Asymptotic analysis of a pile-up of edge dislocation walls

by

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Abstract

The idealised problem of a pile-up of dislocation walls (that is, of planes each containing an infinite number of parallel and identical dislocations) was presented by Roy et al. (*Mater. Sci. Eng. A* 486:653-661, 2008) as a prototype for understanding the importance of discrete dislocation interactions in dislocation-based plasticity models. They noted that analytic solutions for the dislocation wall density are available for a pile-up of screw dislocation walls, but that numerical methods seem to be necessary for investigating edge dislocation walls. In this paper, we use the techniques of discrete-to-continuum asymptotic analysis to obtain a detailed description of a pile-up of edge dislocation walls. To leading order, we find that the dislocation wall density is governed by a simple differential equation and that boundary layers are present at both ends of the pile-up.

*Keywords:* dislocations, asymptotic analysis, modeling, pile-up
1. Introduction

The high concentration of dislocations in a typical metal sample means that the well-established models of discrete dislocation interactions do not translate easily into models of macroscopic plasticity. Although considerable progress has been made in recent years (see, for example, the review by Groh and Zbib [1]), the problem of tracking all of the dislocations in a reasonably sized body remains computationally intractable and it is necessary to invoke the concept of a macroscopic dislocation density in order to make mathematical or computational progress.

The discrete nature of dislocation interactions is, however, sometimes important. Roy et al. [2] investigated pile-ups of dislocation walls in order to demonstrate that apparently sensible continuum approximations can occasionally lead to problems. They showed that the inter-dislocation spacing in an infinite and periodic dislocation wall plays an important role in determining the expression for the repulsion between two walls of dislocations. Indeed, the repulsion changes qualitatively if the dislocations in the wall are treated as a continuum of infinitesimal dislocations instead of as discrete entities.

Roy et al. [2] used various methods to analyse the horizontal spacing between walls held at equilibrium by an applied shear stress. They obtained numerical solutions to the full discrete problem and compared these with predictions from the model developed in [3] and with results from ‘semi-continuum models’, in which discreteness is maintained within the walls but a wall density function is introduced. In the case of screw dislocations, the introduction of a wall density function yields a singular integral equation for which an explicit solution is given in [4]. However, applying the same method
to walls of edge dislocations led to a singular integral equation for which no closed form solution was found.

In this paper, we demonstrate that further progress can be achieved using the methods of discrete-to-continuum asymptotics, following the methodology introduced for dislocation pile-ups by Voskoboinikov and coworkers [5, 6, 7] and further extended by Hall and coworkers [8, 9]. These methods provide a rigorous way of deriving semi-continuum models and they can also be used to locate and analyse boundary layer regions in which all continuum assumptions break down.

Importantly, we follow [8] in not making the \textit{a priori} assumption that the total length of the pile-up scales linearly with the number of dislocation walls. For walls of edge dislocations, we actually find that the length of the pile-up is proportional to the square root of the number of walls. Having identified and applied this scaling, we obtain a simple differential equation for the wall density that is appropriate throughout most of the pile-up.

1.1. Unscaled equations

Following [2], we consider a system containing \( n + 1 \) edge dislocation walls within an infinite, homogeneous, isotropic, linearly elastic body. Each wall consists of infinitely many dislocations, and each dislocation is straight and parallel with the \( z \)-axis, having a Burgers vector of \( b \, i \). Within each wall, the dislocations have the same horizontal position and are evenly spaced in the vertical direction with a spacing of \( h \). Thus, there is a dislocation at each \((x, y) = (x_i, m \, h)\), where \( i \) is an integer between 0 and \( n \), \( x_i \) is the horizontal location of the \( i \)th wall and \( m \in \mathbb{Z} \).

The walls are numbered sequentially so that \( x_i > x_j \) wherever \( i > j \). A
constant $x$-$y$ shear stress, $\sigma_{\text{ext}}$, is applied and we seek solutions for $\{x_i\}$ so that the dislocations in each wall are at equilibrium, except for those in the wall at $x = 0$, which are pinned.

As described in [2], the $x$-$y$ shear stress on the slip plane $y = 0$ due to a wall of dislocations located at $x = 0$ is given by

$$
\sigma(x) = \frac{\mu b}{2\pi (1 - \nu) h} F\left(\frac{x}{h}\right),
$$

where $\mu$ is the shear modulus, $\nu$ is Poisson’s ratio, and $F(x)$ is defined so that

$$
F(x) = \sum_{k=-\infty}^{\infty} \frac{x (x^2 - k^2)}{(x^2 + k^2)^2} = \pi^2 x \text{csch}^2 (\pi x).
$$

Hence, the $x$-$y$ shear stress experienced by the dislocations in a wall located at $x = x_i$ due to the dislocations in a wall located at $x = x_j$ is given by

$$
\sigma_{\text{int}} = \frac{\mu b}{2\pi (1 - \nu) h} F\left(\frac{x_i - x_j}{h}\right).
$$

We nondimensionalise space so that $x_i = \bar{x}_i h$ and we introduce the nondimensional applied shear stress $\tilde{\sigma}_{\text{ext}} = \frac{\sigma_{\text{ext}}}{2\pi (1 - \nu) h \mu b}$. With this notation, we are left with the following system of equations for $\{\bar{x}_i\}$:

$$
\sum_{j=0, j \neq i}^{n} F(\bar{x}_i - \bar{x}_j) = \tilde{\sigma}_{\text{ext}}, \quad i = 1, 2, \ldots, n,
$$

subject to

$$
\bar{x}_0 = 0.
$$

This system has only two dimensionless parameters, $\tilde{\sigma}_{\text{ext}}$ and $n$, and is in a form similar to the system analysed in [8]. We will use methods like those described in [8] to obtain the leading-order problem in the asymptotic limit $n \to \infty$.  

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2. Leading-order asymptotic analysis

Firstly, let us suppose that $\bar{x}_n \sim n^q$ as $n \to \infty$ for some $q > 0$, and we rescale $\bar{x}$ in (2) by introducing $\bar{x} = \xi n^q$ and $\bar{x}_i = \xi_i n^q$. We note that $q$ must be positive because every wall repels every other wall regardless of the distance between them; with a constant applied stress, this indicates that the total length of the pile-up must increase as the number of walls increases. Applying the rescaling gives

$$\sum_{j=0, j \neq i}^n F(n^q[\xi_i - \xi_j]) = \sigma_{\text{ext}}, \quad i = 1, 2, \ldots, n,$$  \hspace{1cm} (3a)

$$\xi_0 = 0.$$  \hspace{1cm} (3b)

We also define $\xi^*$ so that

$$\xi^* = \lim_{n \to \infty} \xi_n = \lim_{n \to \infty} \frac{\bar{x}_n}{n^q},$$

and we define a density function, $\rho(\xi; n)$, that is sufficiently smooth for our analysis and that satisfies

$$\int_0^{\xi_i} \rho(\xi; n) d\xi = i n^{-1},$$  \hspace{1cm} (4)

We expect that $\rho(\xi; n)$ can be expressed as an asymptotic series as $n \to \infty$ and we ultimately seek an equation for the leading-order density,

$$\rho_0(\xi) = \lim_{n \to \infty} \rho(\xi; n).$$

It follows from the definitions of $\rho(\xi; n)$ and $\xi^*$ that

$$\int_0^{\xi^*} \rho_0(\xi) d\xi = 1,$$  \hspace{1cm} (5a)
and that
\[ \rho_0(\xi^*) = 0. \] (5b)

These observations give us the necessary boundary conditions.

Since \( F(x) \sim x^{-1} \) as \( x \to 0 \), it is appropriate to use the first method described in [8], in which sums are approximated by integrals using Euler-Maclaurin series [10]. With some rearrangement, we find that the sum in (3a) becomes

\[
\sum_{j=0, j\neq i}^n F(n^q[\xi_i - \xi_j]) \sim n \int_0^{\xi_1} \frac{F(n^q[\xi_i - \xi'])}{\rho(\xi'; n)} d\xi'
\]

\[
- n \int_{\xi_{i-1}}^{\xi_i+1} \frac{F(n^q[\xi_i - \xi'])}{\rho(\xi'; n)} d\xi' + \frac{F(n^q[\xi_i - \xi_{i-1}]) + F(n^q[\xi_i - \xi_{i+1}])}{2} 
\]

\[
+ \frac{F(n^q\xi_i) + F(n^q[\xi_i - \xi_n])}{2} + \ldots, \quad (6)
\]

where

\[
\int_a^b \rho(\xi'; n) F(n^q[\xi - \xi']) d\xi'
\]

\[
= \lim_{\epsilon \to 0} \left[ \int_{\xi - \epsilon}^{\xi_{i-1}} \rho(\xi'; n) F(n^q[\xi - \xi']) d\xi' + \int_{\xi_{i+1} + \epsilon}^b \rho(\xi'; n) F(n^q[\xi - \xi']) d\xi' \right],
\]

for any \( \xi \in (a, b) \).

From (4), we note that

\[
\int_{\xi_i}^{\xi_i+1} \rho(\xi'; n) d\xi = \pm n^{-1}.
\]

Using a Taylor series for \( \rho(\xi; n) \) around \( \xi = \xi_i \), it follows that

\[
\xi_i - \xi_{i+1} = \mp \frac{1}{\rho(\xi_i; n)} n^{-1} + \frac{\rho'(\xi_i; n)}{2 \rho(\xi_i; n)^3} n^{-2} + O(n^{-3}), \quad (7)
\]
where all derivatives are taken with respect to $\xi$.

Now, we exploit the fact that $F(x)$ is an odd function to show that

$$T_2 = n \int_{\xi_i - \xi_{i-1}}^{\xi_{i+1} - \xi_i} \rho(\xi + t; n) F(n^q t) \, dt.$$  

Applying (7) then gives

$$T_2 = n \int_{\rho(\xi_i; n)}^{\rho(\xi_{i+1}; n)} \rho(\xi + t; n) F(n^q t) \, dt.  \quad (8)$$

From the definition of $F(x)$, we observe that

$$F(x) = x^{-1} + O(x) \quad \text{as} \quad x \to 0, \quad (9)$$

and that

$$F(x) \sim \pm 4 \pi x e^{-2 \pi |x|} \quad \text{as} \quad x \to \pm \infty. \quad (10)$$

Assuming that $\rho(\xi; n)$ and its derivatives are of order one (which will be valid outside boundary layers), we can now determine how the sizes of $T_2$ and $T_3$ depend on $q$. If $0 < q < 1$, it follows from (8) and (9) that $T_2$ and $T_3$ are both $O(n^{-q})$ terms, while if $q > 1$, we can use (8) and (10) to show that $T_2$ and $T_3$ are both exponentially small. In the case where $q = 1$, a Taylor expansion of $F(\xi)$ about $\xi = \xi_i$ can be used to demonstrate that $T_2$ and $T_3$ are $O(n^{-1})$.

Since $\hat{\sigma}_{\text{ext}}$ is an order one term that we expect to participate in the leading order balance of (3a), it follows that neither $T_2$ nor $T_3$ contributes to the leading order equation for the dislocation wall density, regardless of the value of $q$. Also, we note that $T_4$ will be negligible outside boundary layers near $\xi = 0$ and $\xi = \xi_n$. 

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Away from the boundary layers, we therefore find that (3a) becomes

\[ \hat{\sigma}_{\text{ext}} = n \int_{0}^{\xi_n} \rho(\xi'; n) F(n^q[\xi_i - \xi']) \, d\xi' + E(n), \]  

(11)

where the error term, \( E(n) \), is \( O(n^{-q}) \) if \( 0 < q \leq 1 \) and exponentially small if \( q > 1 \).

It is interesting to note that our equation (11) is equivalent to equation (11) in [2] if the transformations \( x = -n^q \xi \) and \( f(x) = n^{1-q} \rho(-n^{-q}x; n) \) are applied. However, our rescaling has the advantage that \( \rho(\xi; n) \) tends to some well-defined limit as \( n \to \infty \). Moreover, we are able to estimate the size of the error associated with going from a discrete formulation to a continuum formulation, and we can simplify our equation (11) further by using Laplace’s method to exploit the fact that \( n^q \) is large.

Since \( F(x) \) is odd, we note that

\[
n \int_{0}^{\xi^*} \rho(\xi'; n) F(n^q[\xi_i - \xi']) \, d\xi' = n \lim_{\epsilon \to 0} \left( \int_{\epsilon}^{\xi_i} F(n^q y) \rho(\xi_i - y; n) \, dy - \int_{\epsilon}^{\xi^* - \xi_i} F(n^q y) \rho(\xi_i + y; n) \, dy \right).
\]

Assuming that \( \min[\xi_i, \xi^* - \xi_i] \gg n^{-q} \), and so we are sufficiently far from boundary layers near \( \xi = 0 \) and \( \xi = \xi^* \), we can rearrange this expression and make the substitution \( n^q y = Y \) to obtain

\[
n \int_{0}^{\xi^*} \rho(\xi'; n) F(n^q[\xi_i - \xi']) \, d\xi' = n^{1-q} \lim_{\epsilon \to 0} \int_{\epsilon}^{n^q Y} \left( \rho(\xi_i - n^{-q}Y; n) - \rho(\xi_i + n^{-q}Y; n) \right) F(Y) \, dY + \text{exponentially small terms},
\]
where $\lambda$ is chosen so that $\lambda < \min[\xi, \xi^* - \xi]$ and $n^{-q} \ll \lambda \ll 1$.

Since $\lambda \ll 1$, it is appropriate to use a Taylor series about $\xi_i$ to approximate $\rho(\xi_i \pm n^{-q} Y)$. Since $\lambda \gg n^{-q}$, we can take the resulting integrals to infinity while only introducing exponentially small errors. Thus, we find that

$$n \int_0^{\xi^*} \rho(\xi; n) F(n^q[\xi_i - \xi']) d\xi = -2 n^{1-2q} \rho'(\xi_i; n) \int_0^{\infty} Y F(Y) dY$$

$$- n^{1-4q} \rho''(\xi_i; n) \int_0^{\infty} Y^3 F(Y) dY + O(n^{-6q}),$$

and hence,

$$n \int_0^{\xi^*} \rho(\xi'; n) F(n^q[\xi_i - \xi']) d\xi = -n^{1-2q} \frac{\pi}{3} \rho'(\xi_i; n) + O(n^{-4q}).$$

In order to balance with the $O(1)$ term in (11), it follows that $q = \frac{1}{2}$ and that the leading-order density, $\rho_0(\xi)$, satisfies

$$\rho'_0(\xi) = -\frac{3 \tilde{\sigma}_{\text{ext}}}{\pi}. \quad (12)$$

Applying the conditions in (5), we therefore find that

$$\xi^* = \sqrt{\frac{2 \pi}{3 \tilde{\sigma}_{\text{ext}}}}, \quad (13)$$

and that

$$\rho_0(\xi) = \sqrt{\frac{6 \tilde{\sigma}_{\text{ext}}}{\pi}} - \frac{3 \tilde{\sigma}_{\text{ext}}}{\pi} \xi. \quad (14)$$

3. Comparison with numerical solutions

The system in (2) can be solved using Newton’s method. As in [8], the solver is constructed so that the unknown variables are $\Delta x_i = x_i - x_{i-1}$ rather
than $x_i$; this leads to a better conditioned system. The initial state for the Newton iteration was given by

$$\Delta x_i = \hat{\sigma}_{\text{ext}}^{-1}(n + 1 - i)^{-1},$$

which is the exact solution to the problem where each wall only feels its nearest neighbours and the repulsion between walls is approximated by $F(x) \approx x^{-1}$. In order to obtain convergence, the numerical method incorporated a correction mechanism where linear interpolation/extrapolation was used to fix any $\Delta x_i$ that became negative during the first iteration.

The numerical solutions for $x_i$ can be rescaled to find $\xi_i$ and approximate densities obtained by noting that

$$\rho(\xi; n) \approx (\xi_i - \xi_{i-1})^{-1} n^{-1},$$

for $\xi \in (\xi_{i-1}, \xi_i)$. In Figure 1, we plot numerical results for $(\xi_i - \xi_{i-1})^{-1} n^{-1}$ against $\frac{1}{2}(\xi_{i-1} + \xi_i)$ when $\hat{\sigma}_{\text{ext}} = 1$ and compare this with the asymptotic $\rho_0(\xi)$ from (14).

Our results clearly indicate that we have found the correct scaling and that (14) is a good approximation for $\rho(\xi; n)$ throughout most of the domain. However, a boundary layer is clearly present near $\xi = 0$, where the density increases rapidly, and our analysis also suggests that there will also be a boundary layer near $\xi = \xi^*$. In the present work, we do not consider the boundary layers further.

4. Discussion and conclusions

Our analysis has shown that discrete-to-continuum asymptotics can be used to obtain useful information about the structure of a pile-up of edge
Figure 1: Numerically calculated wall densities for $\tilde{\sigma}_{\text{ext}} = 1$ compared with the leading-order asymptotic density (dashed). From top to bottom in the left-hand side of the domain, the continuous curves represent $n = 20$, $n = 50$, $n = 100$ and $n = 200$. In each case, the numerical density is given by $(\xi_i - \xi_{i-1})^{-1} n^{-1}$, while the corresponding $\xi$ coordinate is given by $(\xi_i + \xi_{i-1})/2$. For $n = 20$, the individual data points are shown as $\bigcirc$, while for $n = 50$, they are shown as $\triangle$. 
dislocation walls. An advantage of discrete-to-continuum asymptotics is that it makes explicit the assumptions that underly the conventional semi-continuum approach. While it is possible to go directly from equation (2) to the integral equation given in [2] using Euler-Maclaurin summation, the correction terms obtained cannot be shown to be smaller than the main integral term unless some further assumptions are made about $f(x)$. In contrast, assuming a smooth density function that satisfies (4) makes it easy to show that the Euler-Maclaurin correction terms are small outside boundary layers near the ends of the pile-ups.

It should also be noted that simply replacing a sum with a singular integral is not always appropriate. For example, [8] considers the situation where the repulsion function is of the form $F(x) = x^{-a}$ for some $a \geq 2$. In this situation, Euler-Maclaurin series cannot be used to replace the sum with an integral because the correction terms are not asymptotically smaller than the main integral. It is still possible to adapt discrete-to-continuum asymptotic techniques to deal with cases like this, but it would be difficult to determine the right way to proceed if semi-continuum methods were used.

Our work reinforces the central message of [2] about the importance of discrete dislocation interactions. As noted in [2], the correct system of equations will not be obtained if one begins by replacing the discrete dislocations in each wall with a continuum distribution. We can see this clearly in our analysis from the nondimensionalisation, since replacing discrete dislocations with a continuum distribution of infinitesimal dislocations is equivalent to taking the limit where $b$ and $h$ approach 0 but $bh^{-1}$ is held constant. In this situation, we find that $\hat{\sigma}_{\text{ext}}$ remains unchanged, meaning that we recover the
same dimensionless system of equations, but that the dimensional length of
the pile-up will vanish because $x$ was originally scaled with $h$ and $h \to 0$.

Interestingly, our analysis also suggests that even the semi-continuum
assumption breaks down in certain regions. While we leave the boundary
layer analysis as an open problem, analogy with [5] and [8] leads us to expect
regions where a discrete formulation is necessary, which must be matched
with the continuum approximations that are appropriate throughout the rest
of the domain. Further work is needed on applying discrete-to-continuum
asymptotic methods to these problems.

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