Operation of a 3D Frank–Read source in a stress gradient and implications for size-dependent plasticity

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Abstract

The operation of a single Frank–Read (FR) source in the presence of a spatial stress gradient is studied using 3D discrete-dislocation dynamics (DDD) simulations and analytic models. Under a sufficiently large stress gradient, the FR source shows a new stable configuration controlled by the low-stress region of the graded stress field. Successive emissions from the source generate a growing dislocation pile-up that exerts an increasing back stress on the source, leading to hardening. The operation of the FR source in the gradient field can be well-approximated by a single critical stress at a unique critical location, allowing for the development of an analytic model of the source operation. These results are applied to rationalize the size-scaling of strength measured in simulations of single-crystal beam bending using DDD and in experiments on bending of single-crystal cantilever beams. This work demonstrates that size effects in plasticity emerge naturally from the mechanics of dislocation sources operating within a stress gradient, and in this case the relevant material length scale is the length of the FR source.
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1. Introduction

Size effects in crystalline plasticity at the micron scale are now well established experimentally in various materials, geometries [1,2] and loading configurations [3–8]. While the origins of these effects have been attributed to geometrically necessary dislocation hardening [9–13], dislocation starvation [14–18] and dislocation source truncation [19–25], predictive models associated with many of these mechanisms are lacking, as is an understanding of the material length scales that govern the observed size effects. As technological systems move increasingly toward smaller scales, the understanding and description of size-dependent plasticity gains increasing engineering significance.

Taking a different mechanistic view to many current theories [9,26], two of us have recently demonstrated that size effects can emerge due to stress gradients [27–29] acting on the dislocation source–obstacle configurations that control the initiation of plastic flow. This “stress gradient plasticity” was analyzed within the context of plane-strain dislocation pile-ups, and was demonstrated numerically using two-dimensional (2-D) plane-strain dislocation dynamics models [27]. The plane strain derivation and demonstration do not reflect the state-of-the-art level of full 3-D discrete dislocation dynamics (DDD) simulations [30–32] and lack a description of the precise details responsible for the source operation in a gradient.

Here we seek to understand the role of stress gradients on the operation of a 3-D Frank–Read (FR) source. Operation of an FR source of length ℓ and Burgers vector b under constant shear stress τ [33] is well known: the dislocation bows out under increasing load until an instability is
reached at approximately $\tau_{FR} \approx \mu b/l$, beyond which a full loop is formed, the source is reconstituted and it begins to operate again, leading to repeated nucleation of loops. Operation of an FR source in a spatially varying stress field has not been studied directly. The structure of 2-D dislocation pile-ups in a linear stress gradient is well established [34], and these results have been used together with some approximations to estimate the back stresses acting on a 2-D FR source in a beam bending configuration [35]. However, the approximations made in Ref. [35] have not been validated and the model predictions deviate from the trends in our full 3-D simulations here. Therefore, in this paper, we use 3-D discrete dislocation simulations to study the operation of a real FR source in a stress gradient. In a linearly varying stress field, we show that the source operation changes fundamentally, with the dislocation unable to cross the “neutral axis” or position of zero stress, preventing pinch-off on the lower-stress side of the pinned FR source. The emitted loop pinned at the neutral axis then exerts a back stress on the reformed source and inhibits further operation. Increasing the stress leads to the eventual operation of the source, but each emitted loop joins a pile-up around the neutral axis. The simulations reveal a new set of metastable states and an associated strengthening of the source as a function of the stress gradient and of the number of previously nucleated dislocation loops. We present and validate a simple 2-D analytic model that captures key features of the operation of an FR source operation in the presence of a stress gradient. We then apply both the simulation results and the analytic model to rationalize some experimental and numerical results on the size dependence of plasticity in the bending of single-crystal beams.

2. Methodology

The 3-D DDD code ParaDiS [31] was used to conduct the simulations. ParaDiS allows for the implementation of arbitrary dislocation configurations with prescribed material properties, boundary conditions, and loading conditions. The initial configuration of an FR source is shown in Fig. 1a: a single straight edge dislocation segment along the $y$ axis is pinned at its two ends and is centered at $x = y = z = 0$ within a large cubic simulation box for which image forces are verified to be negligible. The prescribed boundary conditions are periodic along the faces normal to $y$ and traction free along the faces normal to $x$ and $z$. Four initial source lengths are analyzed, $l = 250b$, $500b$, $1000b$ and $2000b$. While the results are essentially independent of physical material properties, values are needed in the code and we use a shear modulus $\mu = 130 \, \text{GPa}$, a Poisson’s ratio $\nu = 0.305$ and $b = 2.725 \, \text{Å}$. A simple face-centered cubic mobility slip law is used, where slip is only permitted on the $z = 0$ (001) plane containing the source, with no cross-slip and a maximum dislocation segment velocity of $5 \times 10^7 \, \text{b s}^{-1}$. A dislocation core cut-off radius of $r_c = 2b$ was selected such that an FR source in a constant stress field operates at exactly $\tau_{FR} = \mu b/l$ over all lengths investigated here. ParaDiS adaptively discretizes the dislocation segment as the simulation evolves, with a maximum segment length of $l/2$. Of most importance here is that a spatially varying shear stress $\tau_{xz} = \tau_0 (1 - \chi x)$ is imposed, where $\tau_0$ is the magnitude of the stress at the initial source location and $\chi$ is a normalized measure of the stress gradient $\chi = \frac{1}{l} \frac{d\tau_{xz}}{dx}$. The distance $l/2$ is then also the distance from the source to the plane at which the applied stress becomes zero (the neutral axis or neutral plane), and we use a simulation box length of size $4l/\chi$. The evolution of the dislocations is examined for increasing values of the “applied” stress $\tau_0$, for a range of dimensionless gradient values $0.2 \leq \chi l \leq 1$.

The simulations proceed as follows. The stress $\tau_0$ is incremented, inducing dislocation glide. During glide, the cumulative average velocity of every node is recorded. Once (i) at least 400 time steps have passed, (ii) the ratio of the change in the cumulative average velocity of each node to the cumulative average velocity of each node is less than 0.1% for 300 steps and (iii) the maximum node velocity is less than $5 \times 10^7 \, \text{b s}^{-1}$, the stress is incremented again, by 0.5% of the current value. During glide, two types of segment collisions can occur. First, the dislocation can reach the periodic boundaries of the simulation cell and react with itself to form two separate dislocations, one that glides out of the simulation space at $x < 0$ and the other that glides toward $x = l/\chi$. Second, dislocation segments on the two sides of the latter dislocation can meet and annihilate, forming a new FR source and a separated dislocation. The stress at which the latter event occurs is recorded as the operating stress for the source. Fluctuations present within the data are attributable to numerical issues resolving the equilibrium position of all nodes. As the simulation proceeds with continued operation of the source, we obtain the FR source strength $\tau_0$ as a function of the positions of all prior $N - 1$ nucleated dislocations and the stress gradient $\chi$.

3. Results and analysis

Fig. 1 shows a sequence of dislocation configurations under increasing load in the presence of a high stress gradient. The source first bows out into the increasing stress region ($x < 0$), and becomes unstable (Fig. 1b), similar to an FR source in a constant stress field but at a lower applied stress $\tau_0 < \tau_{FR}$ because the local stress fields on the dislocation segments are larger than $\tau_0$ in the $x < 0$ regime. However, as the dislocation expands and loops round into the region $x > 0$, the decreasing stress field inhibits further glide. The loop can expand in $x < 0$ and laterally along $y < 0$ and $y > 0$, exiting the periodic boundaries and creating a dislocation in the region $x < 0$ that moves off to $x = -\infty$. The remaining dislocation remains trapped in the region $x > 0$ and is unable to pinch-off and reconstitute the source. Trapping and inhibition of the pinch-off are the key features of the FR operation in a
gradient field. With increasing applied stress (Fig. 1c), the first dislocation bows increasingly inward and eventually reaches pinch-off, but the new nucleated dislocation rapidly becomes straight and glides to $x = 1/\chi$, where $\tau = 0$. The reconstituted FR source then starts to act again (Fig. 1d), but when this second dislocation enters the $x > 0$ regime there is a back stress due to the first dislocation that impedes the glide and further inhibits pinning (Fig. 1e). The first dislocation does move into the region where $\tau < 0$ due to the forces exerted by the second dislocation, but the overall interactions inhibit pinch-off. With further increased load, pinch-off is achieved, a two-dislocation pile-up is formed (Fig. 1f) centered around $x = 1/\chi$, and the source begins to operate again. But, pinch-off of the next emitted dislocation is further inhibited by the back stresses from the two-dislocation pile-up. This evolution continues, with increasing applied stress needed to pinch-off each subsequent dislocation and an increasing dislocation pile-up around $x = 1/\chi$.

The applied stress required to nucleate successive dislocations from the FR source in the presence of a stress gradient, i.e. to achieve pinch-off and reconstitute the FR source, is shown in Fig. 2. The source strength is normalized by the standard FR strength and is shown as a function of the number of emitted dislocations for a range of normalized stress gradient values $\chi \ell$.

For the initial source operation ($N = 1$) there is a slight weakening effect ($\tau_0 < \tau_{FR}$) for low gradients ($\chi \ell < 0.4$). In
Results here use $l = 250b$, $r_c = 1.16r_F$ and $x_c = 0.44l$ in Eq. (6); similar results are obtained for other values of $l$.

In this domain, the region of higher stress ($x < 0$) drives the initial loop instability and the lower stresses in $x > 0$ are insufficient to inhibit pinch-off. However, for larger gradients ($\chi^f \geq 0.4$), a strengthening effect is observed due to the inhibition of pinch-off (Fig. 1c), a new feature that is unique to the stress gradient problem. In this strengthening regime, the strengthening scales approximately linearly with $\chi^f$. We can estimate the pinch-off stress for the first dislocation by approximating the interactions between the two arc-like segments. We equate the self-force of a bowing arc segment to the sum of the attractive force between two opposite signed screws (treated as straight, and of length $1/\chi^f$) and the integrated applied force. The result qualitatively captures the linear strengthening with respect to $\chi^f$ observed in the simulations ($N = 1$) but is quantitatively quite poor. To make any quantitative comparison requires a priori knowledge of the exact length, orientation and shape of the two arc-like segments, which rapidly becomes unwieldy and approaches execution of precisely what is computed in the ParaDiS simulations.

Fig. 2 shows that, after the first dislocation ($N = 1$) is emitted, operation of the source to emit additional dislocations ($N > 1$) requires an increasing applied stress at any normalized gradient $\chi^f$. Even at the smallest gradient values studied here ($\chi^f = 0.2$) there is some strengthening effect due to the gradient field after a few dislocations ($N = 4$) are emitted. Overall, the magnitude of the strengthening is significant – twice the nominal source strength $\tau_{FR}$ can be achieved for moderate gradients ($\chi^f = 0.4$) and moderate numbers of dislocations ($N = 7$) emitted. Overall, Fig. 2 demonstrates a clear effect of a spatial stress gradient on the operation of a full 3-D FR source and is the first main result of this paper.

We can understand and unify the simulation results shown in Fig. 2 for $N > 1$ through a model that considers the back stresses due to the previously emitted dislocations. First, we ignore the two curved segments of the current dislocation that has not yet pinched off, and treat it as a long straight edge dislocation. The positions of the prior $N - 1$ dislocations and this last dislocation are then the equilibrium positions of an $N$-dislocation pile-up in a linear gradient field, a problem solved by Eshelby and Bilby [34] and shown schematically in the inset of Fig. 3. The Peach–Koehler force on each edge dislocation in a stress field of the form $\tau = -\tau_{0}x$ is satisfied by [34].

$$H_N'' - 2\tau_{0}xH_N' + 2N\tau H_N = 0 \tag{1}$$

where $H_N$ is the $N$th Hermite polynomial, and the equilibrium positions $x_i$, $i = 1, \ldots, N$ are associated with the roots of $H_N$, i.e.

$$0 = H_N\left(\frac{x}{\tau_{0}}\right) = H_N\left(\frac{x}{2\pi(1-v)^{1/2}}\right) \tag{2}$$

The solutions of Eq. (2) are in excellent agreement with our discrete simulations over the entire range of parameters studied, with the trivial difference that our coordinate system is shifted relative to that of Eshelby and Bilby by $l/\chi^f$. For instance, Fig. 3 shows the normalized position of the $N$th dislocation, $x_N/\ell$, as a function of the normalized gradient $\chi^f$, for several values of $N$, as measured in our simulations and as predicted by Eq. (2). Now, given the positions $x_i$ of the $i = 1, \ldots, N$ dislocations, the total resolved shear stress at a point $x$ due to the first $N - 1$ dislocations is

$$\tau(x) = \tau_{0}(1 - \chi x) - \frac{\mu b}{2\pi(1-v)} \sum_{i=1}^{N-1} \frac{1}{x_i - x} \tag{3}$$

This stress field operates on the $N$th dislocation, influencing its pinch-off and reconstitution of the FR source for the next emission. Qualitatively, the prior $N - 1$ edge dislocations emitted from the source symmetrically pile up around $x = l/\chi^f$ and produce a back stress on the $N$th dislocation connected to the source, pushing the long, straight...
segments back toward the source and thus decreasing the ability of the two arc-like segments to bow out (Fig. 1e), thereby inhibiting their intersection and reconstitution of the FR source.

Eq. (3) requires the solution of Eq. (2), which must be done numerically. To obtain a very useful analytical approximation, we first note that half of the dislocations are at distances $x > l/\gamma$ and half at $x < l/\gamma$ (when $N$ is odd, one dislocation sits exactly at $x = l/\gamma$). Therefore, we group the initial $N − 1$ dislocations into a single super-dislocation located at $x = l/\gamma$ and approximate Eq. (3) as

$$\tau(x) = \tau_0(1 - \chi x) - \frac{\mu b f(N - 1)}{2\pi(1 - v)(1 - \chi x)}$$

(4)

The position $x_N$ of the $N$th dislocation satisfies $\tau(x_N) = 0$ and is given by

$$x_N = \frac{1}{\chi} - \left( \frac{\mu b}{2\pi(1 - v)} \right)^{1/2} \left( \frac{(N - 1)}{\tau_0 \chi} \right)^{1/2}$$

(5)

The prediction of Eq. (5) is compared to our simulation data in Fig. 3 for several of the initially emitted dislocations following the initial pinch-off. The error in using the super-dislocation approach is consistently $\sim 0.1\ell$ for $N = 2$, $\sim 0.05\ell$ for $N = 3$ and negligible for higher $N$. We thus proceed to use the super-dislocation approximation below.

We now postulate that pinch-off of the two arcs of the $N$th dislocation (see Fig. 1c) is determined by the attainment of some critical stress $\tau_c$ at some critical location $x_c$, both to be determined, independent of any other details of the configuration (e.g. independent of the magnitude of the gradient, the applied stress or the number of previously emitted dislocations). To test this postulate, we plot the normalized stress field $\tau(x)$ vs. $x$ computed via Eq. (4) for every value of $(\tau_0, \gamma, N)$ ($N > 1$) at which source operation is observed in the simulations (i.e. the data of Fig. 2). We then search for a unique point $(x_c, \tau_c)$ through which all these stress fields pass. The result is shown in Fig. 4 for one case ($\ell = 250b$). Although the stress fields do not all pass through exactly one point, there is a remarkable convergence of the stress fields in the vicinity of $x/\ell = 0.44$ and $\gamma/l_{FR} = 1.16$. Similar results are obtained for the other source sizes, as shown in Table 1. The standard deviation in the critical stress at the critical location is on the order of 7% across all source sizes, and most of the error comes from the cases with $N = 2$ and where source operation is controlled by the initial instability rather than the second pinch-off instability; such cases are outside the scope of our model. There is a slight dependence of the optimal values of $x_c$ and $\tau_c$ on the value of $\ell$ but the dependence is weak for $\ell/b \geq 500$. Using the critical stress $\tau_c$ at the critical location $x_c$, we can thus express the strength $\tau_0$ of the FR source in the presence of a gradient field including the effects of all prior source emissions as

$$\tau_0(\gamma, N) = \frac{\tau_c}{1 - \chi x_c} + \frac{\mu b f(N - 1)}{2\pi(1 - v)(1 - \chi x_c)^2}$$

(6)

for $N > 1$. The predictions of Eq. (6) are shown in Fig. 2. The model captures the initial strengthening and subsequent hardening associated with the inhibited FR source operation in the stress gradient. The model is based on the existence of a new stable configuration for the FR source, so is quite accurate in the regime controlled by that stable configuration, i.e. $\gamma \ell \geq 0.44$ and $N \geq 2$. The model is not accurate for low normalized gradients ($\gamma \ell = 0.2$), where the 3-D FR source operation is controlled by the high-stress region $x < 0$, a regime outside the scope of this model. The demonstration that operation of a 3-D FR source in the presence of a stress gradient can be accurately represented by a (nearly) unique critical stress $\tau_c$ at a critical position $x_c$ with an accurate analytic model for the source strength (Eq. (6)), is the second main result of this paper.

4. Applications

4.1. Comparison to 3-D DDD Simulations

Motz et al. [35] performed full-sample 3-D DDD simulations of pure bending of micron-scale beams containing an initial distribution of FR sources, and measured size-dependent strengthening and hardening. Here, we show that the full 3-D DDD simulations can be accurately interpreted simply through consideration of the operation of a single FR source in the stress gradient created by the bending deformation.

The Motz et al. simulations were nominally for a single-crystal Al beam, with the bending moment about the (001) plane and the tensile direction along [010]. Four {111} {110}-type slip directions are active, and intersect the neutral plane of the beam with Schmid factors of 0.408. Motz et al. [35] report the flow stress $M/Br^2$ as a function of the normalized total displacement along the length of the beam $u/l$ for beam thicknesses $t = 0.5, 0.75, 1.0$ and 1.5 mm. In pure bending, plastic flow initiates on the outer surfaces of the specimen where the local tensile stresses are highest. The relationship between the tensile
stress on the surface and the measured bending moment is \( \sigma_s = 6M/(Bl^2) \), where \( B \) and \( t \) correspond to the breadth and thickness of the beam, respectively. The resolved shear stress driving plastic flow is thus related to tensile stress on the surface as \( \tau_0 = 2.45M/(Bl^2) \).

Our simulations and model predict the flow stress for a single FR source as a function of the number of previously emitted dislocations \( N \). To connect to the Motz data we must thus relate dislocation emission to plastic displacement as follows. Each dislocation emitted from an FR source near the surface will produce an edge dislocation that glides a distance \( 1/\chi = t/\sqrt{2} \) along the glide plane to, on average, the neutral plane of the beam, thereby contributing a total plastic displacement \( \vec{u}_p = b/2 \) with components \( u_{p,x} = u_{p,y} = b\sqrt{2}/4 \). After \( N \) dislocations have been emitted from each active source and for a density of active sources \( \rho \) in a beam of length \( L \) (total number of active sources \( \rho L \)), the normalized plastic displacement along the length direction is then \( \vec{u}_p/L = \sqrt{2N\rho Lb}/4t \). Our simulations thus yield a flow stress vs. normalized plastic displacement given a density of active sources along the beam.

We can now make a comparison to the results of Motz et al. [35]. Motz et al. use beams with \( L/t \) fixed at 3. For such sample dimensions, the normalized plastic displacement along the length is \( \vec{u}_p/L = 3\sqrt{2Npb}/4 \). The density of active sources in the Motz simulations is not known, however. A posteriori, dislocation pile-ups are clearly observed along the length of the beams, though no quantitative results are available. We therefore fitted the quantity \( \rho \) to relate our results, based on single-source operation, to the net total response of multiple sources in the Motz model. Motz et al. present the total displacement and so the elastic displacement of the beam is subtracted from that data. Since the plastic displacement depends on the product \( N\rho \), and since our simulations and the Motz et al. data both show nearly linear hardening, our model can be reasonably fitted to the Motz et al. data for any combination satisfying \( Npb \sim 0.0189 \). However, the Motz et al. data shows relatively smooth, continuous evolution of the plastic displacement and clear multi-dislocation pile-ups, so \( N \) cannot be too small (i.e. a few dislocations emitted from a large number of sources). Fig. 5 shows the normalized flow stress \( \tau_0/\tau_{FR} \) vs. normalized plastic displacement \( \vec{u}_p/L \) as predicted by our model, with \( 1/\rho = 152 \text{ nm} \) and \( N = 10 \), and as obtained in the Motz et al. simulations. Our simulations generally agree well with the Motz et al. data at both small and large beam thicknesses (large and small stress gradients, respectively). At the intermediate thicknesses, stress gradient effects do not set in until a few dislocations have been emitted, so our predictions are only in qualitative agreement with the full simulations of Motz et al. [35]. The general ability of the mechanics of a single FR source operating in a stress gradient to capture the full 3-D DDD bending response of a beam is the third main result of this paper.

Application of our analytic model yields results comparable to those shown in Fig. 2. The model agrees with our simulations and the Motz et al. [35] data at the smallest beam size (highest gradient). At the largest beam size (smallest gradient), the analytic model predicts no hardening but has a higher initial flow stress, since \( \tau_c = 1.33\tau_{FR} \) is the smallest possible value in the analytic model. At intermediate beam sizes, corresponding to moderate stress gradients, the analytic model overestimates our simulations at low \( N \), where the analytic model has already been shown to be less accurate.

4.2. Comparison to experiments

In separate work, Motz et al. [7] conducted experiments on the bending of single-crystal Cu microbeams ranging in thickness from 1 to 7.5 \( \mu \text{m} \) and oriented with the bending moment about the (112) plane and the tensile direction along [110]. During loading, the force vs. end displacement of the beam was recorded and beyond a critical displacement the force reached a plateau. Motz et al. proposed...
that, due to strain hardening, the best measure of the flow stress is to assume an even distribution of plastic flow through the thickness of the beam, identical to a plastic hinge. Using equilibrium of moments, the average flow stress is related to the force by

\[ \sigma_f = 4M/(Bt^2) \]

where \( M = F_{\text{max}}L \) is the moment. The flow stress computed in this manner scaled nearly inversely with beam thickness, following the power law fit \( \sigma_f = 140 \text{ MPa} + 881 \text{ MPa} \mu m^{1.14} \ell^{-1.14} \). In our model, we assume that the onset of plastic flow occurs along the outermost surface of the beam so that \( \sigma_o = 6M/(Bt^2) \). This flow stress can thus be computed from the quoted stress of Motz et al. as \( \sigma_0 = 3\sigma_f/2 \).

With a Schmid factor of 0.408 for slip along any of the four \{111\}(110) active slip directions, the average flow stress leads to a critical resolved shear stress \( \tau_0 \) of 86 MPa + 539 MPa- \mu m^{1.14} \ell^{-1.14} \) along the outer surface of the beam. Interpreting the experiments within the context of our model, we first assume that the measured critical resolved shear stress of 86 MPa at large beam thickness is controlled by FR sources of this strength, i.e. 86 MPa = \( \mu \ell/\ell \). We can then calculate the active source length \( \ell = 517b \) using the shear modulus along the slip direction of \( \mu_{110} = 44.3 \text{ GPa} \) for Cu [36]. Manipulation of the experimental results [7] yields the normalized scaling

\[ \frac{(\tau_0 - \tau_{FR})}{\tau_{FR}} = \frac{\Delta \tau}{\tau_{FR}} = 63.1 \left( \frac{\ell}{\ell} \right)^{-1.14} \]

(7)
as shown in Fig. 6 using the right axis. In these experiments, yielding and subsequent plastic flow initiates where the cantilever beam is integrated into the supporting structure. With further displacement, the region of active plastic flow evolves towards the free end of the beam, manifesting in a sequence of visible slip bands. We thus interpret the plateau observed in the measured force as the critical force required to initiate the formation and hardening of successive slip bands down the length of the beam. This interpretation is supported by finite element computations on this geometry using conventional size-independent plasticity models. The flow stress derived from analysis of the experimental data should thus correspond approximately to the stress required to form and strengthen/harden an individual slip band.

Turning to predictions of our model, dislocations glide along the slip plane to the neutral axis and this geometry dictates that the normalized (shear) stress gradient is \( \chi = 1.71/\ell \). The change in plastic displacement in the direction of flow due to the prior \( N - 1 \) dislocations is \( \ell^2 = (N - 1)b/2 \). We can thus take all of our simulation data, subtract the initial strength \( \tau_0(\chi; N = 1) \) and normalize by both the FR strength (similar to above) and the normalized plastic displacement \( \ell^2/\ell \), to obtain a normalized scaling

\[ \frac{\tau_0(\chi; N) - \tau_0(\chi; N = 1)}{\tau_{FR}(\ell^2/\ell)} \sim 2.5 \left( \frac{\ell}{\ell} \right)^{-1.16} \]

(8)
as shown in Fig. 6 using the left axis. This comparison demonstrates the unique size scaling of the hardening found both in our simulations (at any fixed plastic displacement) and in the experiments. Note that, while Eqs. (7) and (8) show similar size scaling of the hardening, they differ in that Eq. (8) is also normalized by the plastic displacement, leading to the use of different axes in Fig. 6.

The analytic model of Eq. (6) can be manipulated similarly to our simulation data, yielding

\[ \frac{\tau_0(\chi; N) - \tau_0(\chi; N = 1)}{\tau_{FR}(\ell^2/\ell)} = \frac{1.71(\ell/\ell^{-1})}{\pi(1 - v)(1 - 0.82(\ell/\ell)^{-1})^2} \]

(9)

where we have substituted the value \( \chi_f/\ell = 0.48 \) derived from our analysis. Eq. (9) is also shown in Fig. 6, using the left axis. Although Eq. (9) shows an asymptotic scaling of \( (\ell/\ell)^{-1} \) in reasonable agreement with the simulations and experiments, the actual values in the simulated range of \( \ell/\ell \) show a slightly stronger size scaling. In Eq. (9) we are analyzing the size scaling of the hardening rate (hardening vs. plastic strain), and the analytical model predictions of the slope are not as accurate as the overall trends with \( \chi_f \).

A quantitative comparison between our results (Eqs. (8) and (9)) and the experiments of Motz et al. (i.e. to connect the right and left scales in Fig. 6) requires additional information on the total plastic displacement. Equating our result of Eq. (8) to the data of Motz et al. as expressed in Eq. (7) requires a plastic displacement per source of \( u_p/b = 63.1/2.5 = 25.2 \). The prediction of Eq. (8) with \( u_p/b = 25.2 \) is shown in Fig. 6 now using the same (right) axis as used for the experiments.

A local plastic displacement of \( u_p/b = 25.2 \) corresponds to \( N \sim 2u_p/b \sim 50 \) dislocations emitted per source, which would produce surface steps of magnitude 50b/13 nm. Shielding of other potential sources by these pile-ups would
lead to a slip plane spacing that scales as $-t/2$ (the glide distance from source to neutral axis). In the scanning electron micrographs, however, larger displacements and smaller spacing are observed. If the beam rotation of $4^\circ$ over a length of 20 $\mu$m, as shown in the micrograph in Fig. 2a of [35], is assumed to be accommodated exclusively by plastic displacement on one of the two active slip systems in all of the ~20 observed slip bands on each side of the specimen, then the step size $Nb$ per slip band can be estimated as $20Nb \sim (20 \mu m)\tan(4^\circ)$ or $Nb \sim 70$ nm, which is more comparable to the observed step sizes. However, the back stresses associated with the associated $N = 275$ in an individual slip band would give a strengthening effect approximately $275/50 = 5.5$ times higher than observed in the experiments. In general, this comparison indicates that, in the experiments, any FR sources behave like conventional FR sources but operate in the presence of the back stress field created by the pile-up of previously emitted dislocations around the neutral plane of the specimen. The hardening behavior is thus attributable to the stress gradient present in the bending problem, but does not reflect a “stress gradient” effect on the source operation itself in this regime of very large $t/\ell$. Overall, our results for operation of a single FR source in a stress gradient can match the size scaling of the strengthening observed in the experiments, which is the fourth main result of this paper. In spite of this success, quantitative predictions remain difficult and undoubtedly the experimental situation is more complicated than envisioned in our basic analysis.

5. Summary

The model presented here demonstrates the strengthening and hardening effects arising when an FR dislocation source operates in a graded stress field. This behavior arises due to the emergence of a new metastable configuration for the FR source, as demonstrated via DDD simulations, and for which the length of the FR source is the physical material length scale controlling the magnitude of the gradient effect. The operation of an FR source in a stress gradient, including pile-up dislocations formed on the low-stress side of the source, can be captured through an effective FR source strength associated with the attainment of a critical stress at a critical location near the FR source. To make connections to full 3-D simulations and experiments requires knowledge of dislocation source densities. Using values estimated from the numerical studies [35,37], we are able to capture key features of the strengthening and hardening size effects measured in the full 3-D DDD simulations. Our analysis also predicts the scaling of experimentally measured strength vs. size in bending of cantilever beams, although quantification remains difficult, suggesting that other factors may enter. These results are achieved without consideration of either dislocation junction formation or “strain gradient plasticity”. While the dislocation pile-ups that form in beam bending do correspond to plastic strain gradients, the “stress gradient plasticity” analysis here is a more physically motivated description of that pile-up phenomenon and has a well-defined material length scale controlling the size-scaling behavior. However, this does not mean that other strain-gradient phenomena are unimportant; rather, our results indicate that the influence of stress gradients should also be considered in understanding size effects in plasticity.

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