Dislocation constriction and cross-slip: An *ab initio* study

Gang Lu,[1] Vasily V. Bulatov,[2] and Nicholas Kioussis[3]
[1]*Department of Physics and Division of Engineering and Applied Science, Harvard University, Cambridge, Massachusetts 02138*
[2]*Lawrence Livermore National Laboratory, Livermore, California 94550*
[3]*Department of Physics, California State University Northridge, Northridge, California 91330*
(Received 10 June 2002; published 9 October 2002)

A model based on the Peierls framework of dislocations is developed. The theory allows the study of dislocations spreading at more than one slip planes. As an example, we study dislocation cross-slip and constriction processes in two contrasting fcc metals, Al and Ag. The energetic parameters entering the model are determined from *ab initio* calculations. We find that the screw dislocation in Al can cross-slip spontaneously in contrast with the screw dislocation in Ag, which splits into partials and cannot cross-slip without first being constricted. The response of the dislocations to an external stress is examined in detail. We determine the dislocation constriction energy and the critical stress for cross-slip, and from the latter, we estimate the cross-slip energy barrier for the straight screw dislocations.

DOI: 10.1103/PhysRevB.66.144103 PACS number(s): 62.20.Fe, 61.72.Lk, 62.20.Mk

The cross-slip process, by which a screw dislocation moves from one slip plane to another, plays an important role for plastic deformation in materials. For example, cross-slip is responsible for the onset of stage III of the stress-strain work-hardening curve and the anomalous high temperature yield stress peak observed in $L1_2$ intermetallic alloys. However, theoretical studies of dislocation cross-slip have been proved to be challenging because one has to deal with both long-ranged elastic interactions between dislocation segments and short-ranged atomic interactions due to the constriction process, in which the two partial dislocations have to be recombined into a screw dislocation before cross-slip takes place.

There are currently two theoretical approaches to study cross-slip. The first is based on the line tension approximation which completely ignores atomic interactions,[1,2] and hence is not reliable in treating the constriction process. The second approach is based on atomistic simulations employing empirical potentials.[3,4] Although this approach is quite powerful in determining the cross-slip transition path and in estimating the corresponding activation energy barrier, it is time consuming and critically depends on the accuracy and availability of the empirical potentials employed in the simulations. In this paper, we present an alternative approach to study the cross-slip process based on the Peierls framework with *ab initio* calculations for the relevant energetics. In fact, there has recently been a resurgence of interest in applying the simple and tractable Peierls-Nabarro (PN) model to study dislocation core structure and mobility in conjunction with *ab initio* γ-surface calculations.[5–10] This approach represents a combination of the atomistic (*ab initio*) treatment of interactions across the slip plane and the elastic treatment for the continua on either side of the slip plane. Therefore, this approach is particularly useful for studying the interactions of impurities with dislocations, when empirical potentials are either not available or not reliable to deal with such multielement systems. However, to date all the models based on the Peierls framework are only applicable to a single slip plane while cross-slip process requires at least two active intersecting slip planes, i.e., the primary and the cross-slip planes. It is the purpose of this paper to introduce a PN model that involves two intersecting slip planes. This development represents an effort to extend the PN model to multiple slip planes, which in turn allows the study of dislocation junctions and other interesting dislocation processes as involving multiple slip planes. We will demonstrate that this approach reproduces in precise detail the cross-slip behavior of the straight dislocations, when it is compared to the results from direct atomistic simulations.

We begin by developing an appropriate energy functional for a Peierls dislocation at two intersecting slip planes. To facilitate the presentation, we adopt the following conventions: In Fig. 1, a screw dislocation placed at the intersection of the primary (plane I) and the cross-slip plane (plane II) is allowed to spread onto the two planes simultaneously. The X (X') axis represents the glide direction of the dislocation at the plane I (II). For a fcc lattice, the two slip planes are (111) and $(\bar{1}\bar{1}1)$, forming an angle $\theta \approx 71°$. The dislocation line is along the $[10\bar{1}]$ (Z axis) direction, and L represents the outer radius of the dislocation beyond which the elastic energy is ignored. In the spirit of the PN model, the dislocation is represented as a continuous distribution of infinitesimal dis-

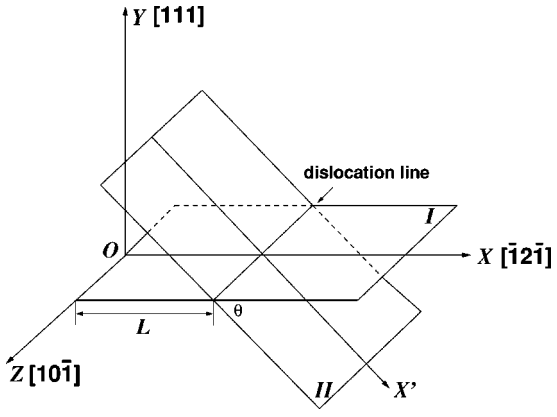

FIG. 1. Cartesian set of coordinates showing the directions relevant to the screw dislocation located at the intersection of the two slip planes.

locations with densities of $\rho^{\mathrm{I}}(x)$ and $\rho^{\mathrm{II}}(x')$ on the primary and the cross-slip planes respectively. Here x and x' are the coordinates of the atomic rows at the two planes. Following the semidiscrete Peierls framework developed earlier,[7,9] we can write the total energy of the dislocation as $U_{tot}=U_{\mathrm{I}}+U_{\mathrm{II}}+\tilde{U}$. Here U_{I} and U_{II} are the energies associated with the dislocation spread on planes I and II, respectively, and $\tilde{U}$ represents the elastic interaction energy between the dislocation densities from the two planes. U_{I} and U_{II} are essentially the same expression given earlier for the single plane case,[7,9] while $\tilde{U}$ is a new term and can be derived from Nabarro's equation for general parallel dislocations[11]:

$$
\begin{aligned}
U_{\mathrm{I(II)}}=&\sum_{i,j}\frac{1}{2}\chi_{ij}\{K_e[\rho_1^{\mathrm{I(II)}}(i)\rho_1^{\mathrm{I(II)}}(j)+\rho_2^{\mathrm{I(II)}}(i)\rho_2^{\mathrm{I(II)}}(j)]\\
&+K_s\rho_3^{\mathrm{I(II)}}(i)\rho_3^{\mathrm{I(II)}}(j)\}\\
&+\sum_i \Delta x\,\gamma_3(f_1^{\mathrm{I(II)}}(i),f_2^{\mathrm{I(II)}}(i),f_3^{\mathrm{I(II)}}(i))\\
&-\sum_{i,l}\frac{x(i)^2-x(i-1)^2}{2}\rho_l^{\mathrm{I(II)}}(i)\,\tau_l^{\mathrm{I(II)}}+Kb^2\ln L,
\end{aligned}
$$

$$
\begin{aligned}
\tilde{U}=&-\sum_{i,j}K_s\rho_3^{\mathrm{I}}(i)\rho_3^{\mathrm{p}}(j)A_{ij}-\sum_{i,j}K_e[\rho_1^{\mathrm{I}}(i)\rho_1^{\mathrm{p}}(j)\\
&+\rho_2^{\mathrm{I}}(i)\rho_2^{\mathrm{p}}(j)]A_{ij}-\sum_{i,j}K_e[\rho_2^{\mathrm{I}}(i)\rho_2^{\mathrm{p}}(j)B_{ij}\\
&+\rho_1^{\mathrm{I}}(i)\rho_1^{\mathrm{p}}(j)C_{ij}-\rho_2^{\mathrm{I}}(i)\rho_1^{\mathrm{p}}(j)D_{ij}\\
&-\rho_1^{\mathrm{I}}(i)\rho_2^{\mathrm{p}}(j)D_{ij}].
\end{aligned}
$$

Here $f_1^{\mathrm{I(II)}}(i)$, $f_2^{\mathrm{I(II)}}(i)$, and $f_3^{\mathrm{I(II)}}(i)$ represent the edge, vertical, and screw components of the general dislocation displacement at the ith nodal point in the plane I(II), respectively, while the corresponding component of dislocation density in plane I(II) is defined as $\rho^{\mathrm{I(II)}}(i)=[f^{\mathrm{I(II)}}(i)-f^{\mathrm{I(II)}}(i-1)]/[x(i)-x(i-1)]$. The projected density ρ^{p}(i) is the projection of the density ρ^{II}(i) from the plane II onto plane I, introduced to deal with nonparallel components of displacement. The γ surface γ_3, which in general includes shear-tension coupling can be determined from *ab initio* calculations. $\tau_l^{\mathrm{I(II)}}$ is the external stress components interacting with the corresponding $\rho_l^{\mathrm{I(II)}}(i)$ $(l=1,2,3)$, which contributes to the total energy as the elastic work done by the external stress.[7] The response of the dislocation to the external stress is achieved by optimization of $\rho_l^{\mathrm{I(II)}}(i)$ at a given value of $\tau_l^{\mathrm{I(II)}}$. The dislocation core energy is defined as a sum of the density-dependent part of the elastic energy and the entire misfit energy, in the absence of external stress. K_e and K_s are the edge and screw components, respectively, of the general prelogarithmic elastic energy factor K. χ_{ij}, A_{ij}, B_{ij}, C_{ij}, and D_{ij} are double-integral kernels defined as follows:

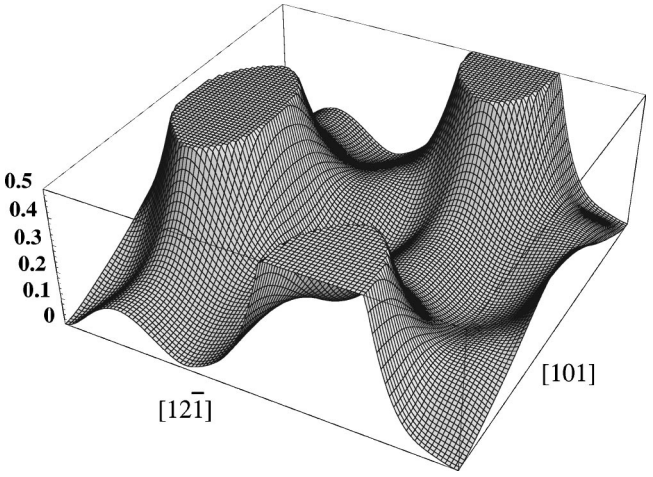

FIG. 2. The γ surface (J/m^2) for displacements along a (111) plane for Ag. The corners of the plane and its center correspond to identical equilibrium configuration, i.e., the ideal lattice. The γ surface is truncated to emphasize the more interesting region.

$$\chi_{ij}=\int_{x_{j-1}}^{x_j}\int_{x_{i-1}}^{x_i}\ln|x-x'|\,dx\,dx',$$

$$A_{ij}=\int_{x'_{j-1}}^{x'_j}\int_{x_{i-1}}^{x_i}\frac{1}{2}\ln(x_0^2+y_0^2)\,dx\,dx',$$

$$B_{ij}=\int_{x'_{j-1}}^{x'_j}\int_{x_{i-1}}^{x_i}\ln\frac{x_0^2}{x_0^2+y_0^2}\,dx\,dx',$$

$$C_{ij}=\int_{x'_{j-1}}^{x'_j}\int_{x_{i-1}}^{x_i}\ln\frac{y_0^2}{x_0^2+y_0^2}\,dx\,dx',$$

$$D_{ij}=\int_{x'_{j-1}}^{x'_j}\int_{x_{i-1}}^{x_i}\ln\frac{x_0y_0}{x_0^2+y_0^2}\,dx\,dx',$$

where $x_0=L-x+x'\cos\theta$, and $y_0=-x'\sin\theta$. The equilibrium structure of the dislocation is obtained by minimizing the total energy with respect to the dislocation density.

To contrast and to understand the different cross-slip behavior in Al and Ag, we have carried out *ab initio* calculations for the γ surface of Ag while the γ surface of Al has been published elsewhere.[9] A supercell containing six atomic layers in the [111] direction is used to calculate the γ surface for Ag. The *ab initio* calculations are based on the pseudopotential plane-wave method[12] with a kinetic energy cutoff of 55 Ry for the plane-wave basis and a k-point grid consisting of (16,16,4) divisions along the reciprocal lattice vectors. Owing to the planar nature of the dislocation core structure of fcc metals, we disregard the displacement perpendicular to the slip planes, and partially consider the shear-tension coupling by performing volume relaxation along the [111] direction in the γ-surface calculations. We present the complete γ surface for Ag in Fig. 2. The most striking difference between the γ surfaces of Ag and Al is the vast difference in the intrinsic stacking fault energy, which is 165 mJ/m^2 for Al

and 14 mJ/m^2 for Ag. This dramatic difference in the γ surface gives rise to very different dislocation core structures and cross-slip behavior that we are going to explore.

The model calculation is set up by introducing a screw dislocation at the intersection of the two slip planes without applying external stress to the system at first. The initial configuration of the dislocation is specified by a step function for the screw displacement $f_3^{\mathrm{I}}(x)=0$ for $x<L$ and $f_3^{\mathrm{I}}(x)=b$ for $x\geqslant L$. All other displacement components, including those on the cross-slip plane, are set to zero initially. This corresponds to a pure screw dislocation with a zero width ''spread'' on the primary plane. We then relax the dislocation structure according to the energy functional. The Burgers vector of Ag, $b=2.84$ Å, is determined from *ab initio* calculations and elastic constants are chosen from the experimental values.[13] The corresponding parameters of Al have been given elsewhere.[9] Having determined all the parameters entering the model, we can calculate the equilibrium structure of the dislocations, represented by their density $\rho(x)$ shown in Fig. 3, using the new PN model. The screw dislocation in Al which starts out at the primary plane spontaneously spreads into the cross-slip plane, as the density peak at the cross-slip plane indicates. As expected, the edge component of the density is zero at the cross-slip plane because only screw displacement can cross-slip. On the other hand, the screw dislocation in Ag dissociates into two partials, separated by $7.8b$ (≈ 22 Å) distance. These partial dislocations cannot cross-slip, as the arrows indicate, without first annihilating their edge component. As a consequence, the dislocation density on the cross-slip plane is essentially zero. The partial separation distance we obtained from the model calculation is in an excellent agreement with the TEM measurement for that in Ag, which is about 20 Å.[14] Obviously, the lack of a clear dissociation in Al results from the fact that the intrinsic stacking fault energy in Al is much higher than that in Ag.

In order to examine the effect of external stress on the dislocation core structure and cross-slip process, we next apply external Escaig stress to the dislocation. The Escaig stress defined as the edge component of the diagonal stress tensor interacts only with the edge component of dislocation densities, extending or shrinking the stacking fault width depending on its sign. The results of the partial separation as a function of Escaig stress are summarized in Fig. 4. Without external stress, the partial separation is $7.8b$ for Ag and zero for Al. Under positive Escaig stress, the partial separation rises rapidly for Ag whereas it remains zero in *A*l until the stress reaches the threshold required to separate the overlapping partials. To activate cross-slip, however, one needs to apply a negative Escaig stress so as to annihilate the edge components of the partials' displacement, known as a constriction process. Upon application of the negative stress, the partials in Ag move toward each other and reduce the width of the stacking fault. During this process, the edge components of displacement from the two partials annihilate each other while the screw component is being built up. However there is a lower limit that the two straight partial dislocations can approach each other, which is $1.7b$ for Ag. This is in good agreement with the atomistic simulations for Cu, reporting a corresponding value of $1.6b$.[15] In the wake of the constriction process, a pure screw dislocation segment is formed at the intersection of the two planes, which in turn can cross-slip. On the other hand, further increasing the negative stress does not complete the constriction but rather increases the partial separation distance. This is due to the fact that the remaining edge component of the partials interacts with the stress, and as a result the two partials exchange signs and move away from each other until the lattice breaks down. Associated with the inversion of the edge component of the partials, a run-on stacking fault is formed between the partials, with an energy of about 1.0 J/m^2. Across the stacking fault plane, the atoms from the neighboring (111) planes sit right on top of each other, and therefore the run-on stacking fault is the most unstable fault configuration in an fcc

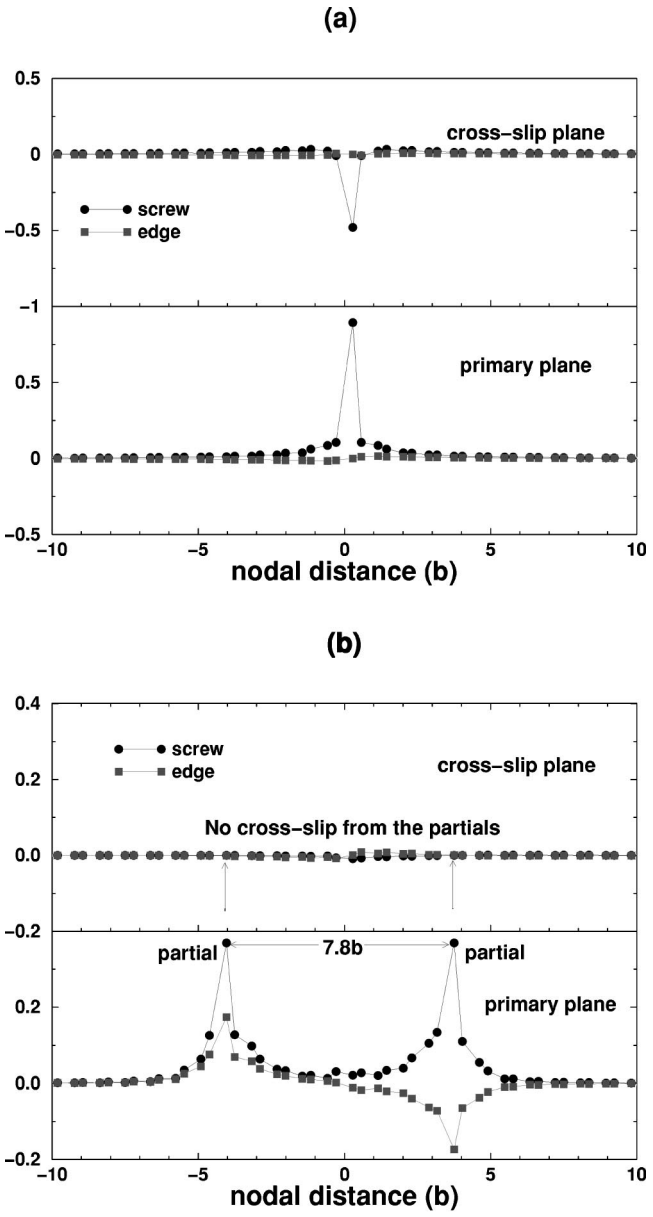

FIG. 3. Dislocation displacement density $\rho(x)$ for Al (a) and Ag (b). The peaks in the density plot represent (partials) dislocations.

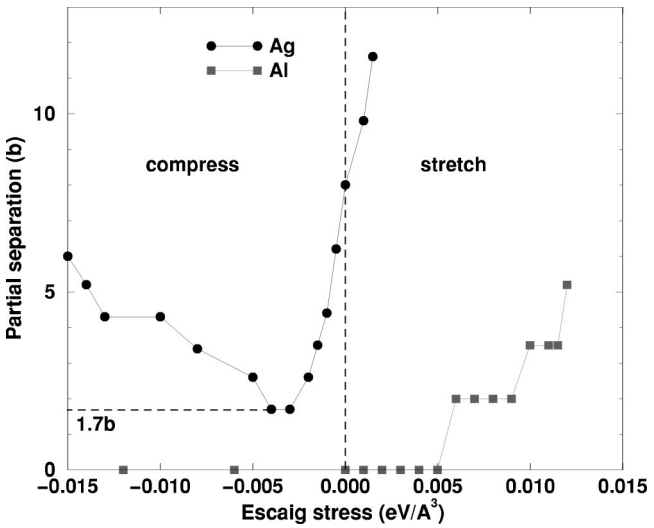

FIG. 4. Partial separation as a function of applied Escaig stress. The vertical dashed line represents the zero stress separating the compress and stretch regions. The horizontal dashed line indicates the minimal separation distance for Ag.

lattice. Such a high energy state of a straight screw dislocation can only exist in real materials under very high stress levels.

We have also estimated critical energetics that are relevant to cross-slip. For example, we calculated constriction energy defined as the difference in dislocation core energy[9] between the normal and the constricted states. By approximating the state with $1.7b$ separation between partials as the constricted state, we were able to estimate the constriction energy for Ag to be 0.14 eV/b. A similar approach has been used to evaluate the constriction energy for a screw dislocation in Cu based on atomistic simulations, reporting a value of 0.17 eV/b, which is in good agreement with our model calculations. Obviously the constriction energy for Al is zero because its normal state is fully constricted. We have also calculated the critical stress for cross-slip which is defined as the glide stress in the cross-slip plane to move a partially constricted dislocation from the primary plane to the cross-slip plane.[15] Of course, this approximation assumes that under the critical glide stress, the constricted dislocation moves to the cross-slip plane. Within this approximation, we determined the critical stress for cross-slip in Ag to be 1.68 GPa, comparing to 0.32 GPa in Al. The critical stress for cross-slip from our calculations is of the same order of magnitude as that required to move a straight screw dislocation in the bcc structure, and shares the same origin of the nonplanar core structure. Finally we estimated cross-slip energy barrier, which in the context of our calculations is defined as the difference in dislocation core energy before and after cross-slip takes place by applying the above mentioned critical stress. In other words, we calculate the core energy difference for the dislocation between its normal state and the state that the dislocation just starts to cross-slip under the application of the critical cross-slip stress. We find that the cross-slip energy barrier for Ag is 0.31 eV/b, much higher than that of 0.05 eV/b for Al. One needs to be cautious when comparing our results for the cross-slip energy barrier directly with experiments, since the dislocations are assumed to be straight in our current implementation of the PN model. Nevertheless the present model is still capable of providing reliable energetics for straight dislocations. Moreover, it is possible to extend the present formalism to deal with an arbitrarily curved dislocation where a more realistic cross-slip energy barrier can be obtained.

To conclude, we have presented a model based on the Peierls framework that allows the study of dislocation cross-slip and constriction. The γ surface entering the model is determined from *ab initio* calculations which provide reliable atomic interactions across the slip plane. We have demonstrated that the model successfully reproduces the different dislocation cross-slip behaviors in Al and Ag. We find that the screw dislocation in Al can spontaneously spread into the cross-slip plane, while in Ag it splits into partials and cannot cross-slip without first being constricted. The response of the dislocations to external stresses is examined, and in particular negative Escaig stresses are applied to the dislocations to simulate the constriction process. It is found that one cannot achieve full constriction for straight partial dislocations. By computing the dislocation core energy in different stress states, we have estimated the dislocation constriction energy for Al and Ag. We have also calculated the critical stress and the energy barrier for dislocation cross-slip, and from which we confirmed that dislocation cross-slip is much easier in Al than in Ag. Since our *ab initio* model calculation is much more expedient than direct *ab initio* atomistic simulations, it can serve as a powerful and efficient tool for alloy design where the goal is to select the ''right'' elements with the ''right'' composition to tailor the desired mechanical, in particular, dislocation properties.

Two of us (G.L. and N.K.) acknowledge the support from Grant No. DAAD19-00-1-0049 through the U.S. Army Research Office. G.L. was also supported by Grant No. F49620-99-1-0272 through the U.S. Air Force Office for Scientific Research. We thank E. Kaxiras for suggesting this interesting problem to us.

[1] J. Friedel, in *Dislocations and Mechanical Properties of Crystals*, edited by J.C. Fisher (Wiley, New York, 1957).
[2] B. Escaig, in *Dislocation Dynamics*, edited by A.R. Rosenfeld, G.T. Hahn, A.L. Bement, and R.I. Jaffee (McGraw-Hill, New York, 1968).
[3] T. Rasmussen, K.W. Jacobsen, T. Leffers, O.B. Pederson, S.G. Srinivasan, and H. Jónsson, Phys. Rev. Lett. **79**, 3676 (1997).
[4] S. Rao, T.A. Parthasarathy, and C. Woodward, Philos. Mag. A **79**, 1167 (1999).
[5] B. Joós, Q. Ren, and M.S. Duesbery, Phys. Rev. B **50**, 5890 (1994).
[6] Y.M. Juan and E. Kaxiras, Philos. Mag. A **74**, 1367 (1996).

[7] V.V. Bulatov and E. Kaxiras, Phys. Rev. Lett. **78**, 4221 (1997).
[8] J. Hartford, B. von Sydow, G. Wahnström, and B.I. Lundqvist, Phys. Rev. B **58**, 2487 (1998).
[9] G. Lu, N. Kioussis, V.V. Bulatov, and E. Kaxiras, Phys. Rev. B **62**, 3099 (2000); Philos. Mag. Lett. **80**, 675 (2000).
[10] G. Lu, Q. Zhang, N. Kioussis, and E. Kaxiras, Phys. Rev. Lett. **87**, 095501 (2001).
[11] F.R.N. Nabarro, Adv. Phys. **1**, 269 (1952).
[12] M.C. Payne, M.P. Teter, D.C. Allan, T.A. Arias, and J.D. Joannopoulos, Rev. Mod. Phys. **64**, 1045 (1992).
[13] J.P. Hirth and J. Lothe, *Theory of Dislocations*, 2nd ed. (Wiley, New York, 1992).
[14] D.J.H. Cockayne, M.L. Jenkins, and I.L.F. Ray, Philos. Mag. **24**, 1383 (1971).
[15] M.S. Duesbery, Modell. Simul. Mater. Sci. Eng. **6**, 35 (1998).