

The DIC results of strains and resolved GNDs are exhibited in **Fig. 3**. After severe plastic deformation, two slip bands occur at the hole edge for orientation #1 (**Fig. 3a**), with 42° and 47° angles to the horizontal direction, which is consistent with the potential directions of slip bands shown in **Fig. 3c**. Based on the strain components shown in

Supplementary Materials S4, the normal strain along the tensile direction is highly localized within the slip bands, accompanied by a pronounced negative lateral strain. The slip band on the left shows a relatively higher strain localization degree. Moreover, the scalar GND density is concentrated at the boundaries of each slip band (**Fig. 3b**), with a roughly symmetrical distribution regarding the central reference line marked in **Fig. 3d**.

As shown in **Fig. 3d**, in contrast to the scalar GND density, the GND densities at individual slip systems show significant asymmetric distributions with respect to the reference line. For example, slip systems of $(1-11)[110]$ and $(-111)[110]$ show edge GND densities localized on the right side of the reference line, while the $(111)[1-10]$ and $(11-1)[1-10]$ exhibit GND densities concentrated on the left. Notably, according to the directions of Burgers vectors that are roughly in-plane, the edge GND-localized strips are approximately perpendicular to the in-plane Burgers vectors for all the slip systems mentioned above. We understand this trend from the original definition of edge GNDs at the s -th slip

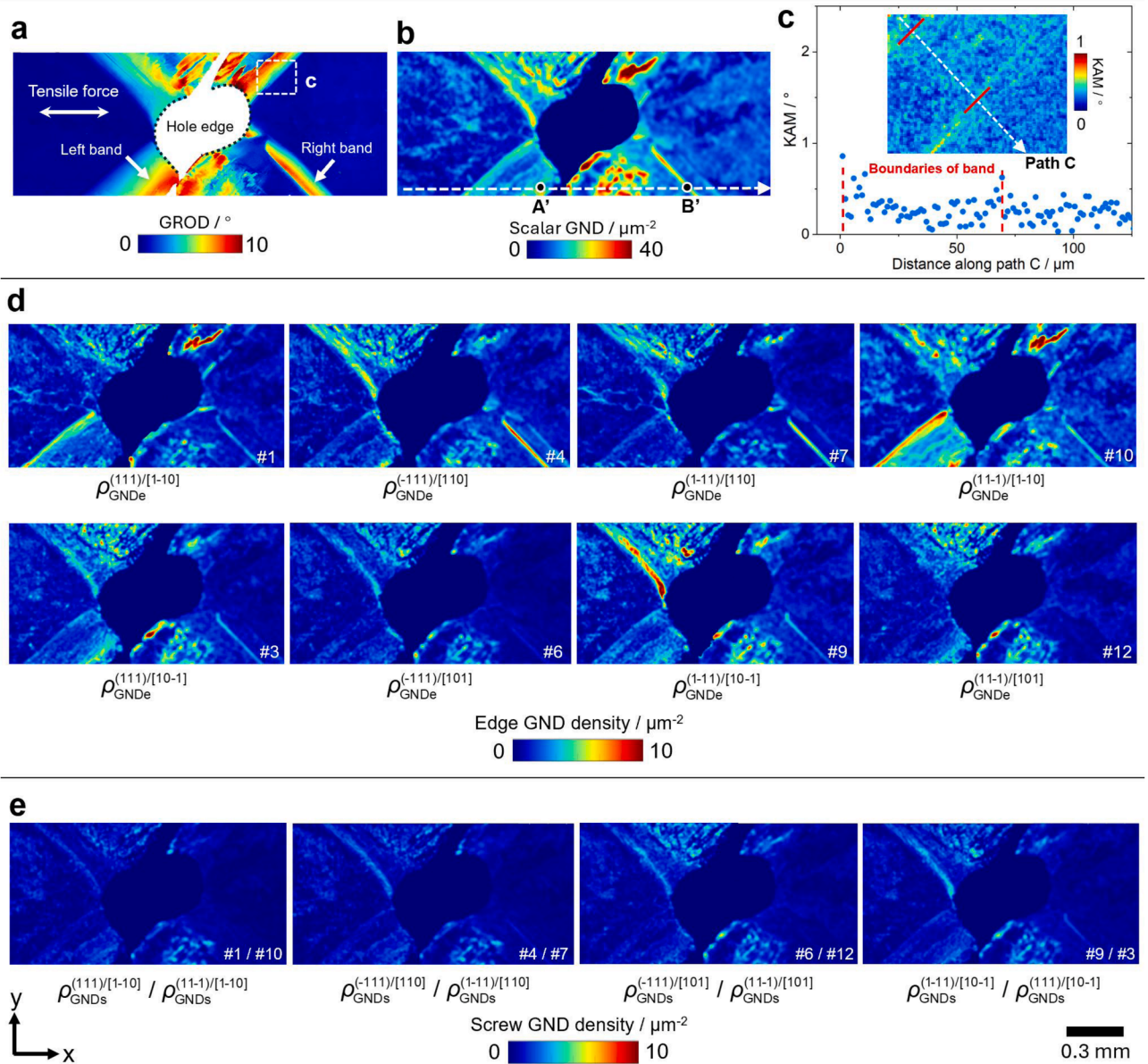


Fig. 4. EBSD-based GNDs resolved at individual slip systems for orientation #1 specimen. (a) GROD map illustrating the degree of plastic deformation [59]. (b) Scalar GND distribution, showing the localization of GNDs at the boundaries of slip bands and regions near the fracture surfaces. Points A' and B' mark the positions with the maximum GND densities within the left and right slip bands, respectively. (c) Kernel average misorientation (KAM) map at the region (c) marked in (a), representing the gradient of orientation change. (d)-(e) Resolved edge and screw GND densities at individual slip systems, respectively.

system [4]:

$$\rho_{\text{GNDe}}^s = -\frac{1}{b} \nabla \gamma^s \cdot \mathbf{s}^s \quad (18)$$

which indicates that edge GND density is proportional to the gradient of plastic shear along the slip direction aligning with the direction of the Burgers vector. For instance, regarding the (1-11)[110] slip system associated with the stronger slip band on the left (Fig. 3a), the strain gradient along the $\vec{p}$ direction is insignificant. Hence, the (1-11)[110] slip system shows minor edge GND densities within the whole left region. On the contrary, the strain gradient along $\vec{q}$ direction is more evident at the boundaries of the left slip band. As a result, the (11-1)[1-10] and (111)[1-10] slip systems, which are roughly parallel to $\vec{q}$, exhibit edge GND densities localized on the boundaries of stronger slip band. This analysis based on the original definition of GND, qualitatively verifies our DIC-based algorithm for resolving GNDs in the scenario of

SXs.

Additionally, compared with edge GNDs, screw GNDs with 4 non-zero independent components show lower densities (Fig. 3e). The lower densities in screw components are consistent with previous EBSD-based studies on resolved GNDs [55,56]. The asymmetry of screw GNDs is less pronounced compared with edge GNDs, which is attributed to the differences in the line directions of dislocations in Eq. (2), as the edge and screw GNDs in FCC metals share the same Burgers vector at each slip system [15].

3.2. EBSD-based resolved GNDs

For the fractured specimen with orientation #1, the resolved GND densities characterized using EBSD are exhibited in Fig. 4. The corresponding global strain is 3.62 %, estimated by proportionally converting the displacements recorded by the tensile machine at 3.5 % global strain to the moment of fracture. As shown in Fig. 4a, the left and right slip

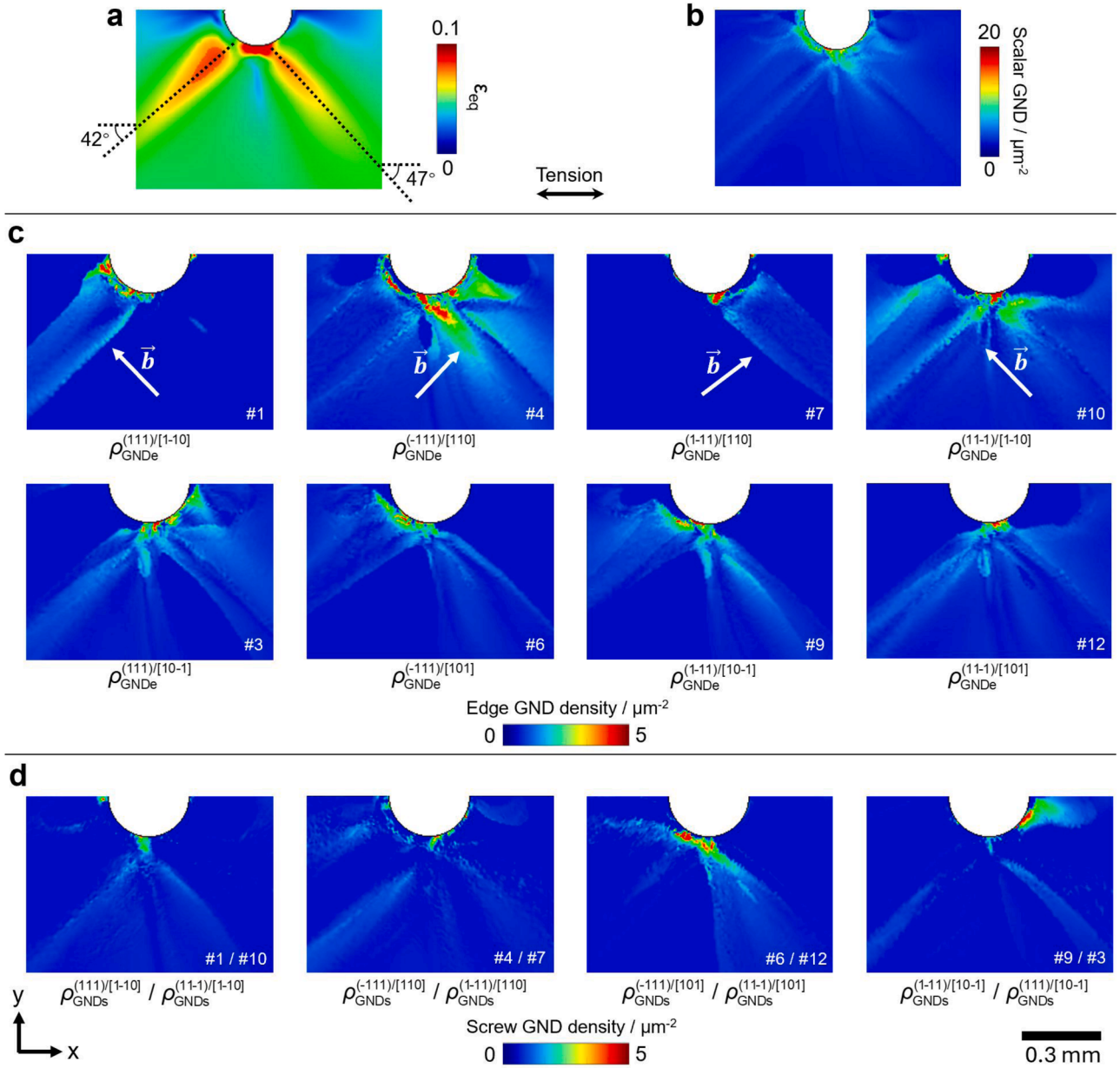


Fig. 5. GND densities at individual slip systems for orientation #1 (~3.5 % global strain) from CPFE simulation. (a) Simulated equivalent strain distributions, derived from ϵ_{xx} , ϵ_{yy} , and ϵ_{xy} . (b) Scalar GND distribution. (c)-(d) Resolved GND densities for individual slip systems: (c) Edge GND densities and (d) screw GND densities.

bands captured in the region of DIC 1 can also be identified in EBSD, where the left one similarly shows a higher degree of plastic deformation. Moreover, the kink bands usually display significant misorientation exceeding 5° at their boundaries, with near-zero misorientation within the bands [57,58]. In this work, however, the misorientation is slightly concentrated at the band boundaries (Fig. 4c) and remains below 1° . Compared to kink bands reported in previous studies, the misorientation in this work tends to be more uniformly distributed within the bands. Additionally, unlike kink bands that exhibit a dramatic change in orientation deviation at their boundaries, Fig. 4a shows a gradual change in orientation deviation around the boundaries. Hence, it is more appropriate to classify the deformation-induced bands observed in this study as slip bands.

Since the crack propagation during the fracture induces additional plastic deformation around the crack growth path, the EBSD-based scalar GND density exhibits a higher magnitude compared with the DIC-based results (Fig. 4b, Fig. 3b). As shown in Fig. 4d and e, the magnitudes of GND densities across different slip systems follow a similar trend with those from DIC, where the highest resolved GND density occurs at the (11–1)[1–10] slip system (edge), and the (111)[1–10] (screw) shows the lowest GND density. The resolved GND patterns obtained from EBSD are comparable to those derived from DIC. For example, the (111)[1–10] and (11–1)[1–10] slip systems show edge GNDs localized around the left slip band, whereas the (–111)[110] and (1–11)[110] exhibit edge GNDs concentrated around the right slip band, which are consistent with the DIC results (Fig. 3d). Similarly, the screw GND densities also show lower magnitudes compared with the edge ones.

3.3. CPFE-based resolved GNDs

Fig. 5 presents the CPFE simulation results on strain distributions and resolved GNDs. As shown in Fig. 5a, the key features of strain pattern in DIC analysis (Fig. 3a) can be reproduced in CPFE simulations, in terms of slip band directions, width of slip band, and strain localization degree. The angles between the slip bands and the horizontal direction are 42° and 47° for the left and right bands, respectively, which align well with the DIC results. Similarly, the CPFE results show that the width of the left band is larger than that of the right band, and the left slip band exhibits a larger degree of strain localization compared to the right band, both of which are in good agreement with the DIC results. A detailed comparison of the strain components is provided in **Supplementary Materials S4**. The simulated scalar GND density is localized at the boundaries of each slip band, which is consistent with DIC-based scalar GND, by comparing Fig. 5b with Fig. 3b. Additionally, the CPFE-based resolved GNDs (Fig. 5c) also show some similarities with the DIC results. Specifically, the (111)[1–10] and (11–1)[1–10] slip systems show edge GND localization at the boundaries of the left slip band, while screw GNDs generally show lower densities compared with the edge GNDs (Fig. 5d).

However, there are still notable differences between CPFE- and DIC-based resolved GNDs. First, both scalar and resolved GNDs exhibit lower magnitudes in CPFE, which is attributed to weaker strain localization and reduced strain gradients of slip bands in the CPFE simulation, compared with the strain patterns in DIC. Secondly, some GND components in CPFE exhibit significant differences in patterns compared with those obtained from DIC. Those differences arise primarily from their distinct abilities in capturing the deformation. CPFE method can simulate the deformation in 3D, enabling the computation of the full components of the Nye tensor. In contrast, the 2D in-plane DIC is limited to resolving only two components of the Nye tensor, leading to differences in the resolved GND patterns. Moreover, the GNDs in DIC and CPFE-based algorithms are resolved under reference and current configurations, respectively, which also contributes to the difference in GND patterns between DIC and CPFE.

3.4. DDP-based resolved GNDs

The comparison between DDP simulation and μ DIC is presented in Fig. 6. The orientation #1 shows the activation of a single slip plane (Fig. 6a), in which the slip traces with a thickness of $2\ \mu\text{m}$ align in the same direction corresponding to (11–1) or (111) slip planes. The number of slip traces and the maximum strains within slip traces, increase with the global strain levels. These features of strain patterns can be successfully captured in DDP simulations. Both μ DIC and DDP indicate that the resolved GNDs are localized at the regions with dense slip traces (Fig. 6b). Nevertheless, the DDP results exhibit a higher resolution of GND density, due to the limitation of DIC in capturing individual dislocations. Moreover, the μ DIC shows that the activation of double slip planes (111) and (–111) occurs at orientation #2 (Fig. 6c), and the interaction between different slip planes enhances strain localization, which can be reproduced in the DDP simulation. Compared with the (111) slip plane, the (–111) slip plane shows more pronounced strain localization, due to a higher Schmid factor as listed in **Table S. 3** in **Supplementary Materials**. Besides, as shown in Fig. 6d, both μ DIC and DDP suggest that resolved GNDs are mainly localized at the region where the (–111) slip plane is activated, while the regions with activation of the vertical (111) slip plane exhibit minor resolved GND densities.

4. Discussion

4.1. Comparison of resolved GNDs among DIC, EBSD, and CPFE

As elaborated in Section 2, the DIC and EBSD-based algorithms are capable of capturing two and five components in the Nye tensor, respectively. Under the 2D conditions, both DIC and EBSD only acquire the limited components in the Nye tensor, leading to comparable results of resolved GNDs. To quantitatively compare the resolved GND patterns between EBSD and DIC across different slip systems, the indicator ψ^s is defined as:

$$\psi^s = \rho_{\text{GND, left}}^s - \rho_{\text{GND, right}}^s \quad (19)$$

where $\rho_{\text{GND, left}}^s$ and $\rho_{\text{GND, right}}^s$ are the maximum GND densities around the left and right slip bands along the path defined in Figs. 3b and 4b. The $\psi^s > 0$ or $\psi^s < 0$ indicates that GND density is localized around the left or right slip band, respectively. As shown in Fig. 7a1, in both EBSD and DIC results, the variations in ψ^s exhibit a similar trend for edge GNDs, where the #1 and #10 slip systems show edge GNDs significantly localized on the left side ($\psi^s > 0$), while the #4 and #7 slip systems present an opposite trend ($\psi^s < 0$). For the screw GNDs with a much lower magnitude, both DIC and EBSD-based analyses reveal a clear concentration of screw GNDs on the left side of the #6 and #12 slip systems. This demonstrates a remarkable consistency between the DIC and EBSD-based algorithms in resolving GND distributions across individual slip systems under 2D conditions.

As presented in Fig. 3d, the (11–1)[1–10] slip system with maximum edge GND density, is selected for quantitatively comparing GND distributions obtained from different methods along path A. Fig. 7b indicates that the GND profiles obtained from DIC, EBSD, and CPFE display similar trends. Both primary and secondary peaks exist on the left side, which is attributed to the strong strain gradient along the slip direction of (11–1)[1–10] at the boundaries of the left slip band. Since the EBSD results are obtained at a larger global strain compared to DIC and CPFE, and crack propagation during fracture may induce additional slip, the resolved GNDs derived from EBSD exhibit the highest magnitudes. Furthermore, in the EBSD results, the horizontal spacing between the primary and secondary peaks on the left of the reference line is larger than that observed in the DIC and CPFE results, as the EBSD-based GNDs are extracted from a highly deformed configuration. On the contrary, the CPFE results show the lowest GND density, owing to the weaker strain

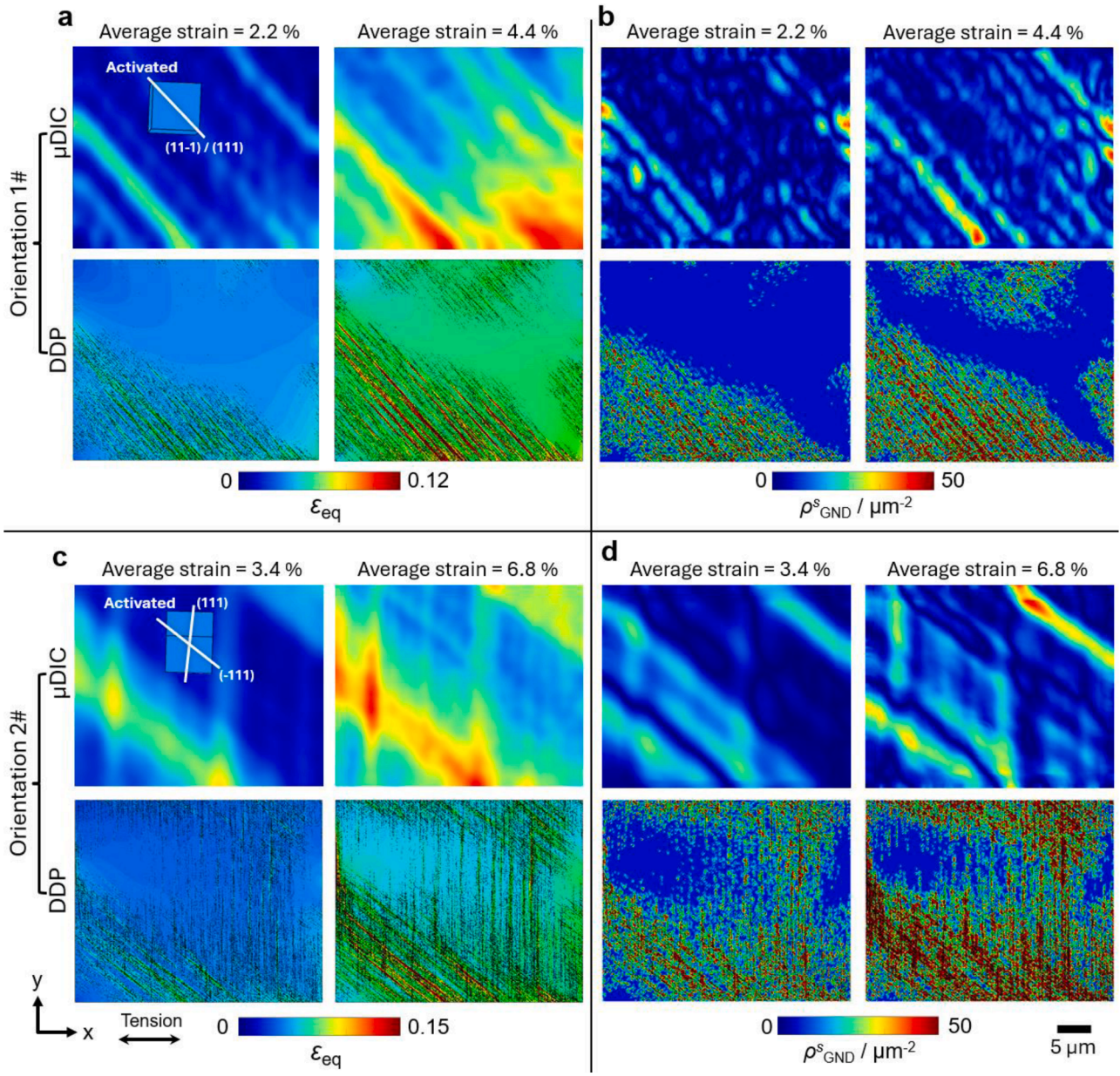


Fig. 6. Comparison of the deformation and the resolved GND densities between DDP and μ DIC for different orientations and global strain levels. (a) Comparison of equivalent strain patterns near the hole for orientation #1, illustrating the activation of a single slip plane. (b) Comparison of GND density at the (111)[10-1] slip system for orientation #1, highlighting differences between DDP and μ DIC results. (c) Comparison of equivalent strain patterns for orientation #2, showing the activation of double slip planes near the hole. (d) GND density comparison at the (-111)[110] slip system for orientation #2.

localization at slip bands in simulations.

Compared to the DIC results, the EBSD results exhibit greater similarity to the CPFE results (Fig. 7b). Unlike the DIC results, both EBSD and CPFE show small peaks of resolved GNDs on the right of the reference line. A possible explanation for this difference is that both EBSD and CPFE use the updated crystallographic orientation in the current configuration to resolve GNDs, whereas the DIC-based approach applies the original orientation from the reference configuration. As a result, different Burgers vectors are employed to resolve GNDs in DIC and EBSD/CPFE, respectively. As detailed in Section 2, two and five components in Nye tensor are accessible in 2D DIC and EBSD, respectively. Hence, the EBSD results are more comparable to the CPFE results capable of resolving full components in the Nye tensor. Besides, in EBSD characterization, there are approximately 0.5° random errors in the measured Euler angles [60]. This error will be greatly enlarged when

solving the second-order partial derivative of Euler angles in Eq. (6), which leads to significant fluctuations in EBSD-based resolved GNDs. As detailed in **Supplementary Materials S2**, the random error of EBSD-based GNDs is estimated to be $4.73 \mu\text{m}^{-2}$, which is consistent with the maximum amplitude of the randomly distributed fluctuations observed in the EBSD-based GND profile shown in Fig. 7b.

4.2. Evolution of resolved GNDs

The DIC-based resolved GND densities evolving with global strains are shown in Fig. 8. The (11-1)[1-10] slip system with maximum edge GND density (Fig. 3d), is selected for a detailed discussion. Based on the DIC strain maps, the width of the slip bands at various global strain levels is carefully measured (Fig. 8a). The results show that the width of the slip band increases with global strain, with a higher growth rate at

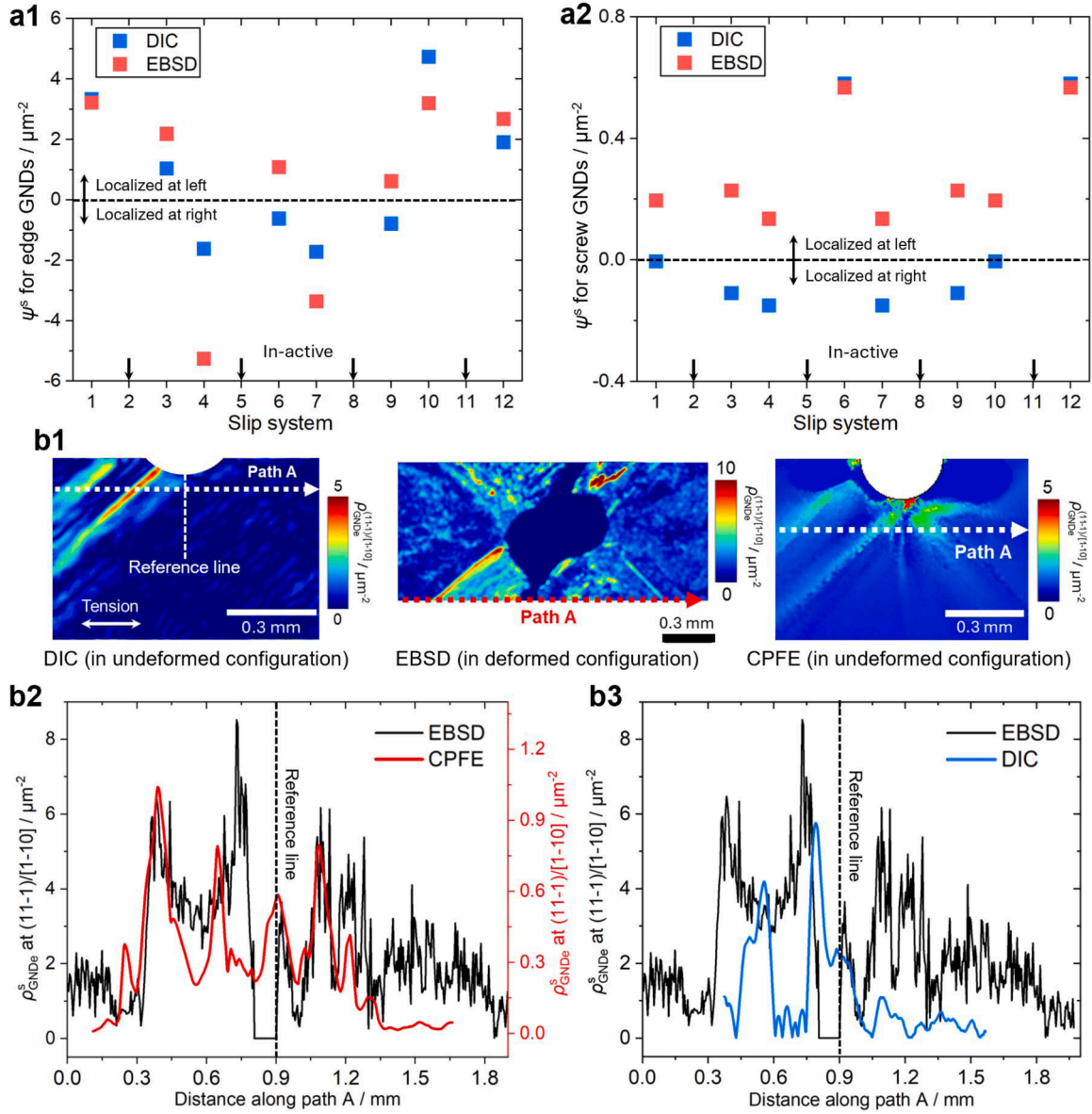


Fig. 7. Quantitative comparison of GNDs resolved using DIC, EBSD, and CPFE methods. (a) Distribution of indicator ψ^s distributed across different slip systems for edge and screw GNDs, respectively. The indices of slip systems correspond to Table S. 3 in Supplementary Materials. The $\rho_{\text{GND, left}}^s$ and $\rho_{\text{GND, right}}^s$ used for calculating the ψ^s are marked as A / B in DIC (Fig. 3b), and A' / B' in EBSD (Fig. 4b). (b) Distributions of edge GNDs at the (11-1)[1-10] slip system along path A, resolved using DIC, EBSD, and CPFE. The definition of path A in different scenarios is shown in (b1).

the early stage following slip band initiation, which is consistent with previous observations in SXs [61]. Additionally, the resolved GND densities are consistently localized at the boundaries of the slip bands (Fig. 8b). As deformation progresses, the locations of the GND peaks shift in alignment with the extension of the slip band boundaries, while the interior of the slip bands exhibits minimal strain gradients and GND densities (Fig. 8c). This observation reinforces the insight that GND densities depend solely on the current deformation state and strain gradients, irrespective of the deformation history [50,62]. Moreover, the magnitudes of the peak GNDs increase with global strain levels. The growth rates of the maximum GNDs at peaks 1 and 2 accelerate in the later stages of deformation (Fig. 8d), driven by enhanced strain gradients around the slip bands.

4.3. CPFE-based resolved SEDs

4.3.1. Crystallographic planes of crack nucleation

Compared with scalar SED, the slip system-dependent SEDs can further capture the crystallographic planes of crack nucleation, which is justified using submillimeter-scale DIC (Fig. 9). Among all slip systems, the ones with maximum SEDs at zones I and II (marked in Fig. 9b1) are selected and shown in Fig. 9a2 and a3. In contrast to the scalar SED (Fig. 9a1), the SEDs at individual slip systems show significant asymmetric distributions relative to the y-axis, with maximum SED at 15° along the circumferential direction in Fig. 9a2 for zone I. This asymmetric SED localization successfully captures the cracking at a position of 10° along the circumferential direction observed from the in-situ tensile test (Fig. 9b2). The comparison of cracking nucleation sites will be further elaborated in orientation #2. In the case of SXs, the crack growth path can be employed to trace the crystallographic plane of crack nucleation [63,64]. From Fig. 9b2 and b3, the angle between the crack

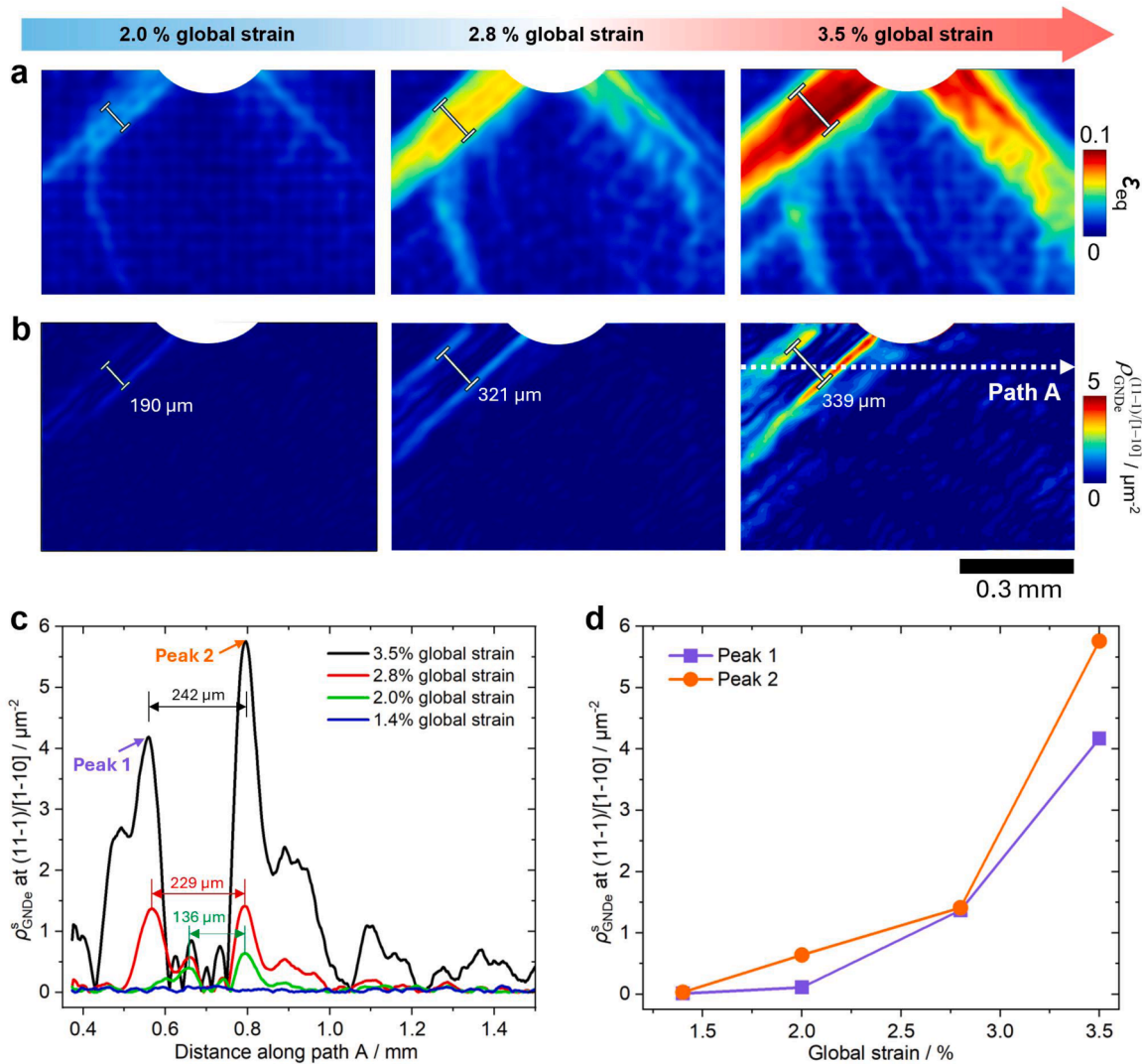


Fig. 8. Evolution of slip system-resolved GND densities. (a-b) Equivalent strains and resolved GND densities at varying global strain levels. (c) Distributions of resolved GND densities along path A marked in (b). (d) Evolution of GND densities at peak 1 and peak 2, as marked in (c). The distance between the primary and secondary peaks along path A is labeled in (c), distinguishing it from the measurements of adjacent GND peaks in (a) and (b), which are taken in the direction perpendicular to the slip band.

growth path and horizontal directions in zone I is smaller than that in zone II. According to the ideal orientations of slip planes, the (1-11) slip plane exhibits a smaller angle to the horizontal direction, compared with the (-111) slip plane. Based on this trend, the cracking crystallographic planes for zones I and II are (1-11) and (-111), respectively. This is further corroborated by the geometries of the fracture surfaces shown in Fig. 9b1. This observation from the in-situ test aligns with the CPFE simulations on the slip planes with maximum resolved SEDs in zones I and II (Fig. 9 a2 and a3), respectively.

4.3.2. Locations of crack nucleation

The specimen with orientation #2 is used to compare the experimental cracking locations along the circumferential direction, with the simulated resolved SEDs obtained from CPFE. In contrast to the scalar SED, the resolved SEDs at some individual slip systems show pronounced asymmetric distributions with respect to the y-axis (Fig. 10a). As shown in Fig. 10c1, the scalar SED exhibits relatively high magnitudes around the positions at 0° and 180°, with each peak falling within a range of $\pm 30^\circ$ where high magnitudes of SEDs exist. Differing from the scalar SED, the resolved GNDs show a higher localization degree, with the peak values occurring at 14° and 195° in CPFE simulations. In the

DIC analysis, the cracking observed at point A (Fig. 10b2) supports the prediction of resolved SEDs, which the scalar SED peaking around 0° fails to capture. For the cracking observed at point B (Fig. 10b3), although both the scalar SED and resolved SED show a peak at 195° (Fig. 10c1), the more pronounced damage localization in the SED resolved at (11-1)[011], suggests a more certain and reliable prediction of the cracking at point B. Therefore, compared with the conventional scalar SED, the slip system-dependent SEDs show better predictions for asymmetric cracking behaviors relative to the x-axis.

Furthermore, for the cracking sites A and B, the SEDs distributed across all slip systems are extracted and shown in Fig. 10c2. Unlike the scalar SED with constant values, the resolved SEDs show lower magnitudes and higher dispersion. The sites A and B share a comparable value of resolved SED at the critical slip systems (#7 slip system for site A, and #11 for B). Therefore, by accounting for the energies distributed across slip systems, the resolved SEDs exhibit enhanced accuracy in predicting crack locations and identifying the crystallographic planes of crack nucleation.

Previous in-situ observations have demonstrated that microcrack initiation in SXs exhibits a strong dependence on the active slip systems [65–67]. This indicates that cracking events are closely linked to

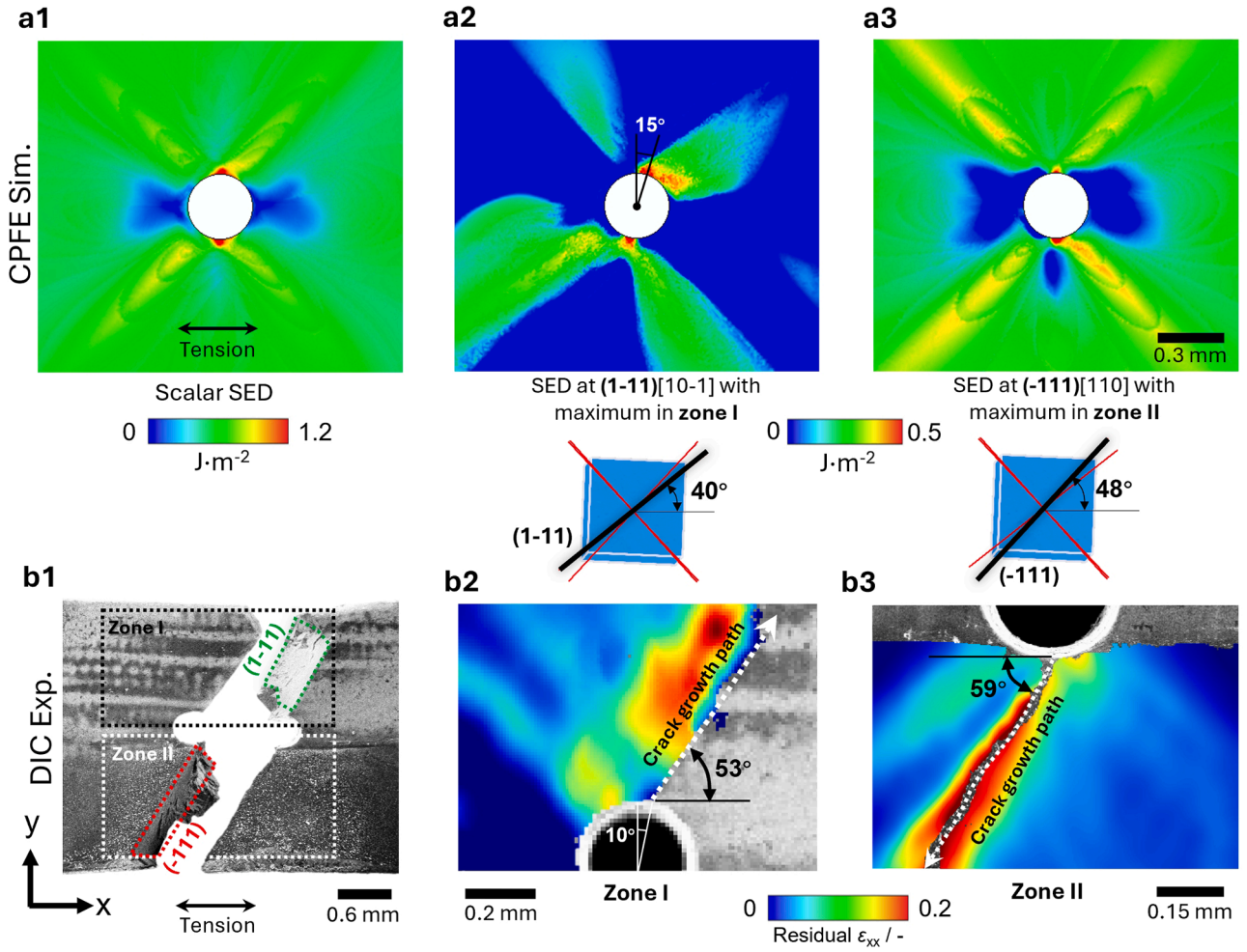


Fig. 9. Crystallographic planes of crack nucleation in orientation #1 sample characterized by DIC and predicted by CPFE simulation. (a) Simulated SED distributions: (a1) scalar SED, (a2) SED at the (1-11)[10-1] slip system showing maximum damage in zone I, (a3) SED at the (-111)[110] slip system, showing maximum damage in zone II. (b) Fractured specimen from the DIC test for orientation #1: (b1) SEM image of the fractured specimen, with crystallographic planes of the crack labeled in both zones I and II. (b2)-(b3) DIC analysis of the fractured specimen, showing the crack growth path mapped on the undeformed configuration. Except for (b1), all DIC and CPFE results are plotted in undeformed configurations for more accurate comparisons.

damage occurring within individual slip systems. On the other hand, scalar dissipative energy density and SED represent the total energy contribution from all slip systems. While localized scalar strain energies indicate a higher probability of crack nucleation, these slip system-independent quantities neglect the energy densities distributed across slip systems that are critical to cracking behavior. For instance, as illustrated in Fig. 10c2, under the same scalar SED at a given point, SED concentrated on a specific slip system indicates a higher likelihood of crack nucleation, whereas uniformly distributed SEDs across all slip systems suggest a lower likelihood of crack initiation.

4.4. DDP-based resolved SEDs

To further justify the slip system-dependent SEDs at the micro-scale, the DDP-simulated SEDs are compared with the cracking locations observed in μ DIC (Fig. 11). During the in-situ tests (Fig. 11c), multi-source crack initiations at the hole edge are captured within the region of DIC 2 for orientation #2. Under intense slip along the (-111) plane, four slip trace-induced cracks appear at the bottom of slip traces. In order to compare with DDP results, the cracking sites are mapped onto the undeformed configuration using μ DIC (Fig. 11d). There are pronounced strain localizations around the slip traces, and the hot spots at the bottom are employed to identify the cracking locations at the hole edge. On the other hand, as shown in Fig. 11b, the DDP-simulated SEDs

similarly show the damage localization at the bottom region within each slip trace, providing better predictions compared with the slip system-independent CED which displays a more random distribution (Fig. 11a). As qualitatively shown in Fig. 11e, the cracking locations of #2 and #3 are successfully captured in the DDP-simulated SEDs, with two prominent SED peaks corresponding to the initiation areas of #2 and #3 cracks in experiments. Moreover, the SED increases dramatically in the latter part of path B, approaching the location of the main crack observed in the in-situ DIC experiment (Fig. 10b2), which also corroborates the accuracy of slip system-dependent SEDs in predicting crack nucleation. Therefore, the SEDs at individual slip systems also can effectively capture the cracking locations at the micro-scale.

The proposed framework demonstrates strong potential for generalization to various alloys due to its ability to resolve the deformation, dislocation densities, and damage at individual slip systems. Further enhancements can be made to accommodate other lattice structures, such as BCC and HCP, by incorporating more intricate slip systems. Besides, alloys often exhibit distinctive microstructural features, including crystallographic texture [68], grain size distribution [8], GBs [69], and phase boundaries [70]. The CPFE approach effectively captures texture and gradient grain sizes at larger scales, while DDP is capable of modeling GBs and phase boundaries at smaller scales. In the future, the proposed framework for slip system-resolved GNDs and SEDs will be further validated through in-situ observations across a range of

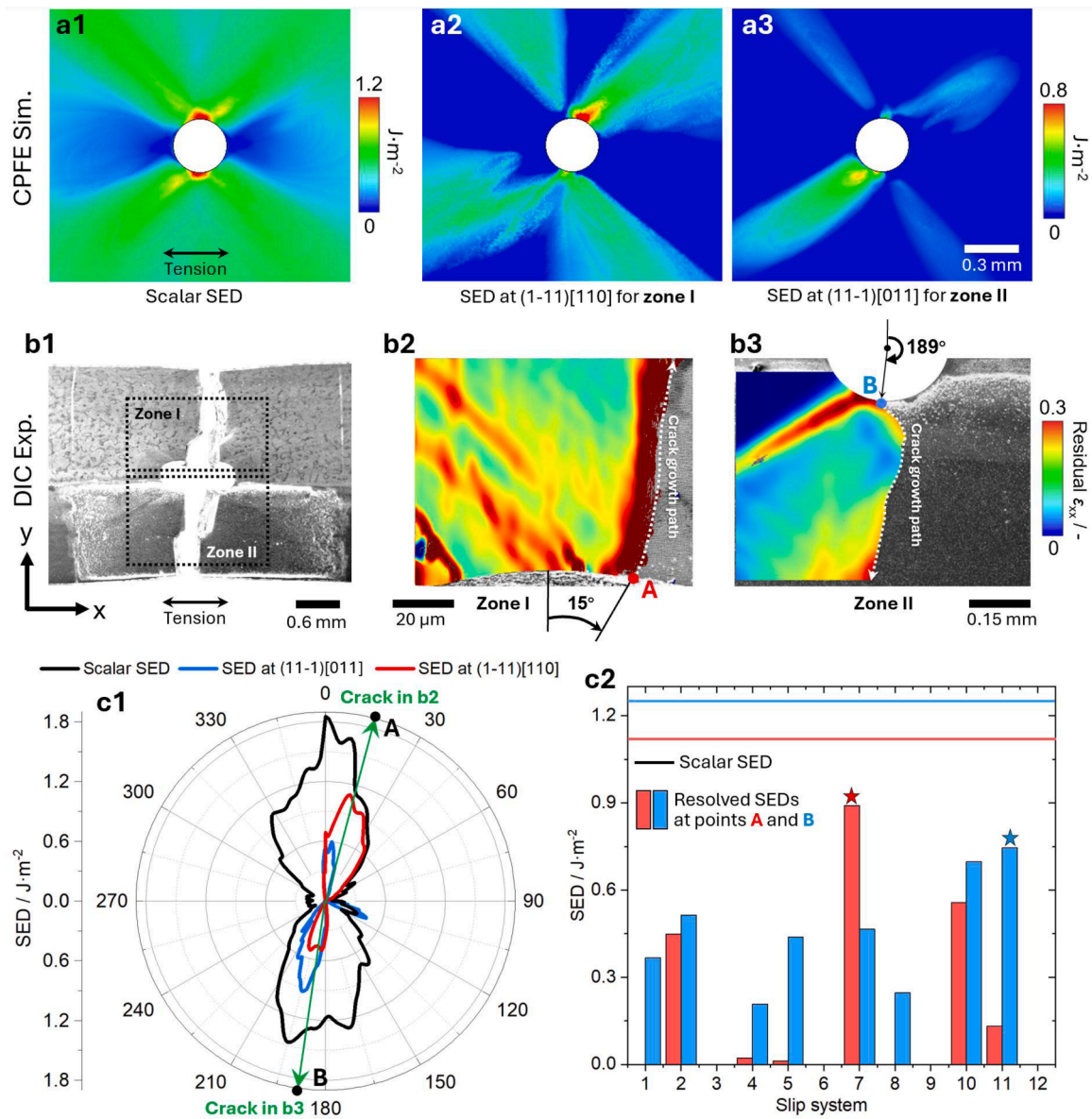


Fig. 10. Crack nucleation sites in orientation #2 sample characterized by DIC and predicted by CPFE simulations. (a) Simulated SED distributions: (a1) scalar SED, (a2) SED at the (1-11)[110] slip system with maximum damage in zone I, (a3) SED at the (11-1)[011] slip system with maximum damage in zone II. (b) fractured specimen, (b1) SEM image of the fractured specimen with orientation #2. (c) Analysis of SED distributions: (c1) Comparison of SED distributions around the hole edge between scalar SED and slip system-dependent SEDs. (c2) Histogram of SED distributions across slip systems at cracking locations A and B marked in (b2) and (b3). The indices of slip systems correspond to Table S. 3 in Supplementary Materials. Except for (b1), all DIC and CPFE results are plotted in undeformed configurations for more accurate comparisons of crack nucleation sites.

alloys.

The proposed framework shows great potential for extension to materials with significant pre-existing dislocations. Without incorporating pre-existing dislocation distributions, it is difficult to directly identify the resolved GNDs and SEDs using DIC, CPFE, and DDP. However, the EBSD-based approach can be employed to map slip system-resolved GNDs, using EBSD data as input for materials with pre-existing dislocations. Additionally, in our previous work [71], the distribution of the residual plastic deformation gradient was estimated based on EBSD by applying the pseudo-inverse solution of Eq. (1). By developing methods to further calculate residual resolved shear strains, the EBSD-based approach holds significant promise for mapping slip system-resolved SEDs in materials with pre-existing dislocations.

5. Conclusions and outlooks

In this paper, EBSD and multi-scale DIC analyses were performed to characterize GNDs at individual slip systems, which were then compared with the corresponding CPFE and DDP simulations. These experimental and simulation approaches were applied to investigate the deformation and damage behaviors in SX plates with a circular hole, avoiding the interference on GND determination from the crystallographic orientations and GBs typically presented in polycrystalline samples. The GNDs-mediated SEDs at individual slip systems were incorporated into CPFE and DDP frameworks, demonstrating improved accuracy and sensitivity for capturing crack nucleation. The key findings are summarized as follows.

1. In contrast to the conventional scalar GNDs, which show symmetric distributions around the slip bands, the resolved GNDs exhibit

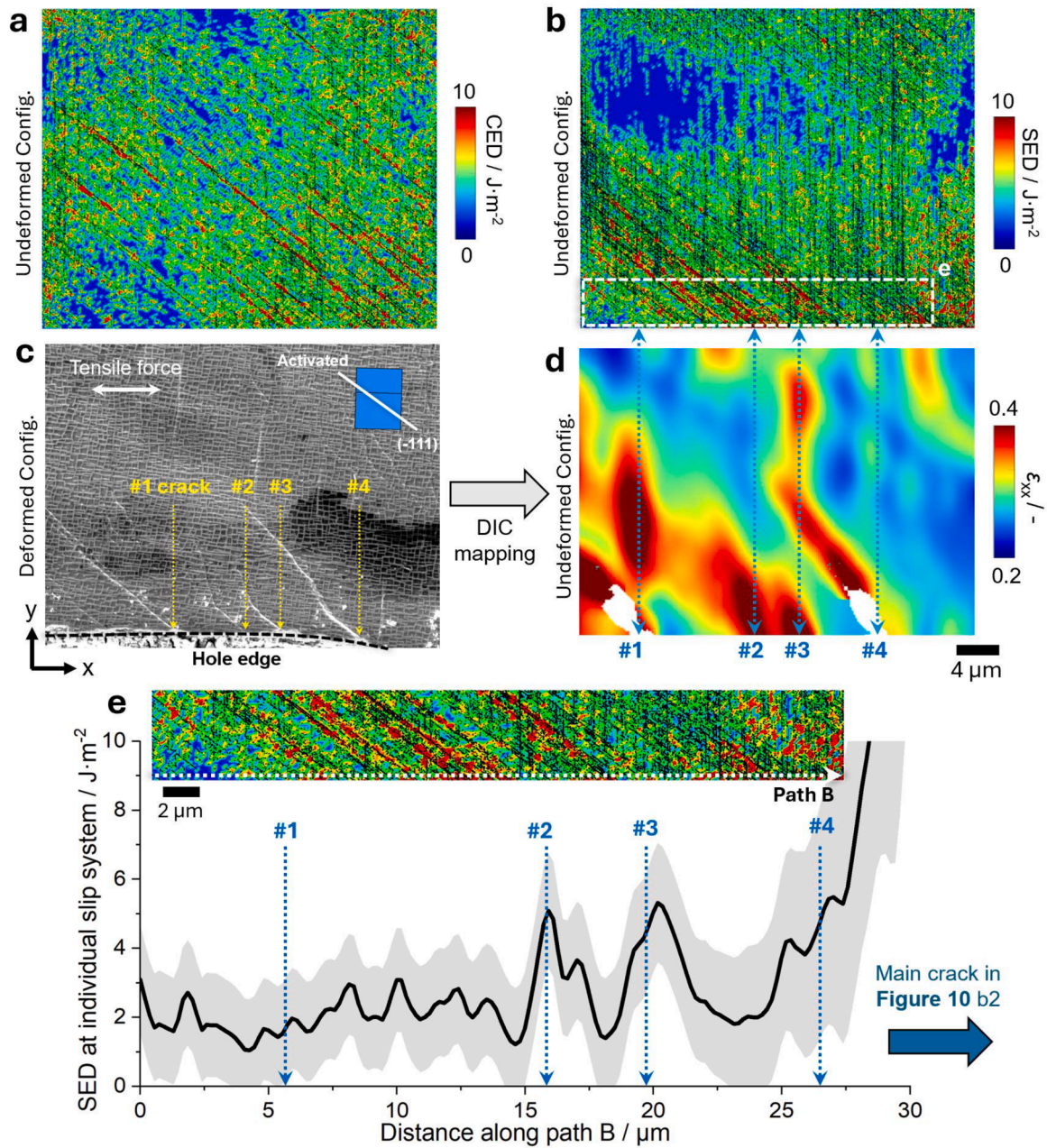


Fig. 11. Crack nucleation sites in orientation #2 sample characterized by μDIC and predicted by DDP simulations. (a)-(b) Comparison of slip system-independent CED and slip system-dependent SED. (c) SEM image showing four crack nucleation sites near the hole edge, as observed during in-situ tensile tests. (d) Cracking locations mapped onto the undeformed configuration using DIC, overlaid with the strain distribution for better visualization of deformation zones. (e) SED distribution along path B. The error band is determined using the standard deviation of SED values within 0.9 μm of path B. The solid black curve indicates the mean SED along this path.

significantly asymmetric distributions around the circular hole in SX plates. These features are captured by DIC, EBSD, and CPFE-based algorithms at the submillimeter-scale.

2. The resolved GNDs migrate along with the extension of slip band boundaries, with the growth rate accelerating in the later stages of deformation.
3. Slip system-dependent SEDs obtained from CPFE reveal asymmetric patterns around the circular hole, providing more accurate predictions of crystallographic planes of crack nucleation and asymmetric cracking locations at the submillimeter-scale, compared with conventional scalar SEDs.
4. At the micro-scale, the DDP simulations demonstrate that slip system-resolved SEDs successfully capture slip trace-induced crack

nucleation near the hole edge, providing a more accurate prediction compared with the CED quantity independent with slip systems.

This study has convincingly demonstrated that slip system-resolved SEDs can serve as a robust damage gauge for SX. It is anticipated that this metric will be applicable to other polycrystalline metals. When applying the proposed framework to polycrystalline materials, the deformation behavior specific to GBs requires further consideration. GB sliding, which is prevalent at high temperatures, should be incorporated into the framework. Additionally, the presence of secondary phases at GBs in some alloys can further complicate GB deformation, necessitating more in-depth investigation. Furthermore, the proposed framework needs to be validated for other geometries, such as micro-cracks and V-type

notches, where more significant stress concentrations and strain gradient effects are present.

Data availability

The data will be available upon reasonable request.

CRediT authorship contribution statement

Zixu Guo: Writing – review & editing, Writing – original draft, Visualization, Software, Methodology, Formal analysis, Data curation. **Xiaochong Lu:** Writing – review & editing, Writing – original draft, Visualization, Software, Methodology, Formal analysis. **Chaitanya Paramatmuni:** Writing – review & editing, Investigation. **Huajian Gao:** Writing – review & editing, Validation, Supervision, Project administration. **Fionn P.E. Dunne:** Writing – review & editing, Conceptualization. **Wentao Yan:** Writing – review & editing, Supervision, Project administration, Funding acquisition. **Yong-Wei Zhang:** Writing – review & editing, Validation, Supervision, Project administration. **Yilun Xu:** Writing – review & editing, Writing – original draft, Visualization, Software, Methodology, Investigation, Formal analysis, Data curation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at [doi:10.1016/j.actamat.2025.120853](https://doi.org/10.1016/j.actamat.2025.120853).

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