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► **To cite this version:**

Cameron Luke Hall. Asymptotic expressions for the nearest and furthest dislocations in a pile-up against a grain boundary. *Philosophical Magazine*, 2010, 90 (29), pp.3879. 10.1080/14786435.2010.499859 . hal-00608030

HAL Id: hal-00608030

<https://hal.science/hal-00608030>

Submitted on 12 Jul 2011

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Journal:	<i>Philosophical Magazine & Philosophical Magazine Letters</i>
Manuscript ID:	TPHM-10-Jan-0005.R2
Journal Selection:	Philosophical Magazine
Date Submitted by the Author:	24-May-2010
Complete List of Authors:	Hall, Cameron; Oxford University, OCCAM, Mathematical Institute
Keywords:	dislocation theory, dislocation interactions, grain boundaries
Keywords (user supplied):	asymptotic analysis
<p>Note: The following files were submitted by the author for peer review, but cannot be converted to PDF. You must view these files (e.g. movies) online.</p> <p>Resubmission ArmstrongNote.zip</p>	



RESEARCH ARTICLE

Asymptotic expressions for the nearest and furthest dislocations
in a pile-up against a grain boundary

Cameron L. Hall

(Received 00 Month 200x; final version received 00 Month 200x)

In 1965, Armstrong and Head (*Acta Metall.* 13(7):759–764, 1965) explored the problem of a pile-up of screw dislocations against a grain boundary. They used numerical methods to determine the positions of the dislocations in the pile-up and they were able to fit approximate formulae for the locations of the first and last dislocations. These formulae were used to gain insights into the Hall-Petch relationship. More recently, Voskoboynikov *et al.* (*Phil. Mag. Lett.* 87(9):669–676, 2007) used asymptotic techniques to study the equivalent problem of a pile-up of a large number of screw dislocations against a bimetallic interface.

In this paper, we extend the work of Voskoboynikov *et al.* to construct systematic asymptotic expressions for the formulae proposed by Armstrong and Head. The further extension of these techniques to more general pile-ups is also outlined. As a result of this work, we show that a pile-up against a grain boundary can become equivalent to a pile-up against a locked dislocation in the case where the mismatch across the boundary is small.

1. Introduction

In their analysis of brittle fracture of polycrystalline materials, Armstrong and Head [1] investigated a pile-up of screw dislocations against a grain boundary. Specifically, they considered the case of an elastically anisotropic material where the crystal orientation changes across a grain boundary. This situation can be dealt with effectively by using the method of images, in which each real dislocation generates a stress field corresponding to a virtual dislocation situated at the image point opposite the grain boundary. The strength of the image dislocation is an explicitly known quantity that depends on the degree of elastic anisotropy in the crystal and on the misorientation across the boundary. Analogous pile-ups of screw dislocations against a bimetallic interface have recently been investigated by Voskoboynikov *et al.* [8] in the asymptotic limit as the number of dislocations tends to infinity.

In [1], numerical methods were used to solve the equations of equilibrium for pile-ups of up to 64 dislocations. Based on these results, heuristic formulae were given for the positions of the first and last dislocations in the pile-up. In all cases described, it was found that the dimensionless position of the first dislocation could be simply expressed in terms of the number of real dislocations in the pile-up and the comparative strength of an image dislocation relative to a real dislocation. In this paper, the results of Voskoboynikov *et al.* [8] are used to develop asymptotic expressions for the positions of the first and last dislocations in a pile-up of screw dislocations against a grain boundary. These expressions give a good justification for the formulae obtained in [1], but we also find some important differences.

Armstrong and Head [1] considered the implications of their formulae for predicting brittle fracture of a polycrystalline material. By making appropriate assumptions, they recovered an expression for the yield stress that resembles the Hall-Petch criterion. We also consider this problem and obtain equivalent asymptotic

2

1 totic expressions.

2 In a typical polycrystalline material, a very small mismatch in effective shear
3 modulus occurs across the grain boundary. As a result, the repulsion of the pile-up
4 by the grain boundary is weak and the first dislocation becomes very close to the
5 grain boundary. Indeed, we show that the equations for a pile-up against a grain
6 boundary reduce to the equations for a pile-up against a lock in the asymptotic
7 limit of very weak image dislocations.

8 Although [1] only considered pile-ups of screw dislocations, the asymptotic meth-
9 ods developed by Voskoboynikov and coworkers can readily be extended to more
10 complicated problems. Voskoboynikov *et al.* [7] have already analysed a pile-up of
11 edge dislocations against a bimetallic interface and their techniques could also be
12 used to analyse pile-ups of edge or mixed dislocations in elastically anisotropic
13 materials. Although we concentrate on the simplest problem of screw dislocation
14 pile-ups, we demonstrate that it is again possible to exploit the smallness of the
15 mismatch across the grain boundary to obtain simple results for more complicated
16 configurations.

23 2. Pile-up against a grain boundary

24 Armstrong and Head [1] considered both pile-ups against a grain boundary and
25 pile-ups against a grain boundary and a locked dislocation. The former situation
26 is identical to the problem investigated by Voskoboynikov *et al.* [8] and we analyse
27 it first.

28 Consider a pile-up of n screw dislocations, each with Burgers vector $\mathbf{b} = b \mathbf{k}$, in an
29 infinite material containing a grain boundary at the plane $x = 0$. The dislocations
30 are taken to be parallel with the z -axis and are located in the plane $y = 0$ at
31 positions $x = x_i > 0$, $i = 1, \dots, n$. The pile-up is held $\ll in \gg$ place by a constant
32 applied y - z shear stress of magnitude τ . The ratio of the strength of an image
33 dislocation compared to a real dislocation is represented by λ ; Armstrong and
34 Head [1] observe that $|\lambda| < 0.3$ for both iron and copper.

35 With this notation, the equations for dislocation equilibrium for $\lambda > 0$ are given
36 by

$$37 \frac{\mu}{2\pi} \sum_{j=1, j \neq i}^n \frac{1}{x_i - x_j} + \frac{\mu \lambda}{2\pi} \sum_{j=1}^n \frac{1}{x_i + x_j} = \tau, \quad i = 1, 2, \dots, n,$$

38 where μ is the equivalent shear modulus obtained from the anisotropic elasticity
39 tensor [1]. Nondimensionalising space with respect to $\frac{\mu b}{2\pi\tau}$, this leads to the following
40 dimensionless system:

$$41 \sum_{j=1, j \neq i}^n \frac{1}{x_i - x_j} + \lambda \sum_{j=1}^n \frac{1}{x_i + x_j} = 1, \quad i = 1, 2, \dots, n. \quad (1)$$

42 When $\lambda < 0$, equation (1) cannot be used to find x_1 because the attraction
43 from the image dislocations would make the first real dislocation very close to the
44 grain boundary. This implies the situation of a pile-up against a lock and a grain
45 boundary, which we discuss in Section 3.

2.1. Position of the furthest dislocation

As described by Voskoboinikov *et al.* [8], there are three spatial scalings to consider for (1). In the region where x is sufficiently far from the boundary layers near $x = 0$ and $x = x_n$, the spatial variable can be rescaled by introducing $x = n\xi$ to recover a singular integral equation for the leading-order dislocation density, $\rho_0(\xi)$. This integral equation can be solved using the Wiener-Hopf method, enabling us to find both $\rho_0(\xi)$ and the leading-order scaled location of the last dislocation, ξ_0^* . From $\ll [5] \gg$, these are given by

$$\rho_0(\xi) = \frac{1}{\pi \sin(\pi a/2)} \sinh \left(a \cosh^{-1} \frac{\xi_0^*}{\xi} \right) \quad (2)$$

and

$$\xi_0^* = \frac{\sin(\pi a)}{a}, \quad (3)$$

where

$$a = \frac{\cos^{-1} \lambda}{\pi}. \quad (4)$$

Greater accuracy in the position of the furthest dislocation can be obtained by considering the boundary layer near $x = x_n$. Equation (2) indicates that $\rho_0(\xi) \sim \frac{1}{\pi} \sqrt{c_0 (\xi_0^* - \xi)}$ near ξ_0^* , where

$$c_0 = \frac{2a^3}{\sin^2(\pi a/2) \sin(\pi a)}.$$

Following the procedures in [9], we find that

$$\xi_n = \xi_0^* + q c_0^{-\frac{1}{3}} n^{-\frac{2}{3}} + \mathcal{O}(n^{-1}),$$

where q is the first root of the Airy function, $\text{Ai}(x)$.

Taking Taylor series around $\lambda = 0$, this yields

$$\xi_n = 2 \left(1 + \frac{2}{\pi} \lambda \right) + 2^{\frac{1}{3}} q n^{-\frac{2}{3}} \left(1 + \left(\frac{2}{\pi} - \frac{1}{3} \right) \lambda \right) + \mathcal{O}(n^{-1}, \lambda^2). \quad (5)$$

Ignoring the $n^{-\frac{2}{3}}$ term would give the simpler expression

$$\xi_n = 2 \left(1 + \frac{2}{\pi} \lambda \right) + \mathcal{O}(n^{-\frac{2}{3}}, \lambda^2). \quad (6)$$

Using (5), we find that

$$\begin{aligned} x_n &= 2n \left(1 + \frac{2}{\pi} \lambda \right) + 2^{\frac{1}{3}} q n^{\frac{1}{3}} \left(1 + \left(\frac{2}{\pi} - \frac{1}{3} \right) \lambda \right) + \mathcal{O}(1, n\lambda^2) \\ &\approx 2n(1 + 0.64\lambda) - 2.94n^{\frac{1}{3}}(1 + 0.30\lambda). \end{aligned} \quad (7)$$

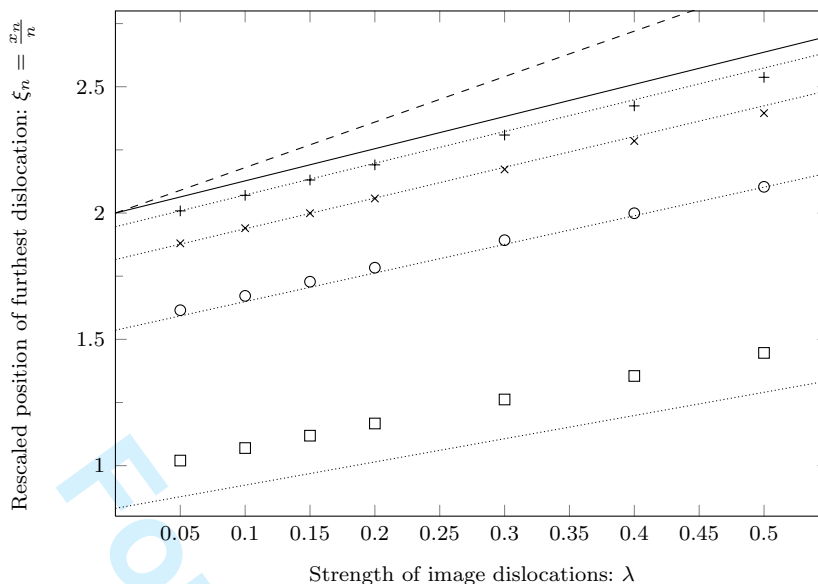


Figure 1. Numerically obtained results for ξ_n using a variety of values of n and λ . Results for $n = 4$ are shown as \square , results for $n = 16$ are shown as \circ , results for $n = 64$ are shown as \times and results for $n = 400$ are shown as $+$. The leading-order asymptotic approximation $\xi_n = 2(1 + \frac{2}{\pi}\lambda)$ is shown as a continuous line while the Armstrong-Head formula $\xi_n = 2(1 + 0.9\lambda)$ is shown as a dashed line. Clearly, the correction due to the boundary layer is important; better asymptotic approximations based on equation (5) are shown as dotted lines.

For comparison, the equivalent expression obtained by Armstrong and Head [1] from curve-fitting is

$$x_n \approx 2n(1 + 0.9\lambda). \quad (8)$$

We have developed a Newton iterative scheme for solving (1), using a starting condition where each dislocation is only able to feel its nearest neighbours and the external stress. This gave the numerical results for ξ_n shown in Figure 1 for a variety of different values of n and λ , including the values used in [1]. Interestingly, equations (6) and (8) both give a fairly poor fit to the final dislocation positions obtained using our numeric scheme. However, including the first correction term associated with the boundary layer gives an expression for ξ_n that *agrees well with the numerical results* over a wide range of λ values and is even *quite* good when n is not very large.

2.2. Position of the nearest dislocation

We now obtain an expression for x_1 , the location of the first dislocation in the pile-up. Since this dislocation will lie in a boundary layer region near $x = 0$, it requires a different spatial scaling from the one described above. Following Voskoboynikov *et al.* [8], we introduce an inner scaling of the form $x = n^{-a/(1-a)}\eta$, where a is defined as above. As shown in [8], the leading-order inner equation takes the form

$$\sum_{j=1, i \neq j}^{\infty} \frac{1}{\eta_i - \eta_j} + \sum_{j=1}^{\infty} \frac{\lambda}{\eta_i + \eta_j} = 0, \quad i = 1, 2, \dots \quad (9)$$

subject to the matching condition

$$\eta_k \rightarrow 2 \left(\frac{k\pi(1-a)\sin(\pi a/2)}{(\xi_0^*)^a} \right)^{1/(1-a)} \quad (10)$$

as $k \rightarrow \infty$.

In Voskoboinikov *et al.* [8], equation (9) is solved using numerical methods. However, it is possible to make further algebraic progress by exploiting the assumption that λ is small. We thus let each η_i be represented as an asymptotic power series in λ :

$$\eta_i \sim \eta_{i,0} + \lambda \eta_{i,1} + \dots$$

Collecting only the leading-order terms in equation (9), we find that

$$\sum_{j=1, i \neq j}^{\infty} \frac{1}{\eta_{i,0} - \eta_{j,0}} = 0, \quad i = 1, 2, \dots \quad (11)$$

Also, we note that $a \sim \frac{1}{2} + \mathcal{O}(\lambda)$ and $\xi_0^* \sim 2 + \mathcal{O}(\lambda)$. Hence, the leading-order matching condition (10) becomes

$$\eta_{k,0} \sim \frac{k^2 \pi^2}{8} \quad (12)$$

as $k \rightarrow \infty$. However, (11) is clearly incorrect when $i = 1$, as all of the terms on the left-hand side are negative. We attempt to resolve this problem by introducing a different scaling for just η_1 . Specifically, we propose $\eta_1 = \lambda \eta_{1,0} + o(\lambda)$ and thus we find that the leading-order equation for $i = 1$ takes the form

$$\frac{1}{2\eta_{1,0}} - \sum_{j=2}^{\infty} \frac{1}{\eta_{j,0}} = 0, \quad (13)$$

while the other leading-order equations are given by

$$\sum_{j=2, i \neq j}^{\infty} \frac{1}{\eta_{i,0} - \eta_{j,0}} + \frac{1}{\eta_{i,0}} = 0, \quad i = 2, 3, \dots \quad (14)$$

Importantly, we note that the system (14) is completely independent of $\eta_{1,0}$. Moreover, this system of equations is identical to the system described in Voskoboinikov *et al.* [9] for the inner problem of a pile-up of dislocations against a lock. Indeed, when λ is small, we find that the dislocation x_1 is precisely equivalent to a locked dislocation to lowest order.

Unlike the system (9), (14) has the advantage that it can be solved exactly. Following Voskoboinikov *et al.* [9] and applying the matching condition (12), we find that

$$\eta_{i,0} = \frac{(\alpha_{i-1})^2}{8}, \quad i = 2, 3, \dots \quad (15)$$

where α_k is the k th positive zero of the Bessel function $J_1(x)$.

6

Rearranging equation (13), this implies that

$$\eta_{1,0} = \frac{1}{16} \left(\sum_{i=1}^{\infty} \frac{1}{\alpha_i^2} \right)^{-1}.$$

We can now exploit the fact that

$$\sum_{k=1}^{\infty} \frac{1}{(j_{\nu,k})^2} = \frac{1}{4(\nu+1)},$$

where $j_{\nu,k}$ is the k th zero of the Bessel function, $J_{\nu}(x)$, and $\nu \geq 0$ to show that

$$\eta_{1,0} = \frac{1}{2},$$

and hence,

$$x_1 \sim \frac{\lambda}{2n^{1-\frac{4}{\pi}\lambda}} \approx \frac{\lambda}{2n^{1-1.27\lambda}}. \quad (16)$$

For comparison, the equivalent expression obtained by Armstrong and Head [1] is

$$x_1 \approx \frac{\lambda}{2n^{1-1.1\lambda}}. \quad (17)$$

The discrepancy between (16) and (17) can be investigated by plotting values of $\log(\frac{2x_1}{\lambda})/\log n$ obtained using the numerical procedure described above against λ , as shown in Figure 2. From this, we clearly see that (16) gives a good approximation of these numerical results when λ is sufficiently small, but that the relationship between $\log(\frac{2x_1}{\lambda})/\log n$ and λ quickly deviates from linearity as λ increases. Indeed, for suitably large values of λ , the Armstrong-Head formula (17) is a better approximation of the numerical results than the asymptotic formula (16).

3. Pile-up against a lock and a grain boundary

Armstrong and Head [1] also consider the situation where there is a locked dislocation at $x = 0$ in addition to image dislocations associated with the grain boundary. In this case, the equations of equilibrium take the form

$$\sum_{j=1, j \neq i}^n \frac{1}{x_i - x_j} + \lambda \sum_{j=1}^n \frac{1}{x_i + x_j} + \frac{1 + \lambda}{x_i} = 1, \quad i = 1, 2, \dots, n. \quad (18)$$

The presence or absence of a locked dislocation at $x = 0$ will not affect the equilibrium equations for the dislocation density in the outer region. Hence, we can repeat the methods of the previous section to find that

$$x_n \sim 2n \left(1 + \frac{2}{\pi} \lambda \right) + 2^{\frac{1}{3}} q n^{-\frac{2}{3}} \left(1 + \left(\frac{2}{\pi} - \frac{1}{3} \right) \lambda \right).$$

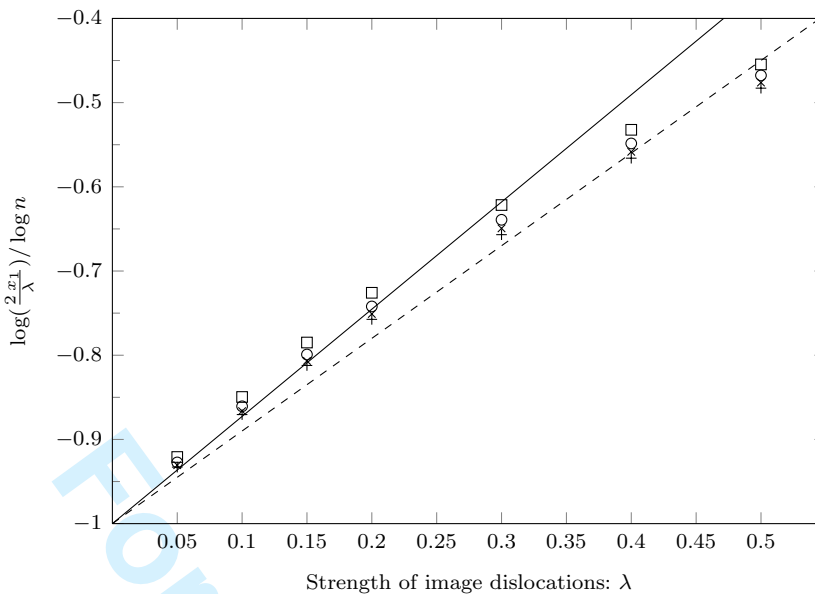


Figure 2. Numerically obtained results for $\log(\frac{2x_1}{\lambda})/\log n$ using a variety of values of n and λ . Results for $n = 4$ are shown as \square , results for $n = 16$ are shown as \circ , results for $n = 64$ are shown as \times and results for $n = 400$ are shown as $+$. The asymptotic approximation $\log(\frac{2x_1}{\lambda})/\log n = -1 + \frac{4}{\pi} \lambda$ is shown as a continuous line while the Armstrong-Head formula $\log(\frac{2x_1}{\lambda})/\log n = -1 + 1.1 \lambda$ is shown as a dashed line.

This is in general agreement with Armstrong and Head [1], who found that the position of the n th dislocation is not noticeably affected by the addition of a locked dislocation at $x = 0$. They reached this conclusion by comparing numerical results for the two cases and finding that they converged as n increased.

However, the locked dislocation will affect the solution in the inner region. In order to match with the unchanged outer region, we find that the same scalings apply as for the simple pile-up against a grain boundary. However, the inner system now takes the form

$$\sum_{j=1, i \neq j}^{\infty} \frac{1}{\eta_i - \eta_j} + \sum_{j=1}^{\infty} \frac{\lambda}{\eta_i + \eta_j} + \frac{1 + \lambda}{\eta_i} = 0, \quad i = 1, 2, \dots$$

As before, we consider the case where λ is small and we propose solutions for η_i as asymptotic power series in λ . This leads us to recover the leading-order system

$$\sum_{j=1, i \neq j}^{\infty} \frac{1}{\eta_{i,0} - \eta_{j,0}} + \frac{1}{\eta_{i,0}} = 0, \quad i = 1, 2, \dots \tag{19}$$

Because of the repulsion from the lock, the $i = 1$ equation is no longer special and we can directly use the solution for a pile-up against a lock given by Voskoboynikov *et al.* [9]. Using this method, we find that

$$\eta_{1,0} = \frac{\alpha_1^2}{8},$$

where α_1 is the first positive zero of the Bessel function $J_1(x)$. Thus,

$$x_1 \sim \frac{\alpha_1^2}{8 n^{1 - \frac{4}{\pi} \lambda}} \approx \frac{1.84}{n^{1 - 1.27 \lambda}}. \tag{20}$$

1 Armstrong and Head [1] observed that plots of $\log x_1$ against $\log n$ based on the
 2 numerical solution of (18) yielded curves that were almost parallel to equivalent
 3 plots of $\log x_1$ against $\log n$ from the numerical solution of (1). This agrees with
 4 the observation that introducing a locked dislocation does not change the scaling
 5 used in the boundary layer.

6 Armstrong and Head [1] also found that, when extrapolated to $n = 1$, the plots
 7 of $\log x_1$ against $\log n$ based on (18) converged to the same point for all values of
 8 λ . Thus, they obtained an expression for x_1 of the form

$$9 \quad x_1 \approx \frac{1.9}{n^{1-1.1\lambda}}. \quad (21)$$

10 Finally, they noted that this agrees well with the approximate result,

$$11 \quad x_1 \sim \frac{\alpha_1^2}{8n} \approx \frac{1.84}{n},$$

12 obtained by Eshelby *et al.* [3] for the well-studied problem of a pile-up against a
 13 locked dislocation (*i.e.* with $\lambda = 0$).

14 4. More general pile-ups

15 One limitation of [1] is that only pile-ups of screw dislocations are considered. For
 16 edge dislocations, more complicated expressions for the image forces are required.
 17 Additionally, it is possible to encounter pile-ups of edge dislocations where the
 18 plane containing the dislocations is not perpendicular to the plane of the grain
 19 boundary. In the simple case of a bimetallic interface (*i.e.* an interface between
 20 two elastically isotropic materials with different elastic constants), the full image
 21 stress is given by Head [4] and perpendicular pile-ups of edge dislocations have
 22 been analysed by Kuang and Mura [5] and by Voskoboynikov *et al.* [7].

23 In the more general case where there is a planar boundary between two different
 24 elastically anisotropic materials, Tucker [6] gives an expression for the interaction
 25 forces between a pair of straight dislocations. Except in the case of a dramatic
 26 change in material properties across the interface, it is found that the interaction
 27 forces can be dealt with by introducing fictional dislocations at the image points.
 28 These image dislocations will have Burgers vectors that are smaller in magnitude
 29 and generally different in orientation from the Burgers vectors of the original dis-
 30 locations.

31 Despite this added complexity, it is still possible to exploit a small discrepancy in
 32 elastic properties across the grain boundary in order to obtain asymptotic expres-
 33 sions for the dislocation density and for the locations of the furthest and nearest
 34 dislocations. In some general pile-up, let x_i represent the nondimensionalised dis-
 35 tance from the point where the plane of dislocations intersects the grain boundary
 36 to the i th dislocation in the pile-up. Then, the equations for a pile-up of dislocations
 37 will be of the form

$$38 \quad \sum_{j=1, j \neq i}^n \frac{1}{x_i - x_j} + \epsilon \sum_{j=1}^n f(x_i, x_j) = 1, \quad i = 1, 2, \dots, n, \quad (22)$$

39 where ϵ is a small parameter representing the change in material properties across
 40 the interface and $f(x_i, x_j)$ is an order one function representing the stress from an
 41 image dislocation at x_j that tends to make the dislocation at x_i glide.

By the intrinsic symmetry of linear elasticity, we note that

$$f(cx_i, cx_j) = c^{-1}f(x_i, x_j). \quad (23)$$

That is, dilating the entire system by a factor of c will reduce all of the interaction stresses by a factor of c^{-1} .

Following [7] and [8], we now consider the asymptotic limit of (22) as $n \rightarrow \infty$. In the outer region away from the boundary layers, we again rescale space by introducing $x = \xi n$. This leads to an integral equation of the form

$$\int_0^{\xi_0^*} \frac{\rho_0(\xi')}{\xi - \xi'} + \epsilon \frac{\rho_0(\xi')}{\xi'} k\left(\frac{\xi}{\xi'}\right) d\xi' = 1, \quad (24)$$

where ξ_0^* is the leading order location of the last dislocation, $\rho_0(\xi)$ is the leading order dislocation density and

$$k\left(\frac{\xi}{\xi'}\right) = \frac{f(\xi, \xi')}{\xi'}.$$

Note that we are only able to construct $k(t)$ in this way because $f(x_i, x_j)$ satisfies (23).

Equation (24) is in the form of the integral equations analysed in [5]. If an appropriate factorisation can be found for

$$K(s) = \int_0^\infty k(u) u^{s-1} du, \quad (25)$$

it is possible to use the Wiener-Hopf method to obtain a closed-form solution for the dislocation density, $\rho_0(\xi)$. Even if a Wiener-Hopf factorisation is unworkable, progress might be made by expressing $\rho_0(\xi)$ and ξ_0^* as asymptotic series in powers of ϵ and seeking a regular perturbation solution to (24).

The next correction in n to the position of the final dislocation can be obtained by proposing a rescaling $\xi = \xi_0^* + n^{-\frac{2}{3}} \tau$ and following the procedure given in [9] for the boundary layer near the turning point.

In order to find the positions of dislocations in the boundary layer near the grain boundary, it is necessary to determine the appropriate scaling in this region, which (unlike the outer scalings) is sensitive to the form of the interaction with the image dislocations. Following [7], it is possible to proceed using a general inner scaling of the form $x = n^{-\frac{a}{1-a}} \eta$ where $0 < a < 1$, leaving a to be determined as a function of λ . More simply, the analogy with [5] indicates that a will be the largest real root of $K(s)$ in $(0, 1)$, where $K(s)$ is defined in (25). Even for complicated functions $K(s)$, an approximation to $a(\lambda)$ can be obtained by performing a regular perturbation expansion in powers of λ for the root of $K(s)$ near $s = \frac{1}{2}$.

Once the rescaling has been found, the procedure in the boundary layer near the grain boundary will be identical to that described in Sections 2.2 and 3 above. As before, we will find that the location of the first dislocation in a pile-up against a grain boundary will scale like $\lambda n^{-\frac{a}{1-a}}$ as $\lambda \rightarrow 0$ and $n \rightarrow \infty$, while the location of the first dislocation in a pile-up against a lock and a grain boundary will scale like $n^{-\frac{a}{1-a}}$.

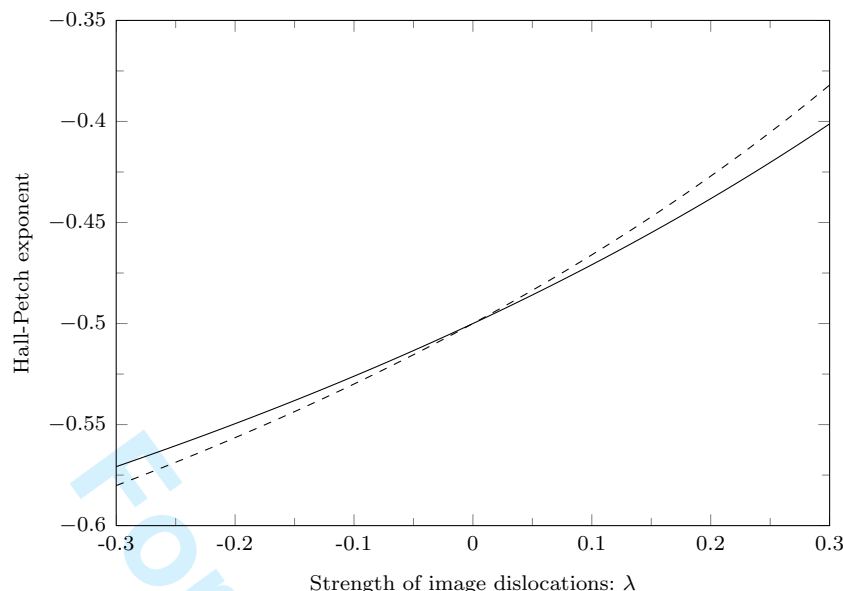


Figure 3. ‘Hall-Petch’ exponents obtained from the Armstrong-Head formula (26), shown as a solid line, and the asymptotic formula (27), shown as a dashed line. Over the physical range of λ values considered, the exponent never deviates far from -0.5 .

5. Discussion

5.1. The Hall-Petch criterion

Armstrong and Head [1] hypothesised that brittle fracture of a polycrystalline material would first occur when a dislocation becomes locked near a grain boundary and then a second dislocation is pushed to within a Burger’s vector length of the locked dislocation. Thus, they considered the stress required to give $\frac{\mu b}{2\pi\tau} x_1 = b$ in the problem of a pile-up against a grain boundary and a lock, assuming that the pile-up took place on the scale of a grain so that $x_n = l$, where l is the grain size.

This led to the formula

$$\tau_{\text{crit}} = \frac{\mu}{\pi} \left(\frac{1.9}{2} (1 + 0.9\lambda)^{1-1.1\lambda} \right)^{\frac{1}{2-1.1\lambda}} \left(\frac{l}{b} \right)^{-\frac{1-1.1\lambda}{2-1.1\lambda}}, \quad (26)$$

where τ_{crit} is the critical stress for fracture. The equivalent expression based on equations (6) and (20) is

$$\tau_{\text{crit}}^{(0)} = \frac{\mu}{\pi} \left(\frac{\alpha_1^2}{16} \left(1 + \frac{2\lambda}{\pi} \right)^{1-\frac{4}{\pi}\lambda} \right)^{\frac{1}{2-\frac{4}{\pi}\lambda}} \left(\frac{l}{b} \right)^{-\frac{1-\frac{4}{\pi}\lambda}{2-\frac{4}{\pi}\lambda}}. \quad (27)$$

Although (5) is more accurate than (6), it is not possible to obtain a closed-form expression for τ_{crit} based on (5) and (20).

As in [1], (27) predicts that τ_{crit} is proportional to a negative power of l that depends on λ . Figure (3) shows that the exponents based on (26) and (27) never vary far from $-\frac{1}{2}$ and the two approaches yield results that are always very close to each other. For small λ , (27) yields

$$\tau_{\text{crit}} \propto l^{-\left(\frac{1}{2} - \frac{\lambda}{\pi}\right)}. \quad (28)$$

As noted by Armstrong and Head [1], taking $\lambda = 0$ leads to $\tau_{\text{crit}} \propto l^{-\frac{1}{2}}$, which is

1 a special case of the Hall-Petch criterion:

$$2 \quad 3 \quad 4 \quad 5 \quad \tau_{\text{crit}} = \tau_0 + k l^{-\frac{1}{2}}, \quad (29)$$

6 where τ_0 and k are material-specific constants obtained by experiment.

7 However, neither (26) nor (27) can account for the τ_0 term in (29). Moreover, it
8 is unlikely that taking further terms in the asymptotic expansions for x_1 and x_n
9 would yield a τ_0 term. Instead, τ_0 needs to be associated with the Peierls friction
10 stress or similar mechanism.
11

12 5.2. Comparison with other work

13 It is interesting to note that Armstrong and Head [1] are not the only researchers to
14 use curve fitting in order to approximate the locations of the nearest and furthest
15 dislocations in a pile-up. Contemporary with their work, Chou [2] considered the
16 problem of finding the position of the furthest dislocation when $\lambda = 0$ or $\lambda = 1$.
17 In [2], as in [9], singular integral equations were used and the results obtained are
18 equivalent. Based on his work, Chou [2] hypothesised a linear relationship between
19 ξ_n and λ :
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$$24 \quad 25 \quad \xi_n = 2 + (\pi - 2)\lambda, \quad 0 \leq \lambda \leq 1.$$

26 Although this expression fails to incorporate the effects of the boundary layer, we
27 find that it gives results that are very close to the leading order expression in (3)
28 for a range of λ values. Equation (6) is, however, a superior approximation to (3)
29 when λ is small and the correction term in (5) is important unless n is very large.
30

31 Wagoner [10] used numerical techniques to find the equilibrium positions of dislo-
32 cations in pile-ups against interfaces in anisotropic materials. Although no attempt
33 was made to fit formulae for the locations of the furthest and nearest dislocations,
34 the position of the dislocation nearest to the interface was estimated by balancing
35 the forces from the real dislocations in the pile-up with the force from the nearest
36 image dislocation. This is analogous to the method described in Section 2.2, but
37 [10] found a surprisingly poor agreement between estimated position and calculated
38 position. The main reason for this is that [10] did not have the correct scaling for
39 the dependence of x_1 on n . Thus, insights from asymptotic analysis can be used to
40 obtain results that are not immediately intuitive.
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44 6. Conclusions

45 We have used the asymptotic methods of Voskoboynikov *et al.* [8] to obtain ex-
46 pressions for the locations of the first and last dislocations in a pile-up against a
47 grain boundary and these expressions have been compared with numerical results.
48 Our asymptotic expressions have the same form as the formulae obtained by Arm-
49 strong and Head [1] using curve fitting, but some of the parameters are different.
50 As expected, the asymptotic expressions are better than the fitted formulae when
51 n is large and λ is small.
52

53 For a pile-up against a grain boundary where the mismatch (and hence λ) is
54 small, we recovered the same system of equations in the inner region as for a
55 pile-up against a locked dislocation. This can be explained by observing that the
56 first dislocation becomes very close to the grain boundary as $\lambda \rightarrow 0$ and the other
57 dislocations begin to feel it as if it were locked at the grain boundary. Thus, pile-ups
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1 against grain boundaries may lead to situations that are physically equivalent to
2 pile-ups against locks. This is true both for the simple pile-ups of screw dislocations
3 analysed in detail and for more complicated configurations.
4

5 6 **Acknowledgements**

7
8 This publication is based on work supported by Award No. KUK-C1-013-04, made
9 by King Abdullah University of Science and Technology (KAUST).

10 I would like to acknowledge the contributions of John R. Ockendon (Ox-
11 ford), S. Jonathan Chapman (Oxford), Roman E. Voskoboynikov (Kurchatov) and
12 Graeme C. Wake (Massey), with whom I discussed various aspects of this work.
13
14

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