A non-local methodology for geometrically necessary dislocations and application to crack tips

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Abstract

A non-local method for the establishment of geometrically necessary dislocation (GND) based on a non-local domain integral has been developed and incorporated into crystal plasticity finite element (CPFE) formulations. The proposed non-local GND method has been validated through a four-point bending case, where the mesh sensitivity of the traditional GND method has been substantially diminished by virtue of the applied non-local domain integral. A comprehensive parametric study has been conducted to investigate the non-local domain effect on the GND calculation. The application of the non-local GND method has resembled the experimental observation of the GND density distribution near a crack tip, and improved the stress field compared to the local method. The improvement on the accuracy of predicting a microstructural driving force at crack tips reveals the necessity of applying the non-local GND method in predicting material fatigue life.

Keywords: geometrically necessary dislocations; crystal plasticity; strain gradient; crack tip

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1 Introduction

Plastic deformation in crystalline metals is critically controlled by dislocation activity. Extensive experimental and computational evidence demonstrates the role of dislocations in controlling the mechanisms associated with the size effect (Dimiduk et al., 2006; Uchic et al., 2004; Uchic et al., 2009), the grain size effect (*i.e.* Hall-Petch effect (Hall, 1951; Petch, 1953)) and the indentation size effect (Nix and Gao, 1998; Pharr et al., 2010). It is hence important to accurately quantify the dislocation density within crystalline materials for both understanding and tailoring material properties and performance.

Crystal plasticity finite element (CPFE) modelling methods focus on microstructure-sensitive plastic deformation through explicit physics-based individual slip behaviour captured by the crystal plasticity slip rule (Roters et al., 2010). While statistically stored dislocation (SSD) distributions evolve from distributed nucleation, slip and stochastic pinning events by obstacles (Ashby, 2006), they give rise to zero net open Burgers circuit. However, geometrically necessary dislocations (GNDs) arise from plastic strain gradients and accommodate the permanent lattice curvature (Arsenlis and Parks, 1999) established during plastic deformation. In addition, GNDs are sessile by nature, and give rise to a length scale effect (Ashby, 2006). The development of strain gradient plasticity (Fleck and Hutchinson, 1997; Fleck et al., 1994) facilitated the capture of experimentally observed size effects either through the introduction of plastic strain gradients into constitutive formulations or through the explicit incorporation of GNDs and their evolutions into the crystal slip rule. As a consequence, the indentation size effect (Wang et al., 2004), the reinforcing phase size effect (Meisssonier et al., 2001), and the grain size effects (Balint et al., 2008; Cheong et al., 2005; Evers et al., 2002;

1 Lim et al., 2014) have been investigated through the introduction of the characteristic
2 length scale. In addition to the strengthening effects on crystalline materials, the GND
3 density has also been shown to contribute significantly to local dislocation stored
4 energy density (Prastiti et al., 2020), which was introduced as a mechanistic driver of
5 fatigue crack nucleation (Chen et al., 2017; Chen et al., 2018a; Wan et al., 2014) and
6 growth (Wilson and Dunne, 2019) in ductile alloys. It is therefore of importance to
7 accurately determine the spatial distributions of density of GNDs as a prerequisite for
8 predicting material lifetime. GND densities are obtained both from experiments and
9 modelling methods by obtaining lattice curvatures which are related to the Nye tensor
10 (Nye, 1953). For example, in experiments, lattice rotations (Kysar et al., 2010) may be
11 measured using high-resolution electron back-scattered diffraction (HR-EBSD)
12 (Wilkinson and Randman, 2010) or X-ray microdiffraction (Ohashi et al., 2009), from
13 which the GND density may be determined. In CPFE modelling, the curl of the plastic
14 deformation gradient is calculated and related to the Nye tensor. Local CPFE
15 approaches for calculating the GND density utilising the curl operation within a single
16 quadratic finite element have been widely used (Aghababaei and Joshi, 2013; Das et
17 al., 2018; Ma et al., 2006; Mayama et al., 2009; Zhang et al., 2020). However, it is
18 known that the local approach shows strong sensitivity to both mesh size
19 (Paramatmuni et al., 2020) and element type (Cheng et al., 2016; Ma et al., 2006), and
20 nonphysical values of GND density can lead to errors of local relevant field quantities
21 (*e.g.* stress and stored energy, etc), which are significant for the identification of crack
22 nucleation sites and corresponding prediction of lifetime. It is noticing that the
23 *introduction* of the GND term to CPFE modelling framework intrinsically results in a
24 non-local effect of the plasticity (Cheng and Ghosh, 2015; Kawano et al., 2020;

1 Sedaghat and Abdolvand, 2021; Shahba and Ghosh, 2016; Voyiadjis et al., 2010).
2 However, the *determination* of GND density still demands a generic non-local
3 methodology that homogenizes (Pierard et al., 2007) the strain gradient contribution
4 from adjacent elements to the element of interest. Inspired by a non-local plasticity
5 formulation (Gao and Huang, 2001), a new non-local GND computational approach is
6 presented in this paper that accounts for neighbouring finite element plastic
7 deformation gradients when the curl operation is performed, which almost entirely
8 eliminates mesh sensitivity.

9 It has been a long-term ambition to predict the fatigue life of ductile alloys, for which
10 it is the short crack growth that dominates in many cases. Much progress (Barabash
11 et al., 2008; Engel et al., 2020; Ghonem, 2010; Pang and Reed, 2008; Sangid et al.,
12 2011; Texier et al., 2019) has been made on correlating the crack growth (including
13 both growth path and rate) to the detailed microstructure (including morphology,
14 grain size, crystallographic orientation, etc.) near the crack (approximately 1-10 grains
15 surrounding). A particular microstructural quantity, namely the stored energy density
16 which depends upon local GND density (Wan et al., 2014; Xu et al., 2021b), has been
17 found to be a useful mechanistic driver in both fatigue crack nucleation (Chen et al.,
18 2017) and growth (Wilson and Dunne, 2019). The localized GND density has also
19 independently been shown as a precursor for fatigue crack propagation (Martínez-
20 Pañeda and Niordson, 2016; Martínez-Pañeda et al., 2016). However, given the
21 existence of strong strain gradients and a heterogeneous stress field near to the crack
22 tip, coupled with the additional complexity arising from the local microstructural
23 influence, the numerical accuracy of GND density determination remains a challenging
24 task. On the other hand, there presents a dislocation free zone ahead of a crack tip

(Chang and Ohr, 1981), as a result of that dislocations are argued to leave from the crack surface. The dislocation free zone has been experimentally observed in various alloys (e.g. (Ohr, 1985; Ohr et al., 1983)), and it has been shown to affect the subsequent crack propagation (Ge et al., 2015). In spite of analytical efforts (e.g. (Huang and Li, 2004; Li et al., 2018)) on understanding the mechanisms of dislocation free zone, few literature has yet addressed the problem at the crystalline slip scale, where the microstructure dominates the crack propagation behaviour (Castelluccio and McDowell, 2016). Experimental results (Wilkinson et al., 2006) show that the peak of GND density deviates an offset distance 5-10 μ m away from a crack tip within a single crystal. Hence, it requires a more accurate (at least of the micro-scale resolution) determination of dislocation density distribution in the vicinity of the crack tip. In this paper, the new non-local GND approach embedded into a CPFE framework is used to investigate the GND density and the resulting stored energy density fields near an edge crackfront.

The remaining sections of this article begin with the proposed new non-local GND computational scheme incorporated into an CPFE modelling framework in Section 2. A beam bending problem is employed in Section 4 to validate and benchmark the non-local GND approach and to provide comparisons to the local method. The non-local GND method is then used to investigate crack tip quantities and energy fields in Section 5 where assessments of the methodology are presented. Concluding remarks are summarized in Section 6.

2 Crystal plasticity finite element formulations

This section begins with a concise summary of the crystal plasticity finite element (CP) formulation which is utilized to investigate the behaviour of four-point bending of an edge-cracked single crystal under Mode I loading. The local and non-local algorithms for determining the geometrically necessary dislocation (GND) density are then detailed.

2.1 Crystal plasticity finite element modeling

A strain-rate dependent, dislocation-based crystal plasticity finite element (CPFE) framework is adopted for the material description in this study. Only a summary is given here, and full details of the framework can be found in (Dunne et al., 2007).

At a given loading instant, the total deformation gradient $\mathbf{F}$ at a material point is decomposed into two terms, namely the elastic $\mathbf{F}^e$ and plastic $\mathbf{F}^p$ deformation gradients

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p \quad (1)$$

The plastic strain rate $\dot{\boldsymbol{\epsilon}}^p$ is determined from the shear rate $\dot{\gamma}^{(i)}$ along all active slip systems, which gives:

$$\dot{\boldsymbol{\epsilon}}^p = \sum_{i=1}^M \dot{\gamma}^{(i)} \mathbf{s}^{(i)} \otimes \mathbf{n}^{(i)} \quad (2)$$

where M is the total number of active slip systems (up to 24 for a Hexagonal Closed Packed (HCP) crystal and a Body Centre Cubic (BCC) crystal considered here), and $\mathbf{s}^{(i)}$ and $\mathbf{n}^{(i)}$ are the slip and normal direction vectors of the i^{th} slip system, respectively. The slip rate $\dot{\gamma}^{(i)}$ along the i^{th} slip system is governed by thermally activated dislocation

1 escape from obstacles (such as lattice defects, impurities, inclusions, etc), which is
 2 given by

$$\dot{\gamma}^{(i)} = \rho_{ssdm} b^2 v_D \exp\left(-\frac{\Delta H}{k\theta}\right) \sinh\left(\frac{\Delta V}{k\theta} \left|\tau^{(i)} - \tau_c^{(i)}\right|\right) \quad (3)$$

3 where ρ_{ssdm} is the initial mobile statistically stored dislocation density, b is the Burgers
 4 vector, v_D the frequency of attempted dislocation jumps over obstacles, ΔH the
 5 activation energy with associated activation volume ΔV , k the Boltzmann constant,
 6 and $\tau^{(i)}$ and $\tau_c^{(i)}$ are the resolved shear stress and critical resolved shear stress on i th
 7 slip system, respectively. The critical resolved shear stress $\tau_c^{(i)}$ evolves with dislocation
 8 density, which is correlated to the effective plastic strain and lattice curvature,
 9 according to a hardening law. The strain rate sensitivity (SRS) of a slip system is
 10 governed by the combination of ΔH and ΔV .

11 A Taylor-based hardening law is adopted for the evolution of shear resistance along
 12 the i th slip system:

$$\tau_c^{(i)} = \tau_{c0}^{(i)} + Gb\sqrt{\rho_{ssd} + \rho_{gnd}} \quad (4)$$

13 where $\tau_{c0}^{(i)}$ is the intrinsic critical resolved shear stress, G the shear modulus, and ρ_{ssd}
 14 and ρ_{gnd} are the density of statistically stored (SSD) and geometry necessary
 15 dislocations (GND), respectively. The evolution of SSD density is proportionally related
 16 to the effective plastic strain rate $\dot{p}$ with small deformation assumption:

$$\dot{\rho}_{ssd} = \lambda \dot{p} \quad (5)$$

17 where the coefficient λ controls the slip system isotropic hardening rate and is
 18 determined from experimental stress-strain data. The effective plastic strain rate $\dot{p}$ is
 19 given by:

$$\dot{p} = \sqrt{\frac{2}{3} \dot{\epsilon}^p : \dot{\epsilon}^p} \quad (6)$$

1 where $\dot{\epsilon}^p$ is the plastic strain rate tensor.

2 Different forms for SSD density evolution can be used to reflect the slip strength
3 hardening under plastic deformation status. For instance, a double exponential
4 evolution formula of SSD density that is based on the thermodynamics theory of
5 dislocation (Langer et al., 2010; Langer and Le, 2020; Le, 2018; Le et al., 2017, 2018)
6 provides satisfactory agreement between simulation and experimental data.

7 The components of GND density tensor are calculated from Nye's dislocation tensor
8 Λ that is related to the curl of plastic deformation gradient F^p :

$$\Lambda = \nabla \times F^p = \sum_{i=1}^M \rho_{Gs}^i \mathbf{b}^i \otimes \mathbf{s}^i + \rho_{Get}^i \mathbf{b}^i \otimes \mathbf{t}^i + \rho_{Gen}^i \mathbf{b}^i \otimes \mathbf{n}^i \quad (7)$$

9 where ρ_{Gs}^i is the screw component, ρ_{Get}^i and ρ_{Gen}^i the edge components, $\mathbf{b}^i$ the
10 Burger's vector, $\mathbf{s}^i$, $\mathbf{t}^i$ and $\mathbf{n}^i$ the unit vectors on the i th slip system, respectively. This
11 curl operator corresponds to the 'curl3' operator (equivalent to the precurl of a
12 transposed tensor) as detailed in (Das et al., 2018) as index notation:

$$\Lambda_{km} = (\nabla \times F^p)_{km} = \epsilon_{ijk} (F^p)_{mj,i} \quad (8)$$

13 where ϵ_{ijk} is the Levi-Civita tensor.

14 The full form of solving the GND density tensor ρ_G is hence given by:

$$A \rho_G = \bar{\Lambda} \quad (9)$$

15 where $\bar{\Lambda}$ is the vectorized Nye's dislocation tensor, A is a $9 \times (3 \times M)$ tensor containing
16 the coefficients of the $\mathbf{b}^i \otimes \mathbf{s}^i$, $\mathbf{b}^i \otimes \mathbf{t}^i$ and $\mathbf{b}^i \otimes \mathbf{n}^i$. The $M \times 3$ independent GND
17 components cannot be uniquely solved with the nine equations from the term Λ .

1 Therefore a minimization algorithm is required to resolve the uniqueness of eqn.(9).
 2 Two extensively used algorithms, namely L1- and L2- normalization that are motivated
 3 by geometry- and energy-orientated minimization respectively are given by (Kysar et
 4 al., 2010):

$$L_1 = \sum_{i=1}^M |\rho^i| \quad (10)$$

$$L_2 = \left[\sum_{i=1}^M (\rho^i)^2 \right]^{1/2} \quad (11)$$

5 In this paper, the L_2 -norm minimization based on minimizing the sum of the squares
 6 of the solved dislocation densities (Arsenlis and Parks, 1999) is utilized to solve eqn.(9)
 7 following singular value decomposition. The scalar GND density is then given by the
 8 by the L_2 -norm minimization of the edge and screw dislocation density components
 9 of Nye's tensor (Cheng and Ghosh, 2015):

$$\rho_{gnd} = \sqrt{\sum_{i=1}^M (\rho_{Gs}^i)^2 + (\rho_{Get}^i)^2 + (\rho_{Gen}^i)^2} \quad (12)$$

10 Based on the discussion above, it is key for determining the GND density to establish
 11 an algorithm for finding the curl of the plastic deformation gradient (*i.e.* eqn.(7)). The
 12 local and non-local methods for this are presented respectively in the following
 13 section.

14 2.2 Material properties for the two investigated problems

15 Two very differing problem types are considered here to investigate the non-local
 16 methodology, namely four-point bending in a ferritic (BCC) single crystal and a mode
 17 I loaded edge-cracked titanium (HCP) single crystal. Crystal properties for the ferritic

1 steel (Barzdajn, 2018) and the commercially pure titanium (Gong and Wilkinson, 2009)
2 are given in Table 1 and

3 Table 2, respectively. The stress strain response curves of the two single crystals
4 subject to monotonic, uniaxial tension are reported in Appendix A.

5 Table 1. Material properties for ferritic phase (BCC) iron-based single crystal

$E(\text{GPa})$	ν	$G(\text{GPa})$	$\lambda(\mu\text{m}^{-2})$	$b(\text{nm})$	$\tau_{c0}(\text{MPa})$
235	0.3	45	0.05	0.25	180
$\rho_{ssdm}(\mu\text{m}^{-2})$	$k(\text{JK}^{-1})$	$\Delta H(\text{eV})$	$\Delta H(\text{J})$	ΔV	
0.01	1.38×10^{-23}	0.16	2.6×10^{-20}	$14.3b^3$	

6

7 Table 2. Material properties for commercial pure titanium (HCP)

$E_{11}(\text{GPa})$	$E_{33}(\text{GPa})$	ν_{12}	ν_{13}	$G_{13}(\text{GPa})$	$b(\text{nm})$	$\rho_{ssdm}(\mu\text{m}^{-2})$
104	143	0.48	0.20	47	0.32	0.01
$\tau_{c0}^{(a)}(\text{MPa})$	$\tau_{c0}^{(c+a)}(\text{MPa})$	$k(\text{JK}^{-1})$	$\lambda(\mu\text{m}^{-2})$	$\Delta H(\text{eV})$	ΔV	
200	500	1.38×10^{-23}	0.05	0.22	$21.3b^3$	

8

9 3 Establishment of GND density

10 There are generally two types of approaches, namely local and non-local, for
11 determining the Nye tensor using eqn.(8) and hence GND density, which are categorized
12 by whether considering the contribution of strain gradients from neighbour finite
13 elements. Both of the approaches are discussed in this section.

14 3.1 Local GND algorithm

15 The local algorithm for Nye tensor and GND calculation considers the differentiation
16 operation in eqn.(8) within a single (appropriate) element, and hence the element
17 shape function has to be at least 2nd order otherwise a constant zero GND density
18 results. We apply the methodology that was proposed in (Kiwanuka, 2013), which

1 finds derivatives of the plastic deformation gradient by constructing an image element
 2 and using the derivatives of the shape functions of a reduced-integration, quadratic
 3 hexahedral element (C3D20R in the ABAQUS element library). This algorithm has been
 4 generalized to be applicable to a quadratic tetrahedral element (C3D10M).

5 3.2 Non-local GND algorithm

6 In contrast to the local approach, a non-local GND approach considers the
 7 contribution of the deformation gradient in the neighbour elements to the element of
 8 interest. Please note that a generic non-local approach (e.g. a numerical
 9 homogenization scheme (Haouala et al., 2020)) that takes account of quantities (e.g.
 10 stress, strain, etc.) from other elements cannot be straightforwardly applied into the
 11 establishment of GND density quantity because the curl operation (eqn. (8))
 12 intrinsically requires a differentiation computation of the deformation gradient
 13 quantities between elements.

14 Gao and Huang (Guo et al., 2001) proposed a non-local integral that approximates the
 15 gradient calculation through an integral method in two-dimensions. The gradient of a
 16 general tensor $\mathbf{H}$ is approximated by ignoring the higher order terms of its Taylor
 17 expansion within an area A_{cell} as:

$$H_{js,r}^{GH} = \frac{\int_{A_{cell}} (H_{js}(\mathbf{x} + \boldsymbol{\zeta}) - H_{js}(\mathbf{x})) \zeta_k dA}{\int_{A_{cell}} \zeta_r \zeta_k dA} \quad (13)$$

18 where $\mathbf{x}$ is the point of interest, $\boldsymbol{\zeta}$ is the local coordinate vector originating from $\mathbf{x}$ with
 19 its components ζ_r, ζ_k , and A_{cell} the finite integral area. However, this integral is still
 20 deemed a local methodology as the integral cell is still limited to an infinitesimal area
 21 (Counts et al., 2008) of the entire material domain by aiming at high local resolution.

1 As opposed to being limited within a cell, Counts et al. (Counts et al., 2008) developed
 2 a two-dimensional non-local integral that was inspired by the general non-local
 3 quantity acquisition in finite element methods (Strömberg and Ristinmaa, 1996) as:

$$H_{js,r}^{NL} = \frac{\int_V (H_{js}(\mathbf{x} + \boldsymbol{\zeta}) - H_{js}(\mathbf{x})) \zeta_k \psi dV}{\int_V \zeta_r \zeta_k \psi dV} \quad (14)$$

4 where the integral volume V is defined as the whole material body domain Ω such
 5 that it overcomes the drawbacks of eqn.(13). ψ is the weighted kernel function based
 6 on the 2nd order norm of vector $\boldsymbol{\zeta}$ as:

$$\psi = \exp \left[-\frac{1}{\omega} \sqrt{\zeta_1^2 + \zeta_2^2 + \zeta_3^2} \right] \quad (15)$$

7 where ω is the damping coefficient that governs the exponential decay rate of the
 8 weighted kernel function. The general scenario of the point of interest and one of its
 9 neighbour nodes in the whole domain Ω (eqn.(14) assuming small deformation and
 10 hence coordinates constant) is sketched in Figure 1(a).

11 The non-local integral eqn.(14) is herein generalized into full three-dimensional space,
 12 and improved by introducing the non-local domain and substituting the weight
 13 function with the corresponding normalized value, which gives:

$$H_{js,r}^{NL} = \frac{\int_{V_{NL}} (H_{js}(\mathbf{x} + \boldsymbol{\zeta}) - H_{js}(\mathbf{x})) \zeta_k \zeta_l \psi_n dV}{\int_{V_{NL}} \zeta_r \zeta_k \zeta_l \psi_n dV} \quad (16)$$

14 Where V_{NL} is the volume of the non-local domain Ω_{NL} , ζ_l is the third coordinate of $\boldsymbol{\zeta}$
 15 and ψ_n is the normalized weight function. The normalized weight function is defined
 16 as:

$$\psi_n = \frac{\psi}{\int_{V_{NL}} \psi dV} \quad (17)$$

Such that the sum of the weights is a unit quantity, which avoids introducing biased magnitude obtained from the non-local integral (Bažant and Lin, 1988). A large damping coefficient ω gives a slower decay of the normalized weight function as an exponential form (Nguyen et al., 2015) with distance, the parametric study of which are shown in Appendix B.

Figure 1. schematic diagrams of the non-local GND scheme (a) the three-dimensional general scenario of the point of interest (in red) and a neighbour element (in black) (b) the element of interest and its neighbour elements within the non-local domain, and the non-local domain definition by the methods of (c) controlled radius and (d) closest neighbour elements

The implementation of the non-local integral eqn.(16) into the CPFE formulation over a discretized domain for finding the Nye tensor at the element of interest gives

$$\Lambda_{js}^{NL} = \frac{\sum_{\alpha=1}^n [(F^p)_{js}^{\alpha} - (F^p)_{js}] \zeta_k \zeta_l \psi_n V^{\alpha}}{\sum_{\alpha=1}^n \zeta_r \zeta_k \zeta_l \psi_n V^{\alpha}} \quad (18)$$

1 Where Λ_{js}^{NL} is the component of Nye tensor i.e. the curl with respect to r direction, n
2 is the total number of non-local elements (NLEs) involved in the non-local domain
3 Ω_{NL} , $(F^p)_{js}^\alpha$ and $(F^p)_{js}$ the deformation gradient component at the α th element in the
4 array of non-local elements and the element of interest, respectively, and V^α the
5 volume of the α th element. The non-local GND scheme is schematically illustrated in
6 Figure 1(b) for an element with its NLEs within a spherical non-local domain Ω_{NL} . Since
7 the non-local Nye tensor is evaluated inter-elementally using eqn.(18), it does not
8 need involving shape function of elements (as most local methods need so) and hence
9 the mesh type sensitivity in local the GND schemes substantially diminishes.

10 By introducing the non-local domain as a subset of the whole finite element domain,
11 it substantially reduces the computational expense without losing much accuracy
12 when a sufficient number of non-local elements is involved (Counts et al., 2008). There
13 are generally two approaches to define the non-local domain (i.e. the non-local
14 elements) of an element of interest, namely, the controlled radius and closest
15 elements approaches, which are schematically illustrated in Figure 1(c) and (d),
16 respectively, in a two-dimensional case. The controlled radius method counts in the
17 elements within the non-local radius R_{NL} while the closest elements method uses a
18 subset of the closest N_{NLE} elements from the complete set. In spite of that the former
19 closely complies with the geometrical principle, the latter approach gives the identical
20 non-local element number for all elements and hence dispels the biased concerns
21 arising when the element of interest is located at the specimen boundary. In addition,
22 the closes element method also resolves the ambiguity of non-local elements when
23 they are located near the surface of the non-local domain (please see the β th element

1 near the boundary of the non-local sphere in Figure 1(b)). The selection of the local
2 domain necessitates excluding the neighbour elements which remain elastic (where
3 the GND density is zero or does not change), which avoids the potential nonphysical
4 underestimated GND density, for instance when a metal matrix is close to hard
5 particles (Kouzeli and Mortensen, 2002).

6 The general procedure of the proposed non-local GND methodology is summarized as
7 following. Before the CPFE analysis, the volume of all elements V^α and the coordinates
8 of all integration points are outputted, respectively, the latter of which allows to
9 compute the distance vector ζ (including three scalars ζ_1 , ζ_2 and ζ_3 along the three
10 dimensions) between each pair of integration points. By assigning the number of non-
11 local elements, the non-local elements can be found and sorted by their distance for
12 each individual element. Please note the non-local elements for the element located
13 along free surfaces of the specimen are defined using the closest elements approach
14 (see Figure 1(d)). The normalized weight ψ_n is then calculated for each non-local
15 element with respect to the element of interest. The implementation of generating
16 the non-local domain information (*i.e.* including the element volume and normalized
17 weights) prior to the CPFE analysis aims to reduce the computational burden. These
18 quantities are assumed to be constant based on the small strain condition. During the
19 CPFE analysis, the solution-dependent deformation gradient $\mathbf{F}^p$ is updated at each
20 integration point in the end of every analysis increment. Therefore, the non-local Nye
21 tensor components are established using eqn. (18), and then the corresponding the
22 GND density scalar is calculated using the L2-norm minimization scheme through
23 eqn.(11) and (12).

1 Errors develop when the Nye tensor is calculated at the current increment but based
2 on the deformation gradient at the previous one. The errors, however, are minimized
3 to no more than 1% (Wilson et al., 2018) by limiting the time increment size (no
4 greater than 10^{-3} s) *i.e.* a quasi-static loading condition is applied.

5 4 Four-point bending

6 An iron-based (BCC) single crystal subjected to four-point bending is used as a
7 validation and benchmark problem for the proposed non-local GND methodology. The
8 four-point bending case has been extensively applied to understand the mechanical
9 behaviour of crystalline materials (e.g. (Nixon et al., 2010)) because the strain field
10 within the beam are well established as linear variation towards the neutral axis and
11 such that a constant GND density is expected (Li and Fang, 2020). The problem is
12 schematically shown in Figure 2, and the material properties are provided in Table 1.
13 The half-beam, with full dimensions of $200 \times 20 \times 20 \mu\text{m}$, is supported and displacement-
14 loaded at distances of $10 \mu\text{m}$ and $40 \mu\text{m}$ from the free end, respectively. The single
15 crystal is orientated such that its $\langle 100 \rangle$ is parallel to the global x-axis, which is shown
16 in Figure 2(a). A symmetry model (*i.e.* one-half beam) is used to reduce the
17 computational expense, and hence a symmetry boundary condition with respect to
18 the x-axis, $U_x=0$, is imposed on the left face. The beam is also constrained in the z-
19 direction on front and back surfaces ($U_z=0$ at $z=0$ and $z=20 \mu\text{m}$) such that a state of
20 plane strain state is imposed. Appropriate small regions near the loading and support
21 lines are assigned anisotropic elastic properties (with no plasticity) to avoid an
22 unphysical stress concentration. Various element sizes and types are applied to
23 investigate the mesh sensitivity of the local and non-local GND methods. A total

1 deflection of $2\mu\text{m}$ is applied in 10s illustrated in Figure 2(b). In this verification study,
2 the GND term in eqn.(4) is generally decoupled from the hardening (*i.e.* the GND
3 density does not affect the material response) in order to validate the non-local GND
4 method. The GND term is however then coupled in a subsequent analysis to study the
5 effect of the non-local GND method on material response.

6 In the following contents, we firstly validate the proposed non-local methodology by
7 comparing the GND density distribution generated by the local and non-local methods,
8 respectively, with the same hexahedral element type (C3D20R), and element size
9 ($1\mu\text{m}$). The element type and size are changed respectively to show how the non-local
10 method outperforms the traditional local one on the perspective of their sensitivity in
11 determining the GND density. A typical combination of the non-local parameters, *e.g.*
12 the number of non-local element (NLE, represented by the equivalent non-local
13 domain radius R_{NL}) and the damping coefficient (ω) is used in the validation example.
14 Parametric studies on the non-local parameters are then performed to investigate
15 their role in determining the GND density distribution. Another example at the end of
16 this section shows the effect of non-local GND hardening with a specific combination
17 of non-local parameters.

Figure 2. Schematic diagram of the benchmark 4-point beam bending problem. (a) Section view of the beam and crystallographic orientation of the BCC single crystal in the X-Y plane, and (b) the three-dimensional half-beam model with boundary and displacement-controlled loading conditions, and applied displacement shown.

The plastic strain developed within the beam is shown to be approximately 0.9% at the base, and linearly decreases along y-axis to zero close to the neutral axis, as shown along Path A-A' in Figure 3(a). The GND density is approximately constant at $\rho_{gnd}=2.7\mu m^{-2}$ within the plastic zone calculated both by the local and non-local methods. An analytic estimation of the GND density based on the plastic strain gradient (Ashby, 2006) $\rho_{gnd} = \frac{1}{b} \frac{\partial \gamma}{\partial y} \approx \frac{1}{b} \frac{\partial \epsilon_{eff}^p}{\partial y} = 3.5\mu m^{-2}$. Both the local and non-local methods in this example predict the GND density reasonably. Compared to the local method (b), the non-local method predicts a more homogenous distribution of GND density with the same element size ($h=1\mu m$) and element type (C3D20R, a reduced-integral, hexahedral and second-order element). The spot-like extreme GND density values (both low and high which deviate greatly from the mean) obtained by

1 the local method are substantially reduced by the non-local method arising from the
2 non-local domain integral. A further statistical examination of the GND density within
3 the plastic zone (areas framed by dash lines in (c)) obtained by both methods is shown
4 in Figure 3(d). The homogenizing effect of the non-local method given by the non-local
5 integral soothes the GND density distribution within the plastic zone. For instance, the
6 maximum GND density is reduced from 4,000 to $8.5\mu\text{m}^{-2}$ (recall the theoretical
7 solution is $3.5\mu\text{m}^{-2}$ throughout the plastic zone) in the non-local results. An
8 appropriate combination of the non-local domain parameters is hence able to
9 effectively reduce the extreme GND density values that are observed in a local method.

Figure 3. The distribution of (a) effective plastic strain (b) GND density using the local method, (c) GND density using the non-local method (with $R_{NL}=2.1\mu\text{m}$ and $\omega=0.3$) of the beam after deflection. Results are shown in the undeformed frame for clearer illustration. (d) shows the statistical analysis of the GND density within the plastic deformed zone (shown in (c)) using the local and non-local methods. This set of calculations is performed with element size $h=1\mu\text{m}$ and second-order reduced-integration, hexahedral element type.

The mesh sensitivities of both local and non-local GND methods are investigated in Figure 4 with two element sizes $h=1$ and $2\mu\text{m}$ for C3D20R hexahedral elements. The GND density predicted by the local method shows strong mesh sensitivity that can be identified from the contour plots (a) and (b) for mesh size $h=1$ and $2\mu\text{m}$. In addition,

1 the statistical analysis shows that a fine mesh predicts a distinctly narrow
2 frequency distribution of GND density, which is given rise by the local numerical
3 gradient algorithm (Kiener et al., 2011; Kiwanuka, 2013). The proposed non-local
4 method substantially diminishes the mesh sensitivity as the contour plots in (d) and
5 (e) are visually similar for the two mesh sizes. A more comprehensive statistical
6 analysis (f) also verifies the robustness of the GND density upon the mesh size. The
7 computational efficiency of both methods is assessed by varying the nonlocal radius
8 R_{NL} in the non-local method. The CPU time (in Appendix C) is reported to be still
9 determined by the mesh size (*i.e.* the element number) as opposed to the nonlocal
10 radius R_{NL} (*i.e.* the nonlocal element number), which proves the proposed algorithm
11 does not raise the computational demanding much.

12
13 Figure 4. Mesh refinement sensitivity of the local and non-local methods showing the
14 GND density distribution with the local method within the beam discretized with
15 element size (a) $h=2\mu\text{m}$ and (b) $h=1\mu\text{m}$, and (c) the statistical analysis, and the GND
16 density distribution with the nonlocal method with element size (d) $h=2\mu\text{m}$ and (e)
17 $h=1\mu\text{m}$, and (f) the statistical analysis. All simulations employ C3D20R elements, and
18 the same non-local domain parameters ($R_{NL}= 2.1\mu\text{m}$ and $\omega=0.5$) are assigned to the
19 nonlocal calculations.

1 The local GND method is also criticised for its element type dependence by virtue of
2 the utilization of various corresponding shape functions, which are presented in Figure
3 5 (a)-(c). The GND value is predicted to be systematically higher by the model (a)
4 discretized by a second order tetrahedral element (C3D10M in ABAQUS) than that (b)
5 by a second order, reduced integral hexahedral element (C3D20R) with identical
6 element *edge* size $h=1\mu\text{m}$. The statistical analysis (c) also shows the median values by
7 the two element types apparently separate. The proposed non-local method, on the
8 contrary, benefiting from the non-local domain integral, shows limited element type
9 dependence as shown in the GND density distribution in (d) and (e) for the tetrahedral
10 and hexahedral elements, respectively. The GND density histograms for two distinct
11 element types show good overlap for the non-local method, which is important since
12 tetrahedral elements are widely used and necessary in applications for which complex
13 geometries are involved, *e.g.* a particle matrix composite (PMC) modelling (Chawla et
14 al., 2006; Xu et al., 2021a).

Figure 5. Element type sensitivity of the local and non-local GND methods. The GND density distribution within the beam with (a) tetrahedral (C3D10M), (b) hexahedral (C3D20R) obtained by the local method and (c) the statistical analysis of GND

1 distribution by the two element types. The GND density distribution within the beam
 2 with (a) tetrahedral, (b) hexahedral obtained by the non-local method and (c) the
 3 statistical analysis. All simulations use the same basic element size $h=1\mu\text{m}$, and the
 4 same non-local domain parameters ($R_{NL}=2.1\mu\text{m}$ and $\omega=0.5$) are assigned to the
 5 nonlocal calculations.

6 The GND density determined by the nonlocal integral eqn.(14) is regulated by the non-
 7 local domain size R_{NL} and the damping coefficient ω (through the normalized
 8 weighting function). The effects of the two non-local factors on the GND density
 9 distribution within the 4-point bending beam are detailed in Figure 6. A large non-local
 10 domain enhances the homogenization effect on the GND density field, and hence
 11 extreme values (for instance, the ones indicated in the circled regions) are brought
 12 down towards the mean, which is seen in Figure 6(a), (b) and (c). On the other hand,
 13 a large damping coefficient also enhances the homogenization effect of the non-local
 14 method, which can be seen in Figure 6(d), (e) and (f). The effects of large local domain
 15 size and a high damping coefficient arises because more elements with more uniform
 16 weighting are included in the non-local integral, respectively. The parametric study
 17 suggests an appropriate combination of the non-local parameters $R_{NL}=2-3\mu\text{m}$
 18 (equivalent to 18-32 elements) and $\omega=0.5$ for achieving a satisfactory GND distribution
 19 in the 4-point bending case.

1 Figure 6. Effect of nonlocal domain size and damping coefficient on the GND density.
2 The same damping coefficient $\omega = 0.5$ but various non-local domain sizes apply in (a),
3 (b) and (c) while the same non-local domain size $R_{NL} = 2.1 \mu\text{m}$ but various damping
4 coefficients apply in (d), (e) and (f).

5 The non-local GND effect on the material response is investigated by comparing the
6 stress distribution of the beam predicted by the two GND methods in Figure 7. In this
7 case, slip strength increases due to GND and SSD hardening (eqn.(4)) and results are
8 shown for (a) the local method and (b) the non-local method with a typical
9 combination of parameters, and the stress distribution without GND hardening is
10 presented in (c) for reference. The stress response for the case of non-local GND
11 density shows a more homogenous distribution compared to that from the local
12 method, because of the homogenizing effect of the non-local method, and reflects the
13 anticipated result in four-point bending.

14 Figure 7. GND effect on xx-stress distribution predicted by (a) local and (b) non-local
15 GND methods (non-local domain parameters as $R_{NL} = 2.1 \mu\text{m}$ and $\omega = 0.5$), and (c) no
16 GND hardening as a reference case. A hexahedral element with size $h = 1 \mu\text{m}$ is used.

18 5 Edge crack under Mode I loading

19 The proposed non-local GND method has been validated in Section 4 through a four-
20 point bending benchmark, where the deformation fields are generally homogenous

1 away from the loading and support points. The highly heterogenous deformation field
2 in the vicinity of an edge crack tip under Mode I loading in a commercially pure Ti (HCP)
3 single crystal (the material properties listed in

4 Table 2) is now examined using the non-local GND method. The problem setup is
5 schematically illustrated in Figure 8 showing half plane dimensions of
6 $4500\mu\text{m} \times 1500\mu\text{m} \times 5\mu\text{m}$ with a $270\mu\text{m}$ through-thickness edge crack, which is
7 monotonic loaded under Mode I stress-control. The single crystal is assigned
8 crystallographic orientation such that its c -axis out-of-plane and parallel to the z -axis,
9 and hence the two prism- $\langle a \rangle$ slip systems are anticipated to be activated. C3D20R
10 (second-order hexahedral) elements are applied to discretize the specimen, and the
11 crackfront region (circled in red dashed line in (a)) is assigned a highly refined element
12 size with $h=2\mu\text{m}$ to resolve the deformation field near the crack tip. Only the back face
13 of the specimen is constrained along z -direction (in (b)) such that a plane stress state
14 is achieved along the front face, which aims to mimic the free surface scenario
15 normally observed in experiments. The applied force is monotonically ramped up to a
16 stress level of 400MPa within 10s , which gives an applied stress intensity factor of K_{app}
17 $= 15.5\text{MPa}\cdot\text{m}^{-0.5}$ according to the geometry of the specimen and crack. The GND
18 density hardening in eqn.(4) is switched on throughout in this case.

Figure 8. Schematic diagram of an edge crack problem showing (a) plate dimensions and single crystal orientation, and (b) the imposed boundary conditions and loading.

The xx -stress fields near the crack front are shown in Figure 9 (a) and (b) predicted by the non-local and local GND methods, respectively. The stress predicted by the non-local GND method shows a more homogenous distribution near the crack tip compared to that with the local method, and the latter contains isolated peak value spots by virtue of the localized GND density (as also seen in Figure 7(a)). Despite the complexity of the deformation field of a single crystal (i.e. a continuum) in the vicinity of a crack tip, analytical solutions (Nakamura and Parks, 1988), low-scale simulations (discrete dislocation plasticity with high dislocation density (Cleveringa et al., 2000), distributed dislocation techniques (Mousavi and Lazar, 2015), atomistic dynamics (Shi et al., 2020) and strain gradient plasticity (Martínez-Pañeda and Niordson, 2016) have demonstrated that the strain and stress fields are generally smooth near the crack tip as opposed to the presence of local peak hotspots. Therefore, with comparison of the

1 stress fields, the proposed non-local GND method closely reflects the deformation
2 field in a single crystal near an edge crack front, which improves the prediction of the
3 conventional local GND method.

4 The GND density field near the crackfront is shown in Figure 9(c) and (d) predicted by
5 the non-local and local GND methods, respectively. The non-local GND density shows
6 a more continuum distribution near the crack tip compared that of the local GND
7 method. The averaged GND density along the 'mountain ridge' paths (labelled as 'Left'
8 and 'Right' in Figure 9(c)), where the density decreases from the crack tip to the
9 material bulk, are reported in Figure 9 (e) for both methods. The local method predicts
10 a peak value at the crack tip and the density abruptly reduces to a small value at about
11 $15\mu\text{m}$ away from the crack tip. In contrast, the non-local method predicts the GND
12 density to have a more steady dependence on the distance from the crack tip, which
13 is more consistent with the GND density distribution experimentally measured using
14 X-ray diffraction (XRD) (Goswami et al., 2017) and EBSD (Kysar and Briant, 2002) as a
15 continuum field near a short crack. Of more significance, the non-local method
16 captures the feature that the GND density peaks at $\sim 1.5 \times 10^{14} \text{m}^{-2}$ at an offset distance
17 $\Delta x = 6\text{--}8\mu\text{m}$ away from the crack front, as opposed to at exactly at the crack tip. Both
18 the magnitude and offset distance of the predicted GND distribution highly resemble
19 the experimental GND measurement using EBSD (Wilkinson et al., 2006), whose
20 results are also plotted in blue squares in (e). They argued the peak GND value position
21 may indicate the outer circumference of cyclic zone. However, the monotonic loading
22 condition in the CPFE modelling also shows the offset distance. The material region
23 showing the peak lattice rotation is less constrained compared to that at the crack tip
24 (*i.e. the dislocation free zone*) due to the strong stress concentration, which drives

1 dislocations to leave the materials from crack surfaces (Huang and Li, 2004) , at the
2 latter position. Hence the peak GND density (manifesting itself as lattice rotation) is
3 observed with an offset distance from the crack tip, which is similar to the discussion
4 in the microstructure change under tribological constraint (Chen et al., 2018b;
5 Ruebeling et al., 2021). Besides, an asymptotic analysis (Le and Tran, 2016) by applying
6 the continuum dislocation theory for a single crystal with a plane strain crack also
7 shows that there is an offset of the maximum dislocation density location with respect
8 to the crack tip. Despite of the discrepancy of GND density between the non-local CPFE
9 modelling and the experiment, which may origin from the material properties and slip
10 systems, the proposed non-local method nonetheless substantially improves the
11 prediction of the GND density distribution compared to experimental observations in
12 the vicinity of a crack tip, where a highly heterogenous deformation presents. In
13 addition, the application of the proposed non-local GND methodology on the edge
14 crack problem has captured the feature of dislocation free zone ahead of an edge
15 crack tip, and hence provides potential mechanisms for the development of the
16 dislocation free zone.

Figure 9. the stress field predicted by (a) the non-local GND method and (b) the local GND method near the crack front. The GND density distribution computed by the (c) the non-local GND method and (d) the local GND method near the crack front. (e) the GND density along two paths (indicated in (d)) from the crack tip to the far field by both methods. The mesh size is $h=2\mu m$ for both methods, and a combination of non-local domain parameters $R_{NL}=6\mu m$ and $\omega=0.5$ is applied for the non-local GND method.

The stored energy density G proposed in (Wan et al., 2014) is given as:

$$G = \int \frac{\xi |\boldsymbol{\sigma} : d\boldsymbol{\varepsilon}^p|}{\sqrt{\rho_{ssd} + \rho_{gnd}}} \quad (19)$$

where ξ is the fraction of dissipated energy stored as dislocation structures and often estimated to be ~ 0.05 (Kamlah and Haupt, 1997). The stored energy density distribution is shown in Figure 10(a) and (b) near the crackfront region predicted by the non-local and local GND method, respectively. The diffused distribution with multiple-peak spots of stored energy computed by the local GND method would make

1 the crack growth and nucleation ambiguous. In contrast, a more concentrated
2 distribution near the crack tip is observed in the stored energy field predicted by the
3 non-local method, which is given by the GND density regulation shown in Figure 9(c).
4 The definitive prediction of the stored energy unambiguously indicates the crack
5 growth rate and/or potential crack nucleation site. It hence necessitates to apply the
6 non-local GND methodology and appropriate non-local domain parameters ($R_{NL}=6\mu\text{m}$
7 and in this case as indicated as the white circle in (a) and $\omega=0.5$) for accurately
8 predicting the vulnerable sites for crack initiation and the fatigue lifetime of materials.

9
10 Figure 10. the stored energy density distribution predicted by (a) the non-local GND
11 method and (b) the local GND method near the crack front. The non-local domain size
12 is indicated as the white circle in (a), and the crack tip is indicated as the black wedge.

13 6 Conclusion

14 A non-local GND methodology that is based on the non-local domain integral has been
15 developed and incorporated into the length scale-dependent, rate-sensitive crystal
16 plasticity finite element framework. The newly proposed non-local methodology
17 features a non-local domain in the full three-dimensional space. Comprehensive study
18 has been conducted on the governing parameters of the non-local GND method.

- 1 • The non-local GND approach has been validated through a four-point bending
2 beam problem, the results of which improves the geometrically necessary
3 dislocation density distribution. The mesh sensitivity in typical local GND
4 methods has been substantially diminished by applying an appropriate non-
5 local domain size.
- 6 • The application of the proposed non-local GND method on investigating the
7 heterogenous deformation of a single crystal near a crack tip has captured the
8 GND density and stress distribution near the crack tip that is observed in
9 independent experiments, which is an example of the dislocation free zone
10 ahead of crack tip.
- 11 • The improvement of the stored energy calculation performed near an edge
12 crack tip sheds light into the potential benefits of applying the proposed non-
13 local GND method in fatigue lifetime prediction.

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1 Appendix A

2
3 Figure A1. stress strain response under monotonic uniaxial tension for the (a) ferritic
4 phase (BCC) for ferritic phase (BCC) iron-based single crystal used in the four-point
5 bending and (b) the commercial pure titanium (HCP) used in the crack tip problem
6 loaded with three strain rates. The crystals are placed as the reference crystal
7 orientation (*i.e.* the major axis parallel to the corresponding global coordinate axis) as
8 sketched in the inset figure.

9 Appendix B

10
11 Figure B1. the normalized weight function against the distance between element
12 centroids for three damping coefficient ω

1 Appendix C

2
3 Figure C1. the CPU time consumed for the 4-point bending benchmark problem solved
4 using the local and non-local GND approaches with two different mesh sizes. The one-
5 off pre-calculation on the non-local domain information is not taken into account.

6

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References

- Aghababaei, R., Joshi, S.P., 2013. Micromechanics of crystallographic size-effects in metal matrix composites induced by thermo-mechanical loading. *International Journal of Plasticity* 42, 65-82.DOI: <http://dx.doi.org/10.1016/j.iijplas.2012.09.013>.
- Arsenlis, A., Parks, D.M., 1999. Crystallographic aspects of geometrically-necessary and statistically-stored dislocation density. *Acta Materialia* 47, 1597-1611.DOI: [http://dx.doi.org/10.1016/S1359-6454\(99\)00020-8](http://dx.doi.org/10.1016/S1359-6454(99)00020-8).
- Ashby, M.F., 2006. The deformation of plastically non-homogeneous materials. *The Philosophical Magazine: A Journal of Theoretical Experimental and Applied Physics* 21, 399-424.DOI: <http://dx.doi.org/10.1080/14786437008238426>.
- Balint, D.S., Deshpande, V.S., Needleman, A., Van der Giessen, E., 2008. Discrete dislocation plasticity analysis of the grain size dependence of the flow strength of polycrystals. *International Journal of Plasticity* 24, 2149-2172.DOI: <http://dx.doi.org/10.1016/j.iijplas.2007.08.005>.
- Barabash, R., Gao, Y.F., Sun, Y.N., Lee, S.Y., Choo, H., Liaw, P.K., Brown, D.W., Ice, G.E., 2008. Neutron and X-ray diffraction studies and cohesive interface model of the fatigue crack deformation behavior. *Phil Mag Lett* 88, 553-565.DOI: <http://dx.doi.org/10.1080/09500830802311080>.
- Barzdajn, B., 2018. A galling failure model: development of predictive framework for iron based hardfacings based on crystal plasticity finite element. Imperial College London.
- Bažant, Z.P., Lin, F.-B., 1988. Non-local yield limit degradation. *Int J Numer Meth Eng* 26, 1805-1823.DOI: <http://dx.doi.org/10.1002/nme.1620260809>.
- Castelluccio, G.M., McDowell, D.L., 2016. Microstructure-sensitive small fatigue crack growth assessment: Effect of strain ratio, multiaxial strain state, and geometric discontinuities. *Int J Fatigue* 82, 521-529.DOI: <http://dx.doi.org/10.1016/j.ijfatigue.2015.09.007>.
- Chang, S.J., Ohr, S.M., 1981. Dislocation-free zone model of fracture. *J Appl Phys* 52, 7174-7181.DOI: <http://dx.doi.org/10.1063/1.328692>.
- Chawla, N., Sidhu, R., Ganesh, V., 2006. Three-dimensional visualization and microstructure-based modeling of deformation in particle-reinforced composites. *Acta Materialia* 54, 1541-1548.DOI: <http://dx.doi.org/10.1016/j.actamat.2005.11.027>.
- Chen, B., Jiang, J., Dunne, F.P.E., 2017. Microstructurally-sensitive fatigue crack nucleation in Ni-based single and oligo crystals. *J Mech Phys Solids* 106, 15-33.DOI: <http://dx.doi.org/10.1016/j.jmps.2017.05.012>.

- 1 Chen, B., Jiang, J., Dunne, F.P.E., 2018a. Is stored energy density the primary meso-
2 scale mechanistic driver for fatigue crack nucleation? International Journal of Plasticity
3 101, 213-229.DOI: <http://dx.doi.org/10.1016/j.ijplas.2017.11.005>.
- 4 Chen, X., Schneider, R., Gumbsch, P., Greiner, C., 2018b. Microstructure evolution and
5 deformation mechanisms during high rate and cryogenic sliding of copper. Acta
6 Materialia 161, 138-149.DOI: <http://dx.doi.org/10.1016/j.actamat.2018.09.016>.
- 7 Cheng, J.H., Ghosh, S., 2015. A crystal plasticity FE model for deformation with twin
8 nucleation in magnesium alloys. International Journal of Plasticity 67, 148-170.DOI:
9 <http://dx.doi.org/10.1016/j.ijplas.2014.10.005>.
- 10 Cheng, J.H., Shahba, A., Ghosh, S., 2016. Stabilized tetrahedral elements for crystal
11 plasticity finite element analysis overcoming volumetric locking. Computational
12 Mechanics 57, 733-753.DOI: <http://dx.doi.org/10.1007/s00466-016-1258-2>.
- 13 Cheong, K.S., Busso, E.P., Arsenlis, A., 2005. A study of microstructural length scale
14 effects on the behaviour of FCC polycrystals using strain gradient concepts.
15 International Journal of Plasticity 21, 1797-1814.DOI:
16 <http://dx.doi.org/10.1016/j.ijplas.2004.11.001>.
- 17 Cleveringa, H.H.M., Van der Giessen, E., Needleman, A., 2000. A discrete dislocation
18 analysis of mode I crack growth. J Mech Phys Solids 48, 1133-1157.DOI:
19 [http://dx.doi.org/10.1016/S0022-5096\(99\)00076-9](http://dx.doi.org/10.1016/S0022-5096(99)00076-9).
- 20 Counts, W.A., Braginsky, M.V., Battaile, C.C., Holm, E.A., 2008. Predicting the Hall-
21 Petch effect in fcc metals using non-local crystal plasticity. International Journal of
22 Plasticity 24, 1243-1263.DOI: <http://dx.doi.org/10.1016/j.ijplas.2007.09.008>.
- 23 Das, S., Hofmann, F., Tarleton, E., 2018. Consistent determination of geometrically
24 necessary dislocation density from simulations and experiments. International Journal
25 of Plasticity 109, 18-42.DOI: <http://dx.doi.org/10.1016/j.ijplas.2018.05.001>.
- 26 Dimiduk, D.M., Woodward, C., Lesar, R., Uchic, M.D., 2006. Scale-free intermittent
27 flow in crystal plasticity. Science 312, 1188-1190.DOI:
28 <http://dx.doi.org/10.1126/science.1123889>.
- 29 Dunne, F.P.E., Wilkinson, A.J., Allen, R., 2007. Experimental and computational studies
30 of low cycle fatigue crack nucleation in a polycrystal. International Journal of Plasticity
31 23, 273-295.DOI: <http://dx.doi.org/10.1016/j.ijplas.2006.07.001>.
- 32 Engel, B., Rouse, J.P., Hyde, C.J., Lavie, W., Leidermark, D., Stekovic, S., Williams, S.J.,
33 Pattison, S.J., Grant, B., Whittaker, M.T., Jones, J.P., Lancaster, R.J., Li, H.Y., 2020. The
34 prediction of crack propagation in coarse grain RR1000 using a unified modelling
35 approach. Int J Fatigue 137, 105652.DOI:
36 <http://dx.doi.org/10.1016/j.ijfatigue.2020.105652>.
- 37 Evers, L.P., Parks, D.M., Brekelmans, W.A.M., Geers, M.G.D., 2002. Crystal plasticity
38 model with enhanced hardening by geometrically necessary dislocation accumulation.

- 1 J Mech Phys Solids 50, 2403-2424.DOI: [http://dx.doi.org/10.1016/S0022-5096\(02\)00032-7](http://dx.doi.org/10.1016/S0022-5096(02)00032-7).
- 2
- 3 Fleck, N.A., Hutchinson, J.W., 1997. Strain gradient plasticity. Adv Appl Mech 33, 295-361.DOI: [http://dx.doi.org/10.1016/s0065-2156\(08\)70388-0](http://dx.doi.org/10.1016/s0065-2156(08)70388-0).
- 4
- 5 Fleck, N.A., Muller, G.M., Ashby, M.F., Hutchinson, J.W., 1994. Strain Gradient Plasticity - Theory and Experiment. Acta Metall Mater 42, 475-487.DOI: [http://dx.doi.org/10.1016/0956-7151\(94\)90502-9](http://dx.doi.org/10.1016/0956-7151(94)90502-9).
- 6
- 7
- 8 Gao, H., Huang, Y., 2001. Taylor-based nonlocal theory of plasticity. Int J Solids Struct 38, 2615-2637.DOI: [http://dx.doi.org/10.1016/s0020-7683\(00\)00173-6](http://dx.doi.org/10.1016/s0020-7683(00)00173-6).
- 9
- 10 Ge, J., Sun, Y., Wang, T., Liu, S., Bai, Y., 2015. Fatigue crack growth based on the dislocation-free zone (DFZ) model. Engineering Fracture Mechanics 149, 111-118.DOI: <http://dx.doi.org/https://doi.org/10.1016/j.engfracmech.2015.10.001>.
- 11
- 12
- 13 Ghonem, H., 2010. Microstructure and fatigue crack growth mechanisms in high temperature titanium alloys. Int J Fatigue 32, 1448-1460.DOI: <http://dx.doi.org/10.1016/j.ijfatigue.2010.02.001>.
- 14
- 15
- 16 Gong, J., Wilkinson, A.J., 2009. Anisotropy in the plastic flow properties of single-crystal α titanium determined from micro-cantilever beams. Acta Materialia 57, 5693-5705.DOI: <http://dx.doi.org/10.1016/j.actamat.2009.07.064>.
- 17
- 18
- 19 Goswami, R., Qadri, S.B., Pande, C.S., 2017. Fatigue mediated lattice rotation in Al alloys. Acta Materialia 129, 33-40.DOI: <http://dx.doi.org/10.1016/j.actamat.2017.02.061>.
- 20
- 21
- 22 Guo, Y., Huang, Y., Gao, H., Zhuang, Z., Hwang, K.C., 2001. Taylor-based nonlocal theory of plasticity: numerical studies of the micro-indentation experiments and crack tip fields. Int J Solids Struct 38, 7447-7460.DOI: [http://dx.doi.org/10.1016/S0020-7683\(01\)00047-6](http://dx.doi.org/10.1016/S0020-7683(01)00047-6).
- 23
- 24
- 25
- 26 Hall, E., 1951. The deformation and ageing of mild steel: III discussion of results. Proceedings of the Physical Society. Section B 64, 747.
- 27
- 28 Haouala, S., Lucarini, S., Llorca, J., Segurado, J., 2020. Simulation of the Hall-Petch effect in FCC polycrystals by means of strain gradient crystal plasticity and FFT homogenization. J Mech Phys Solids 134, 103755.DOI: <http://dx.doi.org/10.1016/j.jmps.2019.103755>.
- 29
- 30
- 31
- 32 Huang, M., Li, Z., 2004. Dislocation emission criterion from a blunt crack tip. J Mech Phys Solids 52, 1991-2003.DOI: <http://dx.doi.org/https://doi.org/10.1016/j.jmps.2004.03.003>.
- 33
- 34
- 35 Kamlah, M., Haupt, P., 1997. On the macroscopic description of stored energy and self heating during plastic deformation. International Journal of Plasticity 13, 893-911.DOI: [http://dx.doi.org/10.1016/S0749-6419\(97\)00063-6](http://dx.doi.org/10.1016/S0749-6419(97)00063-6).
- 36
- 37

- 1 Kawano, Y., Sato, M., Mayama, T., Mitsuhashi, M., Yamasaki, S., 2020. Quantitative
2 evaluation of slip activity in polycrystalline α -titanium considering non-local
3 interactions between crystal grains. International Journal of Plasticity 127,
4 102638.DOI: <http://dx.doi.org/10.1016/j.iijplas.2019.12.001>.
- 5 Kiener, D., Guruprasad, P.J., Keralavarma, S.M., Dehm, G., Benzerga, A.A., 2011. Work
6 hardening in micropillar compression: In situ experiments and modeling. Acta
7 Materialia 59, 3825-3840.DOI: <http://dx.doi.org/10.1016/j.actamat.2011.03.003>.
- 8 Kiwanuka, R., 2013. Micro-deformation and texture in engineering materials. Oxford
9 University, UK.
- 10 Kouzeli, M., Mortensen, A., 2002. Size dependent strengthening in particle reinforced
11 aluminium. Acta Materialia 50, 39-51.DOI: [http://dx.doi.org/10.1016/S1359-6454\(01\)00327-5](http://dx.doi.org/10.1016/S1359-6454(01)00327-5).
- 12
13 Kysar, J.W., Briant, C.L., 2002. Crack tip deformation fields in ductile single crystals.
14 Acta Materialia 50, 2367-2380.DOI: [http://dx.doi.org/10.1016/S1359-6454\(02\)00070-](http://dx.doi.org/10.1016/S1359-6454(02)00070-8)
15 [8](http://dx.doi.org/10.1016/S1359-6454(02)00070-8).
- 16 Kysar, J.W., Saito, Y., Oztop, M.S., Lee, D., Huh, W.T., 2010. Experimental lower bounds
17 on geometrically necessary dislocation density. International Journal of Plasticity 26,
18 1097-1123.DOI: <http://dx.doi.org/10.1016/j.iijplas.2010.03.009>.
- 19 Langer, J.S., Bouchbinder, E., Lookman, T., 2010. Thermodynamic theory of
20 dislocation-mediated plasticity. Acta Materialia 58, 3718-3732.DOI:
21 <http://dx.doi.org/10.1016/j.actamat.2010.03.009>.
- 22 Langer, J.S., Le, K.C., 2020. Scaling confirmation of the thermodynamic dislocation
23 theory. Proc Natl Acad Sci U S A 117, 29431-29434.DOI:
24 <http://dx.doi.org/10.1073/pnas.2018647117>.
- 25 Le, K.C., 2018. Thermodynamic dislocation theory for non-uniform plastic
26 deformations. J Mech Phys Solids 111, 157-169.DOI:
27 <http://dx.doi.org/10.1016/j.jmps.2017.10.022>.
- 28 Le, K.C., Tran, T.M., Langer, J.S., 2017. Thermodynamic dislocation theory of high-
29 temperature deformation in aluminum and steel. Phys Rev E 96, 013004.DOI:
30 <http://dx.doi.org/10.1103/PhysRevE.96.013004>.
- 31 Le, K.C., Tran, T.M., Langer, J.S., 2018. Thermodynamic dislocation theory of adiabatic
32 shear banding in steel. Scripta Mater 149, 62-65.DOI:
33 <http://dx.doi.org/10.1016/j.scriptamat.2018.02.011>.
- 34 Le, K.C., Tran, V.N., 2016. Stress and dislocation distributions near a crack tip in ductile
35 single crystals. Int J Eng Sci 102, 4-11.DOI:
36 <http://dx.doi.org/10.1016/j.ijengsci.2016.02.005>.

- 1 Li, F.F., Fang, G., 2020. Modeling of 3D plastic anisotropy and asymmetry of extruded
2 magnesium alloy and its applications in three-point bending. International Journal of
3 Plasticity 130, 102704.DOI: <http://dx.doi.org/10.1016/j.iijplas.2020.102704>.
- 4 Li, X., Li, X., Yang, H., Jiang, X., 2018. Analysis of the effect of a micro-crack on plastic
5 zone of the edge macro-crack tip by macroscopic and microscopic methods.
6 Engineering Fracture Mechanics 201, 1-12.DOI:
7 <http://dx.doi.org/https://doi.org/10.1016/j.engfracmech.2018.08.023>.
- 8 Lim, H., Carroll, J.D., Battaile, C.C., Buchheit, T.E., Boyce, B.L., Weinberger, C.R., 2014.
9 Grain-scale experimental validation of crystal plasticity finite element simulations of
10 tantalum oligocrystals. International Journal of Plasticity 60, 1-18.DOI:
11 <http://dx.doi.org/10.1016/j.iijplas.2014.05.004>.
- 12 Ma, A., Roters, F., Raabe, D., 2006. A dislocation density based constitutive model for
13 crystal plasticity FEM including geometrically necessary dislocations. Acta Materialia
14 54, 2169-2179.DOI: <http://dx.doi.org/10.1016/j.actamat.2006.01.005>.
- 15 Martínez-Pañeda, E., Niordson, C.F., 2016. On fracture in finite strain gradient
16 plasticity. International Journal of Plasticity 80, 154-167.DOI:
17 <http://dx.doi.org/10.1016/j.iijplas.2015.09.009>.
- 18 Martínez-Pañeda, E., Niordson, C.F., Gangloff, R.P., 2016. Strain gradient plasticity-
19 based modeling of hydrogen environment assisted cracking. Acta Materialia 117, 321-
20 332.DOI: <http://dx.doi.org/10.1016/j.actamat.2016.07.022>.
- 21 Mayama, T., Ohashi, T., Kondou, R., 2009. Geometrically necessary dislocation
22 structure organization in FCC bicrystal subjected to cyclic plasticity. International
23 Journal of Plasticity 25, 2122-2140.DOI:
24 <http://dx.doi.org/10.1016/j.iijplas.2009.02.001>.
- 25 Meissonnier, F.T., Busso, E.P., O'Dowd, N.P., 2001. Finite element implementation of
26 a generalised non-local rate-dependent crystallographic formulation for finite strains.
27 International Journal of Plasticity 17, 601-640.DOI: [http://dx.doi.org/10.1016/S0749-
28 6419\(00\)00064-4](http://dx.doi.org/10.1016/S0749-6419(00)00064-4).
- 29 Mousavi, S.M., Lazar, M., 2015. Distributed dislocation technique for cracks based on
30 non-singular dislocations in nonlocal elasticity of Helmholtz type. Engineering Fracture
31 Mechanics 136, 79-95.DOI: <http://dx.doi.org/10.1016/j.engfracmech.2015.01.015>.
- 32 Nakamura, T., Parks, D.M., 1988. Three-Dimensional Stress Field Near the Crack Front
33 of a Thin Elastic Plate. Journal of Applied Mechanics 55, 805-813.DOI:
34 <http://dx.doi.org/10.1115/1.3173725>.
- 35 Nguyen, G.D., Korsunsky, A.M., Belnoue, J.P.H., 2015. A nonlocal coupled damage-
36 plasticity model for the analysis of ductile failure. International Journal of Plasticity 64,
37 56-75.DOI: <http://dx.doi.org/10.1016/j.iijplas.2014.08.001>.

- 1 Nix, W.D., Gao, H.J., 1998. Indentation size effects in crystalline materials: A law for
2 strain gradient plasticity. *J Mech Phys Solids* 46, 411-425.DOI:
3 [http://dx.doi.org/10.1016/S0022-5096\(97\)00086-0](http://dx.doi.org/10.1016/S0022-5096(97)00086-0).
- 4 Nixon, M.E., Lebensohn, R.A., Cazacu, O., Liu, C., 2010. Experimental and finite-
5 element analysis of the anisotropic response of high-purity α -titanium in bending.
6 *Acta Materialia* 58, 5759-5767.DOI:
7 <http://dx.doi.org/https://doi.org/10.1016/j.actamat.2010.06.051>.
- 8 Nye, J.F., 1953. Some geometrical relations in dislocated crystals. *Acta Metallurgica* 1,
9 153-162.DOI: [http://dx.doi.org/10.1016/0001-6160\(53\)90054-6](http://dx.doi.org/10.1016/0001-6160(53)90054-6).
- 10 Ohashi, T., Barabash, R.I., Pang, J.W.L., Ice, G.E., Barabash, O.M., 2009. X-ray
11 microdiffraction and strain gradient crystal plasticity studies of geometrically
12 necessary dislocations near a Ni bicrystal grain boundary. *International Journal of*
13 *Plasticity* 25, 920-941.DOI: <http://dx.doi.org/10.1016/j.iplas.2008.04.009>.
- 14 Ohr, S.M., 1985. An electron microscope study of crack tip deformation and its impact
15 on the dislocation theory of fracture. *Materials Science and Engineering* 72, 1-35.DOI:
16 [http://dx.doi.org/https://doi.org/10.1016/0025-5416\(85\)90064-3](http://dx.doi.org/https://doi.org/10.1016/0025-5416(85)90064-3).
- 17 Ohr, S.M., Horton, J.A., Chang, S.-J., 1983. Direct Observations of Crack Tip Dislocation
18 Behavior During Tensile and Cyclic Deformation. Springer Netherlands, Dordrecht, pp.
19 3-15.
- 20 Pang, H.T., Reed, P.A.S., 2008. Effects of microstructure on room temperature fatigue
21 crack initiation and short crack propagation in Udimet 720Li Ni-base superalloy. *Int J*
22 *Fatigue* 30, 2009-2020.DOI: <http://dx.doi.org/10.1016/j.ijfatigue.2008.01.001>.
- 23 Paramatmuni, C., Zheng, Z.B., Rainforth, W.M., Dunne, F.P.E., 2020. Twin nucleation
24 and variant selection in Mg alloys: An integrated crystal plasticity modelling and
25 experimental approach. *International Journal of Plasticity* 135, 102778.DOI:
26 <http://dx.doi.org/10.1016/j.iplas.2020.102778>.
- 27 Petch, N., 1953. The cleavage strength of polycrystals. *Journal of the Iron and Steel*
28 *Institute* 174, 25-28.
- 29 Pharr, G.M., Herbert, E.G., Gao, Y.F., 2010. The Indentation Size Effect: A Critical
30 Examination of Experimental Observations and Mechanistic Interpretations. *Annu Rev*
31 *Mater Res* 40, 271-292.DOI: [http://dx.doi.org/10.1146/annurev-matsci-070909-](http://dx.doi.org/10.1146/annurev-matsci-070909-104456)
32 [104456](http://dx.doi.org/10.1146/annurev-matsci-070909-104456).
- 33 Pierard, O., Llorca, J., Segurado, J., Doghri, I., 2007. Micromechanics of particle-
34 reinforced elasto-viscoplastic composites: Finite element simulations versus affine
35 homogenization. *International Journal of Plasticity* 23, 1041-1060.DOI:
36 <http://dx.doi.org/10.1016/j.iplas.2006.09.003>.
- 37 Roters, F., Eisenlohr, P., Hantcherli, L., Tjahjanto, D.D., Bieler, T.R., Raabe, D., 2010.
38 Overview of constitutive laws, kinematics, homogenization and multiscale methods in

- 1 crystal plasticity finite-element modeling: Theory, experiments, applications. Acta
2 Materialia 58, 1152-1211.DOI: <http://dx.doi.org/10.1016/j.actamat.2009.10.058>.
- 3 Ruebeling, F., Xu, Y., Richter, G., Dini, D., Gumbsch, P., Greiner, C., 2021. Normal Load
4 and Counter Body Size Influence the Initiation of Microstructural Discontinuities in
5 Copper during Sliding. ACS Appl Mater Interfaces.DOI:
6 <http://dx.doi.org/10.1021/acsami.0c19736>.
- 7 Sangid, M.D., Pataky, G.J., Sehitoglu, H., Rateick, R.G., Niendorf, T., Maier, H.J., 2011.
8 Superior fatigue crack growth resistance, irreversibility, and fatigue crack growth-
9 microstructure relationship of nanocrystalline alloys. Acta Materialia 59, 7340-
10 7355.DOI: <http://dx.doi.org/10.1016/j.actamat.2011.07.058>.
- 11 Sedaghat, O., Abdolvand, H., 2021. A non-local crystal plasticity constitutive model for
12 hexagonal close-packed polycrystals. International Journal of Plasticity 136,
13 102883.DOI: <http://dx.doi.org/10.1016/j.iijplas.2020.102883>.
- 14 Shahba, A., Ghosh, S., 2016. Crystal plasticity FE modeling of Ti alloys for a range of
15 strain-rates. Part I: A unified constitutive model and flow rule. International Journal of
16 Plasticity 87, 48-68.DOI: <http://dx.doi.org/10.1016/j.iijplas.2016.09.002>.
- 17 Shi, M., Admal, N.C., Tadmor, E.B., 2020. Noise filtering in atomistic stress calculations
18 for crystalline materials. J Mech Phys Solids 144, 104083.DOI:
19 <http://dx.doi.org/10.1016/j.jmps.2020.104083>.
- 20 Strömberg, L., Ristinmaa, M., 1996. FE-formulation of a nonlocal plasticity theory.
21 Computer Methods in Applied Mechanics and Engineering 136, 127-144.DOI:
22 [http://dx.doi.org/10.1016/0045-7825\(96\)00997-8](http://dx.doi.org/10.1016/0045-7825(96)00997-8).
- 23 Texier, D., Stinville, J.C., Echlin, M.P., Pierret, S., Villechaise, P., Pollock, T.M., Cormier,
24 J., 2019. Short crack propagation from cracked non-metallic inclusions in a Ni-based
25 polycrystalline superalloy. Acta Materialia 165, 241-258.DOI:
26 <http://dx.doi.org/10.1016/j.actamat.2018.11.051>.
- 27 Uchic, M.D., Dimiduk, D.M., Florando, J.N., Nix, W.D., 2004. Sample dimensions
28 influence strength and crystal plasticity. Science 305, 986-989.DOI:
29 <http://dx.doi.org/10.1126/science.1098993>.
- 30 Uchic, M.D., Shade, P.A., Dimiduk, D.M., 2009. Plasticity of Micrometer-Scale Single
31 Crystals in Compression. Annual Review of Materials Research 39, 361-386.DOI:
32 <http://dx.doi.org/10.1146/annurev-matsci-082908-145422>.
- 33 Voyiadjis, G.Z., Pekmezi, G., Deliktas, B., 2010. Nonlocal gradient-dependent modeling
34 of plasticity with anisotropic hardening. International Journal of Plasticity 26, 1335-
35 1356.DOI: <http://dx.doi.org/10.1016/j.iijplas.2010.01.015>.
- 36 Wan, V.V.C., MacLachlan, D.W., Dunne, F.P.E., 2014. A stored energy criterion for
37 fatigue crack nucleation in polycrystals. Int J Fatigue 68, 90-102.DOI:
38 <http://dx.doi.org/10.1016/j.ijfatigue.2014.06.001>.

- 1 Wang, Y., Raabe, D., Kluber, C., Roters, F., 2004. Orientation dependence of
2 nanoindentation pile-up patterns and of nanoindentation microtextures in copper
3 single crystals. *Acta Materialia* 52, 2229-2238.DOI:
4 <http://dx.doi.org/10.1016/j.actamat.2004.01.016>.
- 5 Wilkinson, A.J., Meaden, G., Dingley, D.J., 2006. High resolution mapping of strains and
6 rotations using electron backscatter diffraction. *Mater Sci Tech-Lond* 22, 1271-
7 1278.DOI: <http://dx.doi.org/10.1179/174328406x130966>.
- 8 Wilkinson, A.J., Randman, D., 2010. Determination of elastic strain fields and
9 geometrically necessary dislocation distributions near nanoindents using electron
10 back scatter diffraction. *Philosophical Magazine* 90, 1159-1177.DOI:
11 <http://dx.doi.org/10.1080/14786430903304145>.
- 12 Wilson, D., Dunne, F.P.E., 2019. A mechanistic modelling methodology for
13 microstructure-sensitive fatigue crack growth. *J Mech Phys Solids* 124, 827-848.DOI:
14 <http://dx.doi.org/10.1016/j.jmps.2018.11.023>.
- 15 Wilson, D., Zheng, Z.B., Dunne, F.P.E., 2018. A microstructure-sensitive driving force
16 for crack growth. *J Mech Phys Solids* 121, 147-174.DOI:
17 <http://dx.doi.org/10.1016/j.jmps.2018.07.005>.
- 18 Xu, Y., Gu, T., Xian, J., Giuliani, F., Ben Britton, T., Gourlay, C.M., Dunne, F.P.E., 2021a.
19 Intermetallic size and morphology effects on creep rate of Sn-3Ag-0.5Cu solder.
20 *International Journal of Plasticity* 137, 102904.DOI:
21 <http://dx.doi.org/10.1016/j.iijplas.2020.102904>.
- 22 Xu, Y., Wan, W., Dunne, F.P.E., 2021b. Microstructural fracture mechanics: Stored
23 energy density at fatigue cracks. *J Mech Phys Solids* 146, 104209.DOI:
24 <http://dx.doi.org/10.1016/j.jmps.2020.104209>.
- 25 Zhang, J., Li, H.W., Sun, X.X., Zhan, M., 2020. A multi-scale MCCPFEM framework:
26 Modeling of thermal interface grooving and deformation anisotropy of titanium alloy
27 with lamellar colony. *International Journal of Plasticity* 135, 102804.DOI:
28 <http://dx.doi.org/10.1016/j.iijplas.2020.102804>.

29