Surface versus bulk nucleation of dislocations during contact

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December 5, 2006

Abstract

The indentation of single crystals by a periodic array of flat rigid contacts is analyzed using discrete dislocation plasticity. Plane strain analyses are carried out with the dislocations all of edge character and modeled as line singularities in a linear elastic solid. The limiting cases of frictionless and perfectly sticking contacts are considered. The effects of contact size, dislocation source density, and dislocation obstacle density and strength on the evolution of the mean indentation pressure are explored, but the main focus is on contrasting the response of crystals having dislocation sources on the surface with that of crystals having dislocation sources in the bulk. When there are only bulk sources, the mean contact pressure for sufficiently large contacts is independent of the friction condition, whereas for sufficiently small contact sizes, there is a significant dependence on the friction condition. When there are only surface dislocation sources the mean contact pressure increases much more rapidly with indentation depth than when bulk sources are present and the mean contact pressure is very sensitive to the strength of the obstacles to dislocation glide. Also, on unloading a layer of tensile residual stress develops when surface dislocation sources dominate.

Keywords: Discrete dislocation plasticity; indentation; residual stress; size effect
1 Introduction

The near-surface plastic deformation induced by contact between two rough surfaces plays a central role in controlling friction, wear and contact fatigue. Considerable effort has therefore been devoted to developing models that predict the influence of surface topography, loading conditions, and the properties of the two contacting materials on the extent and severity of this plastic deformation. Classical models are based on the continuum theory of plasticity, which provides an appropriate description of contacts for crystalline solids (which are the focus of this paper) for sufficiently large asperities, say asperity sizes of the order of tens of microns and larger for typical crystalline metals and ceramics. Asperity contacts between rough surfaces of crystalline solids are often substantially smaller than this, and typically range from a few nanometers to several microns. As a result, there is increasing experimental and theoretical evidence to suggest that classical theories do not accurately model rough surface contact. For example, nanoindentation tests show a strong size dependence of hardness that is not predicted by classical theory, e.g. (Ma and Clarke, 1995; Swadener et al., 2002; Wang et al., 2006b); in addition, recent measurements of residual stresses induced by contact between rough surfaces show the development of a tensile layer near the surface that cannot be accounted for by continuum models (Wang et al., 2006a). These discrepancies are primarily a consequence of the discrete nature of plastic flow, which can be neglected for large contacts, but which plays a dominant role in determining the behavior of typical asperity contacts.

Recent advances in developing and implementing discrete dislocation models of plasticity have provided an opportunity to investigate these issues. A variety of discrete dislocation analyses of indentation have been carried out (Polonsky and Keer, 1996; Fivel et al., 1998; Kreuzer and Pippan, 2004; Widjaja et al., 2005), with much attention given to modeling the size dependence of indentation hardness. In particular, Balint et al. (2006a) have performed a detailed investigation of the influence of contact size, the density of bulk dislocation sources, and the density of obstacles blocking dislocation glide on the behavior of a two-dimensional wedge indenter. They found that the indentation pressure approaches the continuum plasticity solution for sufficiently large contact sizes and transitions towards the elastic solution for small contact sizes. Only bulk dislocation sources were modeled in these cited studies. There is both experimental (Kiely et al., 1998; Gouldstone et al., 2001; De la Fuente et al., 2002) and theoretical evidence (Zimmerman et al., 2001; Li et al., 2002; Yu et al., 2006) that dislocations may nucleate from surface sources under contact loading when the surface has atomic-scale (or larger) roughness. This may play a significant role in governing material behavior near the surface; for example, models of isolated steps show that dislocations nucleated at the surface can remain trapped near the surface, and can generate substantial tensile residual stress (Gao et al., 2006b; Yu et al., 2006), which can lead to crack nucleation and delamination wear.

In general, dislocation nucleation is expected to be possible from both surface and bulk dislocation sources. Here, we investigate the relative roles played by these two sets of dislocation sources on the evolution of plastic flow and the development of residual stresses in contact loading. A second important difference with the study of Balint et al. (2006a) is that we study not an isolated indenter but a periodic array of indenters, taken to be
flat and rigid for simplicity. The collective effect of an array of contacts, thus considered, has important consequences. Although the contacts are taken to be widely spaced (nine times the contact size) in all the results reported here, for representative contact sizes and dislocation densities, the depth of the plastic zone is found to be comparable to the asperity spacing, and much greater than the contact size. This behavior is in sharp contrast to the predictions of continuum plasticity theory, in which the deformation is localized around each contact. Generally, but not in all circumstances analyzed, the smaller contacts are harder. The details vary significantly with the friction between the contacting surfaces, the densities and strengths of dislocation sources and obstacles, the contact size, as well as with the relative number and spacing of surface and bulk dislocation sources.

2 Formulation

![Figure 1: Two-dimensional model of single crystal indented by a rough surface with protrusions having contact width $a$ and center-to-center contact spacing $w$. Calculations are carried out for a unit cell of width $w$.](image)

The problem to be solved is illustrated in Fig. 1. A small strain formulation is used and the material is idealized as a semi-infinite single crystal strip, which occupies the region $0 < x_2 < h$, $-\infty < x_1 < \infty$ and is constrained to deform in plane strain normal to the $x_1-x_2$ plane. The crystal is elastically isotropic, with Young’s modulus $E$ and Poisson’s ratio $\nu$. Plastic flow occurs in the crystal as a result of the nucleation and motion of edge dislocations that glide along three slip systems as indicated in Fig. 1. The Burgers vector for the dislocations has magnitude $b$, and direction parallel to the slip plane. The line direction for the dislocations is perpendicular to the plane of deformation.

The strip is indented on $x_2 = h$ by a periodic array of flat contacts, with contact width $a$ and center-to-center contact spacing $w$. The distribution of dislocation sources and obstacles is taken to be periodic in the $x_1$ direction with period $w$ and the calculations
are carried out for a unit cell that lies between $-w/2 < x_1 < w/2$. Two limiting cases of friction are considered: (i) perfect sticking between the contacts and the crystal; and (ii) frictionless contact between the contacts and the crystal.

The numerical procedure for solving the governing field equations and constitutive equations is described in detail in Nicola et al. (2003, 2006a). The indentation displacement, $u$ in Fig. 1, is applied incrementally. At each time step, the stress and deformation state is determined using superposition of a singular field and an image field, (Van der Giessen and Needleman, 1995). The singular field is associated with the discrete dislocations and is calculated analytically. The image field is obtained from a finite element solution of a non-singular linear elasticity boundary value problem. Once the stresses have been determined the change in position of each dislocation is calculated and dislocations are nucleated into, or removed from, the unit cell according to the constitutive equations outlined in Section 2.1. The procedure is repeated to calculate the stress and dislocation distributions in the crystal as a function of time.

2.1 Constitutive relations for dislocation plasticity

The calculations are carried out using plane strain two-dimensional discrete dislocation plasticity with the evolution of the dislocation structure in the crystal specified by a set of constitutive equations derived from Kubin et al. (1992). These rules control the nucleation, glide, annihilation of dislocations as well as their pinning at obstacles. Although there are aspects of dislocation plasticity that cannot be modeled within the two-dimensional framework used here, such as cross-slip and the dynamic evolution of dislocation sources and obstacles, there is a wide range of complex phenomena involving plastic deformation in small volumes that can be represented qualitatively, e.g. (Nicola et al., 2003; Deshpande et al., 2003, 2005; Balint et al., 2006b), and, to a remarkable extent even quantitatively, e.g. (Nicola et al., 2006a; Chng et al., 2006). In such circumstances, the dislocation–dislocation interactions that are so important for work hardening do not play a major role and long-range elastic dislocation interactions dominate.

In the present calculations, dislocations may nucleate from sources inside the crystal, and/or from sources that lie on the free surface at $x_2 = h$. The constitutive relation for bulk dislocation nucleation is taken to model generation from pre-existing bulk Frank-Read sources. Inside the crystal, dislocation dipoles are nucleated when the Peach-Koehler force at source $n$, $f^n$, exceeds $\tau^n_{\text{bulk}}b$ for the time $t_{\text{nuc}}$ which is needed for the loop to reach its minimum stable size.

Dislocation nucleation from free surfaces, in particular from the stress concentration associated with surface steps provides another possibility for dislocation nucleation (Yu et al., 2006). At present no surface nucleation criterion for use in a discrete dislocation plasticity analysis has been developed. In fact, there is no basis for presuming that a critical Peach-Koehler force is an appropriate criterion for dislocation nucleation at a surface (see Liu et al. (2006)). In the absence of a more appropriate surface nucleation criterion, we use a similar criterion as for bulk sources but with possibly different source strengths $\tau^n_{\text{surf}}$. At a surface source, a single dislocation is nucleated, which travels into
the crystal. The Burgers vector is accommodated by a step at the surface, which is accounted for by means of an appropriate image dislocation above the surface. Thus, the results to be presented here illustrate effects of source location but not any effects that would arise from a stress state needed to activate surface sources that differs from the stress state needed to activate bulk sources. Furthermore, unlike a bulk Frank-Read source that recovers its original state after each dislocation nucleation, the strength of a surface-step dislocation source depends on the number of dislocations it has generated. This step-height dependence is not accounted for in our calculations.

Dislocation sources are randomly distributed through the bulk of the crystal with density $\rho_{\text{bulk}}$ (per unit area) and on the surface with density $\rho_{\text{surf}}$ (per unit length). The strengths of the sources are selected randomly from a Gaussian distribution.

After nucleation, the glide velocity $v^I$ of the $I$th dislocation is proportional to the Peach-Koehler force $f^I$ according to

$$f^I = B v^I$$  \hspace{1cm} (1)

with $B$ the drag coefficient.

Obstacles to dislocation motion are modeled as points on the slip planes which pin dislocations that attempt to pass through them. An obstacle releases a pinned dislocation when the Peach-Koehler force on the dislocation exceeds $\tau_{\text{obs}}b$, where $\tau_{\text{obs}}$ is the obstacle strength. The obstacles are randomly distributed within the crystal with density $\rho_{\text{obs}}$ (per unit area) and all obstacles have the same strength.

Two nearby dislocations with opposite Burgers vector are taken to annihilate when they are within a distance $L_{\text{ann}}$.

### 2.2 Boundary conditions

For the array of flat rigid contacts the contact length is fixed at $a$ and the loading is imposed by prescribing the normal displacement under the contacts

$$u_2(x_1, h) = -\int \hat{u} \, dt, \quad -\frac{a}{2} \leq x_1 \leq \frac{a}{2}. \hspace{1cm} (2)$$

For a perfectly sticking contact, the lateral displacement on the contact surface satisfies

$$u_1(x_1, h) = 0, \quad -\frac{a}{2} \leq x_1 \leq \frac{a}{2}, \hspace{1cm} (3)$$

while for a frictionless contact

$$\sigma_{12}(x_1, h) = 0, \quad -\frac{a}{2} \leq x_1 \leq \frac{a}{2}. \hspace{1cm} (4)$$

Outside the contact region, the top surface ($x_2 = h$) is traction free, which requires

$$\sigma_{12}(x_1, h) = \sigma_{22}(x_1, h) = 0, \quad \frac{a}{2} < |x_1| < \frac{w}{2}. \hspace{1cm} (5)$$
The boundary conditions along the bottom of the unit cell, $x_2 = 0$, are taken to be

$$u_2(x_1, 0) = 0 \quad \sigma_{12}(x_1, 0) = 0$$

(6)

Periodic boundary conditions are imposed on the sides of the simulation cell by requiring

$$u_1\left(\frac{w}{2}, x_2\right) = u_1\left(-\frac{w}{2}, x_2\right) + V$$

(7)

$$u_2\left(-\frac{w}{2}, x_2\right) = u_2\left(\frac{w}{2}, x_2\right).$$

(8)

In addition, we impose

$$u_1\left(-\frac{w}{2}, 0\right) = 0$$

(9)

which, for frictionless contacts, prevents rigid body translation parallel to the $x_1$–axis.

The value of $V$ depends on the friction between the contacting surfaces. For perfectly sticking contacts, the unit cell cannot expand or contract because the indenter is rigid so that $V = 0$. On the other hand, for frictionless contacts, the unit cell may expand horizontally. We assume that there is no remotely imposed loading parallel to the surface, so the resultant horizontal forces acting on any vertical plane $x_1 = \text{constant}$ vanish. The value of $V$ is determined from the condition

$$\frac{1}{h} \int_0^h \sigma_{11}(x_1, x_2) dx_2 = 0.$$  

(10)

### 3 Numerical results

The height of the unit cell is fixed at $h = 50\mu m$ and the contact fraction $a/w$ is fixed at $1/9$. The contact size $a$ is varied between $0.25\mu m$ and $2.0\mu m$ so that $w$, the spacing between contacts (see Fig. 1), varies between $2.25\mu m$ and $18\mu m$. Because both the absolute size of the contacts as well as the ratio $a/w$ affects the response, both $a$ and $w$ are specified; for example, a case with $a = 0.5\mu m$ and $w = 4.5\mu m$ is denoted by $a/w = 0.5\mu m/4.5\mu m$.

Young’s modulus and Poisson’s ratio are taken as $E = 70\text{GPa}$ and $\nu = 0.33$, respectively, values which are representative of aluminum. The Burgers vector is fixed at $b = 0.25 \text{nm}$. There are three potentially active slip systems in the crystal, with orientations $\phi = 0^\circ$, $60^\circ$ and $120^\circ$ as shown in in Fig. 1, and with planes spaced at $200b$. Dislocations may nucleate in the bulk of the crystal, at the surface, or both. When present, the bulk sources are randomly distributed on all three slip systems with total density $\rho_{\text{bulk}} = 30/\mu m^2$, unless otherwise stated. When surface sources are present, they are distributed with density $\rho_{\text{surf}} = 33/\mu m$ on slip planes with $\phi = 60^\circ$ and $120^\circ$. Hence, when there are no bulk sources, there can be no dislocation slip on planes with $\phi = 0^\circ$.

The strengths of both bulk and surface sources are assigned at random from a Gaussian distribution with mean strength 50MPa and a standard deviation of 10MPa. All sources have a nucleation time of $t_{\text{nuc}} = 10\text{ns}$. The drag coefficient for dislocation glide is taken to
be $B = 10^{-4}\text{Pa} \cdot \text{s}$. Obstacles are placed on slip planes where at least one dislocation source is present, with density $\rho_{\text{obs}} = 30/\mu\text{m}^2$ and obstacle strength $\tau_{\text{obs}} = 150\text{MPa}$. The critical distance for annihilation of dislocations with opposite signed Burgers vector is $L_{\text{ann}} = 6b$.

At time $t = 0$ the crystal is stress and dislocation free. Indentation takes place at the constant rate $\dot{u} = 4 \times 10^{-4}\mu\text{m}/\text{s}$ (see Fig. 1). Results are presented for the evolution of the mean contact pressure, $P_m$, defined by

$$P_m = -\frac{1}{a} \int_{-a/2}^{a/2} \sigma_{22}(x_1, h) dx_1,$$

and for the dislocation structures and stress states that emerge as a function of indentation depth $u$. As with all plane contact problems, the elastic compliance of the contact is sensitive to the remote boundary conditions, and would increase in proportion to $\log(h/a)$ as $h/a \to \infty$. However, the values of the mean contact pressure $P_m$ required to initiate plastic deformation or plastic collapse in continuum plasticity (when it occurs) are not sensitive to the cell height, although the corresponding indentation depth values are.

To determine the bulk yield strength with the specified properties, a plane strain frictionless indentation was performed with $a = w = 9\mu\text{m}$. The crystal exhibits approximately elastic-perfectly plastic behavior, with a plateau flow strength of $49 \pm 2\text{MPa}$. The response is approximately equivalent to that of a crystal characterized by nonhardening continuum slip plasticity theory with a slip system strength of $\approx 20\text{MPa}$.

### 3.1 Effect of contact size and friction without surface sources

![Figure 2](image_url)

**Figure 2**: Mean contact pressure, $P_m$, versus indentation depth, $u$, for crystals with bulk dislocation sources and contact size ranging from $a = 0.25\mu\text{m}$ to $a = 2\mu\text{m}$. (a) Frictionless contacts. (b) Perfectly sticking contacts.

Fig. 2 shows the variation of mean contact pressure $P_m$ with indenter displacement $u$ for a crystal containing only bulk sources, for contact sizes ranging from 0.25μm to
2\mu m (with scaling of the contact spacing \( w \) to maintain a contact fraction of 1/9). Under frictionless conditions, Fig. 2a, smaller contacts are harder than larger ones in the early stages of indentation, but at larger values of \( u \), nearly the same plateau value of \( P_m \) (\( \approx 430\text{MPa} \)) is reached for all contact sizes in Fig. 2a. On the other hand, for perfectly sticking contacts, Fig. 2b, smaller contacts are harder for the entire range of indentation depths analyzed. Also, the elastic stiffness is greater for perfectly sticking contacts than for frictionless contacts due to the constraint on Poisson contraction.

The plateau value of the mean contact pressure in Fig. 2a is consistent with the plane strain flow strength of the crystal (i.e. indentation with \( a/w = 1 \)) which was found to be 49MPa. Hence, with a contact fraction of \( a/w = 1\mu m/9\mu m \), from equilibrium, the plane strain deformation mode is consistent with a mean contact pressure of \( 9 \times 49 = 447\text{MPa} \), which agrees quite well with the plateau value of \( \approx 430\text{MPa} \).

For sufficiently small contact sizes, \( a \leq 0.5\mu m \) in Fig. 2, in the plastic range, the mean contact pressure for a perfectly sticking contact is significantly greater than that for the corresponding frictionless contact. However, for \( a/w = 2\mu m/18\mu m \) over the range of indentation displacements calculated, the \( P_m \) versus \( u \) response is independent of the friction condition to within the statistical scatter of the discrete dislocation simulations. This insensitivity to the friction condition is consistent with calculations carried out (but not shown here) using conventional continuum crystal plasticity.

![Figure 3](image-url): The distribution of \( \sigma_{22} \) stress and the dislocation structure near a frictionless indenter at \( u = 0.1\mu m \) in crystals with only bulk sources with contact size (a) \( a/w = 0.25\mu m/2.25\mu m \) and (b) \( a/w = 2\mu m/18\mu m \).

The dislocation and stress distributions at \( u = 0.1\mu m \) are shown for frictionless contacts with sizes of 0.25\mu m and 2\mu m in Fig. 3. One contribution to the size dependence of the mean contact pressure is the limited availability of dislocation sources for small contacts in the highly stressed region. For example, an area \( 3a \times 3a \) contains approximately \( 10^3 \) dislocations for a 2\mu m contact, Fig. 3b, and only 17 dislocations for a 0.25\mu m contact, Fig. 3a. The region over which plastic deformation occurs is much larger in discrete dislo-
cation plasticity than in conventional continuum plasticity where plastic flow is confined to a relatively small region just under the contact. As deformation proceeds, the dislocations emanating from sources near neighboring contacts interact and this contributes to the increased mean contact pressure.

A more detailed study of the role of contact size and contact fraction $a/w$ will be reported in Nicola et al. (2006b). In the remainder of this paper, unless stated otherwise, the contact size is $a = 1\mu m$ and $w = 9\mu m$. For this contact size: (i) the discrete nature of plastic slip plays a dominant role in governing the behavior of the contacts, leading to contact pressures that can exceed the predictions of continuum plasticity theory by a factor of $3 - 8$; and (ii) that are strongly dependent on whether the contact is frictionless or perfectly sticking.

### 3.2 Surface nucleation versus bulk nucleation

![Graph A](image1)

**Figure 4:** Mean contact pressure, $P_m$, versus indentation depth, $u$, for crystals containing surface and/or bulk dislocation sources for $a/w = 1\mu m/9\mu m$. (a) Frictionless contacts. (b) Perfectly sticking contacts.

Fig. 4 shows curves of mean contact pressure versus indentation displacement for $a/w = 1\mu m/9\mu m$ with only bulk sources; only surface sources, or a combination of the two. Results are shown for both frictionless and perfectly sticking contacts. For frictionless contacts, a crystal containing both surface and bulk sources has a slightly lower plateau stress (which occurs at the onset of bulk plane strain compression of the entire crystal) than one with only bulk sources, but otherwise the contact pressures for the two cases are close. Even though the bulk compression mode is not activated when the contacts are perfectly sticking, the addition of surface sources reduces the hardness proportionally by a comparable amount. This is a consequence of high local shear stresses that develop near the edges of a sticking contact that can activate surface sources.

When the crystal contains only surface dislocation sources, there is no plateau in
the mean contact pressure. The value of $P_m$ continues to rise (modulo oscillations associated with discrete dislocation events) with increasing indentation depth $u$ (results in Section 3.5 show that obstacles to dislocation motion play an important role in this regard). Bulk plane strain compression only occurs if bulk sources are present in the crystal. For perfectly sticking contacts, Fig. 4b, both the value of mean contact pressure at which significant plastic deformation occurs and the rate of increase of $P_m$ with indentation depth $u$ are greater than for frictionless contacts, Fig. 4a. A kink occurs in the contact pressure-displacement curves at an indentation depth of approximately $0.1 \mu m$ for both frictionless and sticking contacts, but is more pronounced for frictionless contacts.

Figure 5: The distribution of $\sigma_{22}$ stress and the dislocation structure at an indentation depth $u = 0.14 \mu m$ for frictionless contacts. (a) Surface sources only. (b) Surface and bulk sources. (c) Bulk sources only.

Some insight into the mechanisms responsible for this kink can be obtained by examining the dislocation and stress distributions underneath the contacts; for frictionless contact these are shown in Fig. 5 at an indentation depth of $u = 0.14 \mu m$. The full width of the unit cell, $-w/2 \leq x_1 \leq w/2$, is shown but only the top part $20 \mu m \leq x_2 \leq 50 \mu m$. When bulk sources are present, there is dislocation activity throughout the material, Figs. 5b,c. In contrast, when only surface sources are present, Fig. 5a, dislocation activity is almost entirely confined to bands emanating from under the indenters. In addition, the stress levels in crystals that contain only surface sources are substantially higher than when bulk sources are present, compare Figs. 5a and 5b,c.

A magnified view of the dislocation distribution in the region close to the indenter is shown in Fig. 6. When only surface sources are present, dislocations nucleate mainly on four slip planes that intersect the surface near the contact edges. Dislocation motion on these slip planes gives rise to two regions that are subject to high compressive stress.
Figure 6: The distribution of $\sigma_{22}$ stress and the dislocation structure near a contact at an indentation depth $u = 0.14\mu m$ for frictionless contacts with $a/w = 1\mu m/9\mu m$. Close-up of Fig. 5. (a) Surface sources only. (b) Surface and bulk sources. (c) Bulk sources only.

The two slip planes that bound each region accumulate dislocations with opposite sign: these dislocation dipoles accommodate material that has been forced into the band-like regions by the indenter, inducing the high compressive stress. The dipolar bands (the two-dimensional equivalent of a train of dislocation loops in three-dimensional indentation) increase in length as the indentation depth is increased. At a critical indentation depth (which depends on the absolute contact size, the contact fraction $a/w$, and the source and obstacle densities and strengths) the bands emitted by neighboring contacts intersect and one of the two bands shown in Fig. 6a is blocked. This intersection coincides with the kink in the mean contact pressure-indentation depth curve of Fig. 4. The increased slope of the $P_m$ versus $u$ curve is therefore a consequence of the interaction between such bands emanating from neighboring contacts. Qualitatively similar interactions occur in the presence of bulk sources, but the effect is more pronounced with only surface sources, as deformation is confined to well-defined narrow dipolar bands that are easier to block.

The dislocation and stress distributions for perfectly sticking contacts are shown in Fig. 7. When there are only surface sources, the stress level throughout the bulk is much higher than for a frictionless contact (compare Fig. 5a with Fig. 7a). Also, the length of the dipolar bands emanating from near the contact corners is smaller than for the corresponding frictionless case. With bulk dislocation sources present, dislocations are confined to a layer of about $10\mu m$ below the surface, whereas at the same indentation depth they penetrate deep into the crystal for frictionless contact (compare Fig. 5b,c with Fig. 7b,c).
Figure 7: The distribution of $\sigma_{22}$ and the dislocation structure at an indentation depth $u = 0.14\mu m$ under a perfectly sticking contact with $a/w = 1\mu m/9\mu m$. (a) Surface dislocation sources. (b) Surface and bulk dislocation sources. (c) Bulk dislocation sources.

### 3.3 Effect of surface and bulk source densities

The effect of variations in the densities of surface and bulk dislocation sources on the response to frictionless indentation is presented in Fig. 8. The surface source density in Fig. 8a ranges from $\rho_{\text{surf}} = 8/\mu m$ to $\rho_{\text{surf}} = 132/\mu m$. A surface source density of $\rho_{\text{surf}} = 8/\mu m$ corresponds to a mean source spacing of 0.125$\mu m$ while $\rho_{\text{surf}} = 132/\mu m$ corresponds to a mean spacing of 0.00758$\mu m$ (for the cases with $\rho_{\text{surf}} = 66/\mu m$ and $\rho_{\text{surf}} = 132/\mu m$ the potentially active slip plane spacings are 100b and 50b, respectively). Fig. 8b shows results for crystals with bulk source densities ranging from $\rho_{\text{bulk}} = 15/\mu m^2$ to $\rho_{\text{bulk}} = 60/\mu m^2$, which correspond to mean source spacings of 0.258$\mu m$ and 0.129$\mu m$, respectively. Once plastic deformation occurs, the mean contact pressure for the crystal with $\rho_{\text{surf}} = 8/\mu m$ in Fig. 8a is significantly greater than for the crystal with $\rho_{\text{bulk}} = 60/\mu m^2$ in Fig. 8b, even though the spacings and strengths of sources and obstacles are the same. It is worth noting here that increasing the mean surface source strength, increases the value of $P_m$ at a given value of $u$. Hence, if the nucleation strength of surface sources is actually greater than the nucleation strength of the bulk sources, the increased strength associated with surface nucleation will be even greater than in Fig. 8.

Increasing the surface source density from $8/\mu m$ to $17/\mu m$ to $33/\mu m$ significantly decreases the slope of the mean contact pressure versus indentation depth curve. The effect is particularly strong for indentation depths $u > 0.1\mu m$, where the bands from neighboring contacts interact. In contrast, increasing the source density from $33/\mu m$ to $132/\mu m$ has no appreciable effect on the contact pressure.

With only bulk dislocation sources, Fig. 8b, a factor of four difference in nucleation source density has little effect on the mean contact pressure. For comparison purposes, the
Figure 8: Mean contact pressure, $P_m$, versus indentation depth, $u$, for frictionless indentation of crystals having various source densities. (a) Surface dislocation sources. (b) Bulk dislocation sources.

Figure 9: Mean contact pressure, $P_m$, versus indentation depth, $u$, for crystals with $a/w = 1\mu m/9\mu m$, $\rho_{\text{surf}} = 33/\mu m$ and various densities of bulk sources. (a) Frictionless contacts. (b) Perfectly sticking contacts.

mean contact pressure versus indentation depth curve obtained from conventional continuum crystal plasticity theory with a slip system flow strength of 20 MPa is shown. This is the slip system strength that gives rise to essentially the same plane strain compression response as obtained from discrete dislocation plasticity with $w = 9\mu m$. If continuum crystal plasticity is regarded as corresponding to the limit of infinite source density, then Fig. 8b shows that even with $\rho_{\text{bulk}} = 60/\mu m^2$ the discreteness of dislocation sources has a
large effect on the mean contact pressure. The effect of source density for perfectly sticking contacts is qualitatively similar to that for frictionless contacts and is not reported here.

The influence of the bulk source density, with a fixed density of surface sources $\rho_{\text{surf}} = 33/\mu m$, on the $P_m$ versus $u$ response is shown in Fig. 9. For frictionless contacts, Fig. 9a, with a low density of bulk sources $\rho_{\text{bulk}} = 10/\mu m^2$, the mean contact pressure at small indentation depths ($u < 0.05\mu m$) is essentially the same as for the case where only surface sources are present ($\rho_{\text{bulk}} = 0$). At increased indentation depths, however, the presence of this low bulk source density is sufficient to enable plastic deformation throughout the crystal and the value of $P_m$ reaches a plateau. For perfectly sticking contacts, Fig. 9b, the slope of the mean contact pressure versus indentation depth curve decreases with increasing $\rho_{\text{bulk}}$, and the kink in the curve disappears when bulk sources are present.

### 3.4 Effect of contact size for crystals with surface sources

Results for the dependence of the response of crystals without surface sources on contact size are presented in Section 3.1. Fig. 10 shows the mean contact pressure versus indentation depth curves for crystals that contain only surface sources, with the reference density of $\rho_{\text{surf}} = 33/\mu m$. Both for frictionless and perfectly sticking contacts, decreasing

![Figure 10](image-url)

Figure 10: Mean contact pressure, $P_m$, versus indentation depth, $u$, for crystals having surface sources only with contact size ranging from $a = 0.25\mu m$ to $a = 2\mu m$ and corresponding $w$ to keep $a/w$ at a constant value. (a) Frictionless contacts. (b) Perfectly sticking contacts.

the contact size has two main effects: (i) the kinks in the contact pressure curves shift to smaller indentation depths; and (ii) the slope of the $P_m$ versus $u$ curve generally tends to increase, both before and after the kink.

The dislocation and stress distributions in Fig. 11 provide some insight into the origins of this behavior. When only surface dislocation sources are present, plastic deformation
takes place primarily in the form of two dipolar bands emanating from the edges of the contact. The length of these bands is controlled mainly by the indentation depth and by the obstacle density, and is not strongly influenced by the contact size or the density of dislocation sources. The kink in the contact pressure versus indentation depth curves occurs when the dipolar bands emitted by neighboring contacts intersect. Since the bands have a fixed length for a given indentation depth and obstacle density, this occurs earlier when contacts are more closely spaced. Inspection of Fig. 11 reveals that the width of the dipolar bands does not scale with contact size for the smaller contacts because of insufficient dislocation sources near the edges of a small contact. Wider bands correspond to an increase of the mean contact pressure.

![Diagram](a)  ![Diagram](b)

Figure 11: The distribution of $\sigma_{22}$ stress and the dislocation structure for frictionless contacts at $u = 0.06\mu m$ in crystals with only surface sources with contact sizes (a) $a/w = 0.25\mu m/2.25\mu m$ and (b) $a/w = 2\mu m/18\mu m$.

The effect of the relative densities of surface and bulk dislocation sources on the evolution of the mean contact pressure for a contact size $a/w = 0.25\mu m/2.25\mu m$ is shown in Fig. 12. Comparison of Figs. 12a and 9a shows the effect of contact size for various dislocation source densities. With $\rho_{\text{bulk}} > 0$ and for shallow indentation depths, $u < 0.05\mu m$, the $1\mu m/9\mu m$ contacts (Fig. 9a) show some plasticity and the $P_m$ versus $u$ response is not strongly sensitive to either the surface or bulk source densities, while the $0.25\mu m/2.25\mu m$ contacts remain elastic almost until $u = 0.05\mu m$. For indentation depths exceeding $0.05\mu m$, the mean contact pressure for the frictionless contacts with $\rho_{\text{bulk}} > 0$ reaches a plateau.

For perfectly sticking contacts, (compare Fig. 12b with Fig. 9b), there is a strong influence of contact size irrespective of whether there are surface sources, bulk sources, or both. The slope of $P_m$ versus $u$ increases with decreasing contact size. The size of the region where dislocation glide occurs under a large contact ($2\mu m$ or larger) scales with the contact size. In contrast, the size of this region under a small contact ($1\mu m$ or smaller) is substantially larger in proportion to the contact size. As a consequence, the
interaction between the plastically deforming regions of neighboring contacts occurs at smaller indentation depths for small contact sizes and this interaction acts to increase the slope of the $P_m(u)$ curve.

Figure 13: Mean contact pressure response to frictionless $a/w = 0.25\mu m \text{/} 2.25\mu m$ indentation in crystals with various source distributions for given densities (a) $\rho_{\text{bulk}} = 0$ and $\rho_{\text{surf}}$ as indicated; (b) $\rho_{\text{bulk}} = 10/\mu m^2$ and $\rho_{\text{surf}} = 33/\mu m$. Here, #i ($i = 1, 2, 3$) denotes the $i$th realization.

The location and strength of dislocation sources and obstacles are specified statistically; we refer to a given distribution of sources and obstacles as a “realization.” To ex-
plore the statistical scatter, Fig. 13 compares the mean contact pressure versus indentation depth response for several realizations for frictionless contacts with $a/w = 0.25\mu m/2.25\mu m$ and $\rho_{surf} = 33/\mu m$. While the overall response varies little among the various realizations, the yield point does depend on the exact location and strength of the sources and obstacles, particularly those in the high stressed region near the contact. The statistical variation tends to be greatest at small contact sizes where fewer sources and obstacles are involved. The statistical scatter is smaller than the systematic trends both with (Fig. 13a) and without (Fig. 13b) bulk sources.

### 3.5 Effect of obstacles to dislocation motion

![Image](image.png)

**Figure 14:** The effect of obstacle strength on the mean contact pressure, $P_m$, versus indentation depth, $u$, for crystals with frictionless contacts of $a/w = 1\mu m/9\mu m$. (a) Surface dislocation sources, $\rho_{surf} = 33/\mu m$. (b) Bulk dislocation sources, $\rho_{bulk} = 30/\mu m^2$.

In addition to dislocation source density, the strength and density of pinning obstacles have a significant influence on the response of the crystal. This is illustrated in Fig. 14, which shows contact pressure versus indentation depth curves for crystals with only bulk sources, and also for one with only surface sources. Results are shown only for frictionless contacts, since the behavior of sticking contacts is qualitatively similar. The obstacle strength has a particularly pronounced effect for a crystal containing only surface sources (Fig. 14a). For a high obstacle strength ($\tau_{obs} = 1500\, MPa$) the shear bands that form at the contact edges are blocked and the mean contact pressure increases rapidly with increasing indentation depth. In addition, no kink in the $P_m$ versus $u$ curve occurs, as the shear bands are never long enough to interact. In contrast, for a zero obstacle strength (or density), a single dominant shear band propagates through the unit cell at a contact pressure of approximately 230MPa. In such a case dislocations reach the bottom ($x_2 = 0$) of the unit cell, but over the range of indentation depths in Fig. 14 there is no evident effect
of dislocations being blocked at \( x_2 = 0 \) on the mean contact pressure. Also, with zero obstacle strength (or density) no interaction occurs between dislocation arrays emitted by neighboring contacts.

### 3.6 Residual stress

Residual stresses left inside the material after removal of contact may be crucial for reliability. Tensile stress parallel to the surface may favor crack nucleation and growth orthogonal to the indented surface, while compressive stress generally is favorable to suppress fatigue. To examine the effect of dislocation source distribution and contact size on the residual stress state, we have conducted a series of simulations in which crystals were first indented to \( u = 0.1 \mu m \) and were then unloaded by removing the applied displacement. A constant displacement rate (\( |\dot{u}| = 4 \times 10^4 \mu m/s \)) was used in Eq. (2) for both loading and unloading. This part of the unloading process is terminated when \( P_m \) defined in Eq. (11) vanishes. Then, the boundary conditions are changed to traction boundary conditions on the contact surface and calculation is continued until the contact surface is traction free.

We confine attention to the \( \sigma_{11} \) component of the residual stress, which is the normal stress parallel to the indented surface, and define an \( x_1 \)-average measure of stress as

\[
\langle \sigma_{11} \rangle (x_2) = \frac{1}{w \lambda} \int_{x_2 - \lambda/2}^{x_2 + \lambda/2} \int_{0}^{w} \sigma_{11}(x_1, z_2) dx_1 dz_2 \tag{12}
\]

Thus, \( \langle \sigma_{11} \rangle (x_2) \) is the average value of \( \sigma_{11} \) in an infinitely long strip centered at \( x_2 \) with height \( \lambda \). The height of the region \( \lambda \) is introduced to smooth the results; using \( \lambda = 0.0167 \mu m \) we find values of \( \langle \sigma_{11} \rangle (x_2) \) that are nearly independent of \( \lambda \). The integral in Eq. (12) was evaluated using a \( 5 \times 5 \) trapezoidal quadrature rule in each finite element.

Fig. 15 shows plots of \( \langle \sigma_{11} \rangle (x_2) \), for contacts with \( a = 1 \mu m \). Each figure contrasts the residual stress distribution in a crystal that contains only bulk dislocation sources with that in a crystal containing only surface sources. For frictionless contacts (Fig. 15a), the crystal that contains only bulk sources has a compressive residual stress at its surface, with a peak value \( \simeq -30 \) MPa (or about \( 3/5 \) of the bulk yield strength). The residual stress is compressive down to a depth of \( \simeq 10 \mu m \). This compression is balanced by a small tensile stress, \( \simeq 5 \) MPa in the remainder of the crystal. The residual stress distribution for the crystal that contains only surface sources differs significantly. In this case, there is a thin \( (\simeq 2 \mu m \) thick) layer at the surface where the residual stress is tensile, with a maximum value of around \( 15 \) MPa. A compressive region develops below this, and extends to a depth of about \( 20 \mu m \). As before, the stress near the base of the crystal is tensile.

Corresponding results for perfectly sticking contacts are shown in Fig. 15b. In the presence of bulk sources only, the residual stresses are reduced significantly by friction: the stress near the surface fluctuates between small compression and tension, and a compressive region with magnitude \( \simeq 10 \) MPa has developed \( 5-10 \mu m \) below the surface. In contrast, when there are only surface sources, a slightly larger residual stress develops under the perfectly sticking contacts. In addition, the tensile region shifts to between \( 5 \mu m \) and \( 10 \mu m \) below the surface.
Figure 15: The variation of the $x_1$-averaged residual stress, $\sigma_{11}$, with $x_2$ for two crystals, one with only bulk dislocation sources and one with only surface dislocation sources, for $a/w = 1\mu m/9\mu m$ unloaded from $u = 0.1\mu m$. (a) Frictionless contacts. (b) Perfectly sticking contacts.

Figure 16: Residual $\sigma_{11}$ and dislocation structure for crystals with contact size $a/w = 1\mu m/9\mu m$ and frictionless contacts. (a) Surface dislocation sources. (b) Bulk dislocation sources. Corresponding averaged $\sigma_{11}$ profiles are given in Fig. 15a.

A more detailed picture of the residual stress distribution near the surface is shown in Fig. 16. The stresses fluctuate rapidly around stored dislocations, and local tensile stresses with magnitude up to 70MPa (half the obstacle strength) can develop even at depths where the average stress is compressive. The fluctuations are greater in the crystal with bulk dislocation sources, since the dislocation density is higher. With surface sources only, Fig. 16a, the bands of compressive stress between dislocation arrays on the four dominant slip planes remain after unloading. Near the surface, the stresses outside these
bands are tensile, and high local tensile stresses develop at gaps in the dislocation walls, which form near pinning obstacles on the slip plane.

Figure 17: (a) The variation of the \( x_1 \)-averaged residual stress, \( \sigma_{11} \), with \( x_2 \) for two crystals with contact size \( a/w = 0.25\mu m/2.25\mu m \) after unloading from frictionless contact to \( P_m = 0 \). The crystal with bulk dislocation sources is unloaded from \( u = 0.1\mu m \) to \( u = 0.057\mu m \); the crystal with surface dislocation sources from \( u = 0.1\mu m \) to \( u = 0.013\mu m \). (b) Comparison between crystals with various realizations.

To explore the effect of contact size on residual stress, residual stresses were calculated for frictionless indentation by contacts with size \( a/w = 0.25\mu m/2.25\mu m \). The average stresses \( \langle \sigma_{11} \rangle (x_2) \) are shown in Fig. 17a. The results are qualitatively similar to those for larger contacts, but the residual stresses are confined to a shallower layer near the surface, and their magnitudes increase significantly as the contact size is reduced.

Even though Fig. 13 shows that the overall response is not sensitive to the distribution of sources and obstacles, the local response may depend on this. However, Fig. 17b demonstrates that both the tensile–compression characteristics of the profile and the peak values are quite similar for two different source distributions.

The detailed distribution of residual stress for \( a/w = 0.25\mu m/2.25\mu m \) contacts is shown in Fig. 18. The density of stored dislocations is smaller than for the \( a/w = 1\mu m/9\mu m \) contacts in Fig. 16, so the stress distribution is more uniform. With bulk sources, the compressive layer near the surface appears to be associated with a large density of pinned dislocations. In the material with only surface sources, the region of compressive stress appears to occur at the point where the slip bands emitted from neighboring contacts overlap. The stresses near the surface are predominantly tensile, with peak values exceeding 70MPa (40% greater than the bulk yield strength).

Calculations were also carried out with \( \tau_{obs} = 1500\text{MPa} \) to investigate the effect of obstacle strength on the residual strength distribution and, in particular, on the emergence of the near-surface tensile layer. It was found that although the details of the residual stress distribution did vary with obstacle strength, a similar layer of tensile \( \langle \sigma_{11} \rangle \) developed
Figure 18: Residual $\sigma_{11}$ and dislocation structure for crystals with contact size $a/w = 0.25\mu m/2.25\mu m$ and frictionless contacts. (a) Surface dislocation sources. (b) Bulk dislocation sources. Corresponding averaged $\sigma_{11}$ profiles are given in Fig. 17a. The stress and dislocation distribution in the loaded state are shown in Fig. 11a.

near the surface for the higher obstacle strength.

4 Discussion

Existing models of rough surface contact which account for inelastic deformation are generally based on the continuum theory of plasticity, e.g. (Pei et al., 2005; Gong and Komvopoulos, 2003; Persson, 2005; Majumdar and Bhushan, 1991). These models predict contact sizes that range from several microns down to a few nanometers, depending on how the surface topography is approximated. At these size scales discrete dislocation effects lead to substantial deviations from the predictions of classical plasticity theory. Two features observed in our simulations have particularly important implications: firstly, the contact pressures substantially exceed the predictions of classical plasticity theory; secondly, the plastic zone sizes are predicted to be much greater. As a consequence of the increased strength at small size scales, classical plasticity models of rough surface contact will underestimate the contact pressure under displacement control and, under force control, overestimate the contact area. In addition, the large plastic zone sizes in the discrete dislocation model lead to significant interactions between contacts, even when widely spaced. Many models of rough surface contact are based on superposing the cumulative effects of individual asperities, each of which is assumed to act as an isolated indenter. While these models may accurately characterize the behavior of large contact spots, asperity interactions will play an important role in governing the behavior of small contacts.

For frictionless contacts and with dislocation nucleation from bulk sources, the mean contact pressure $P_m$ reaches a plateau value that is relatively contact size independent.
Under other conditions, for the range of contact sizes considered (between 0.25 and 2µm), the discrete dislocation plasticity analyses give contact pressures that are size dependent and that can be several times higher than predicted by continuum plasticity theory, with smaller being harder. The main contributions to the size-dependent response are: (i) small contacts have only a limited number of dislocation sources in their vicinity; and (ii) the region in which dislocation glide takes place does not scale with contact size, and for small contacts is comparable to the spacing between contacts. This interaction between “plastic zones” emanating from under neighboring contacts also acts to increase the mean contact pressure.

![Dislocation etch pits on a (100) plane of surface plasticity associated with micron scale asperity contacts in an MgO single crystal. Unpublished data from Kim (1980).](image)

In our calculations, the deformation bands that penetrate into the crystal from the contacts are a characteristic feature of the deformation mode with surface sources. Fig. 19 shows dislocation etch pits of bands emanating from asperity contacts in an MgO single crystal (Kim, 1980) exhibiting a similar deformation pattern. The crystal was loaded on a (001) plane by impact of a nominally-flat surface of polycrystalline titanium. Random asperities of the MgO and titanium surfaces induced surface plasticity near the contact surfaces. The MgO crystal was then cleaved on a (100) plane perpendicular to the contact plane and etched. The oblique arrays of etch pits in Fig. 19 correspond to those of edge dislocations on (011) and (011) slip planes. The horizontal arrays of etch pits in Fig. 19 correspond to screw dislocations on other slip systems. The spacing of the dislocation etch pit arrays shows that the major spacing frequencies of the asperities that give rise to the deformation bands are approximately 10/mm and 300/mm for this particular experiment. Our discrete dislocation plasticity analyses suggest that the band-like deformation pattern seen experimentally in Fig. 19 is characteristic of contact plasticity that is dominated by surface dislocation sources.

A strong sensitivity to the friction between the contact and the crystal is found when
the size of the contact is around or below 1 \mu m. This sensitivity is not predicted by classical plasticity theory for contacts having the size and spacing considered here. In our discrete dislocation analyses sticking contacts can have a substantially higher strength than frictionless contacts. In addition, friction has a significant influence on the residual stress distributions. The implications of these results on the behavior of rough surfaces merit further study. In particular, it is not clear whether rough surfaces are most appropriately modeled as frictionless or perfectly sticking. Moreover, perfect sticking conditions require the shear traction under the indenter to be smaller than the adhesive strength, which may be a function of contact pressure. These issues depend on the crystal and contact material properties, and on the surface properties.

Figure 20: Measured residual stress profile in a polycrystalline aluminum alloy after indentation with a nominal contact pressure of 80 MPa. From Wang et al. (2006c).

Our results on the formation of a layer of tensile residual stress at or near the contact surface are in accord with recent analytical models, Gao et al. (2006b); Yu et al. (2006), and experimental observations, Wang et al. (2006c). Fig. 20 shows a measured residual stress corresponding to $<\sigma_{11}> (x_2)$ defined in Eq. (12) versus distance from the surface from Wang et al. (2006c). For a sufficiently large (greater than about 40 MPa) nominal contact pressure, defined as the force per unit total surface area which for the calculations here would correspond to $aP_m/w = P_m/9$ with $P_m$ given by Eq. (11), a narrow tensile layer typically 0.1 to 0.4 \mu m thick is followed by a thick compressive layer. For nominal contact pressures less than 40 MPa a tensile residual stress layer was not observed, which may reflect the need to attain a critical stress to activate surface dislocation sources. The experimental observations are qualitatively similar to the discrete dislocation results in Section 3.6. However, since the experimental specimens are polycrystalline aluminum alloys with a bulk yield strength of 120 MPa so that the slip orientations are random and there are many grain boundaries, the results are not directly comparable to the single crystal simulation results. The analytical modeling in Gao et al. (2006b); Yu et al. (2006) showed that dislocations in certain slip planes can be easily nucleated but
will stay in equilibrium positions very close to the surface step and that such contact-
induced near-surface dislocation segregation would generate a thin tensile-stress sub-layer
adjacent to the surface within the boundary layer of near-surface plastic deformation.
Our calculations, which pertain to a fixed number of surface and bulk dislocation sources,
indicate that such a tensile layer is formed only when surface sources are dominant but
not when there are sufficient bulk dislocation sources. However, dislocations nucleated at
bulk sources that glide to the surface could form surface-step sources so that the surface
source density would evolve with deformation. Possible effects of an evolving density of
surface (and/or bulk) dislocation sources remain to be investigated.

5 Conclusions

The indentation of single crystals by a periodic array of flat rigid contacts was analyzed
as an idealized model of indentation of a ductile single crystal by a rough, hard surface.
Plane strain discrete dislocation plasticity calculations were carried out. The limiting
cases of frictionless and perfectly sticking contacts were contrasted. The ratio of contact
size to spacing was held fixed at $a/w = 1/9$, with the contact size $a$ varying between 0.25
and 2$\mu$m (see Fig. 1). A main focus was on contrasting the response when dislocation
nucleation occurs at surface sources to that when dislocation nucleation occurs from bulk
(e.g. Frank-Read) sources. The main conclusions are:

- For materials containing only bulk sources:
  - Over the range of indentation depths considered, the contact pressure under
    large contacts (order of magnitude 1$\mu$m or larger) is independent of the friction
    between the contacting surfaces, consistent with the prediction of conventional
    continuum crystal plasticity.
  - For contacts sizes below around 1$\mu$m, a substantial difference emerges between
    frictionless and sticking contacts, once significant plastic deformation occurs.
  - For frictionless contacts, the mean contact pressure is size dependent for suf-
    ficiently shallow indentation depths, but a relatively size independent plateau
    value of the mean contact pressure is attained at larger indentation depths.
  - For perfectly sticking contacts, the mean contact pressure is size dependent over
    the entire range of indentation depths analyzed, with smaller being harder.
  - A state of predominantly compressive residual stress is induced near the sur-
    face. The depth of the layer of residual stress is approximately ten times the
    contact width. The magnitude of the residual stress is sensitive to contact size
    and to the friction between the contacting surfaces.

- For crystals containing only surface sources:
Plastic flow occurs primarily as a result of the development of two dipolar bands, which intersect the surface near the edge of the contact, and which induce high compressive stresses.

There is a rapid increase in mean contact pressure with indentation depth. A typical contact pressure-indentation depth curve exhibits two regimes: (i) for shallow indentation depths, obstacles on the active slip systems have the dominant effect on the mean contact pressure; and (ii) for larger indentation depths, interactions between deformation bands emanating from neighboring contacts play a dominant role that increases as the size and spacing of the contacts is reduced.

The value of the mean contact pressure is sensitive to the strength of obstacles to dislocation motion. When there are no obstacles to dislocation glide, the values of the contact pressure are comparable to those obtained with only bulk sources.

A mean tensile residual stress develops near the contact surface after unloading. The magnitude of this residual stress increases with decreasing contact size.

• When both surface and bulk dislocation sources are available, the response is generally dominated by the bulk sources, at least for the range of source densities and strengths considered here.

Acknowledgments

We are pleased to acknowledge support from the Brown/General Motors Collaborative Research Laboratory in Computational Materials Research and from the Materials Research Science and Engineering Center at Brown University (NSF Grant DMR-0520651).

References