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Analytic model of the γ-surface deviation and influence on the stacking fault width between partial dislocations

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ABSTRACT

The stacking fault width (R_{eq}) between partial dislocations within an FCC crystalline lattice characterizes the onset of numerous plastic flow mechanisms, as well as the relationship between material strength and grain size. Continuum models traditionally consider a complete unit of dislocation slip (**b**) along the $\langle 1\,1\,0\rangle$ direction distributed between two discrete partial dislocations, each with a *fixed* partial Burgers vector ($\mathbf{b}_p$), which bound a stacking fault. Across the stacking fault, the vectorial slip is assumed to be constant, yielding a constant intrinsic stacking fault energy density, γ_{isf}. Here, we demonstrate that the vectorial displacement path taken in accomplishing a complete unit of slip (**b**) deviates from the expected displacement path containing the local minima, γ_{isf}, leading to a correction in the nominally derived stacking fault width. The magnitude of the correction depends on both the net orientation of the dislocation within the lattice, and also the degree of relaxation of each partial Burgers vector along the $\langle \bar{1}\,1\,2\rangle$ direction. We derive a simple analytic model for the corrected stacking fault width, explicitly accounting for the deviation, by introducing a variable $\xi\,(0 < \xi < 1)$, which governs the magnitude of each partial dislocation component along the $\langle \bar{1}\,1\,2\rangle$ direction. Significantly, our model predicts a correction to R_{eq} of $\sim\mathcal{O}(|\mathbf{b}|)$ for the nominally screw dislocation, and has no noticeable influence on nominally edge dislocations. We apply our model towards computing the stacking fault width of several FCC metals, and demonstrate excellent agreement both with our own numerical data as well as that obtained from *ab initio* and Molecular Statics (MS) methods within the literature. The results from this study demonstrate that, upon judicious application, discrete linear elastic models are successful in reproducing elastic interactions as computed from higher fidelity models on the spatial scale of metallic dislocation cores.

1. Introduction

Increasingly sophisticated materials systems continue to facilitate the advancement of technology across a broad spectrum of industries. A host of experiments [1–5], simulations [6,7], and theories [8–10] have demonstrated that the interactions between dislocations, interfaces [11–13], grain boundaries [5,7,8], and other defects [14,15] within materials are responsible for dramatic increases in desirable engineering features such as ductility and strength [16–19]. The single intrinsic material length scale with the most notable influence on mechanical behavior is the stacking fault width between partial dislocations (R_{eq}).

The stacking fault width has an unambiguous role in determining mechanical features of interest across a broad range of materials systems. The mobility of screw dislocations within Silicon is largely dependent upon their equilibrium stacking fault width [20]. Moreover, with increased interest in thin films, and microelectromechanical systems, a precise understanding of both the stacking fault width, and interactions with interfaces is of increasing relevance [21]. More recent multiscale simulation methodologies, which are designed upon passing material defects between differing physical domains, rely upon a precise description of the size of the dislocation core to maintain continuity across domain boundaries [22]. Finally, the strongly anisotropic plastic response of α-RDX to flyer plate impact has been attributed to slip system dependent behavior of dislocation stacking fault aggregate [23]. This range of applications motivates the detailed mechanistic study of the features of a dislocation core, and the stacking fault width.

The simplest elastic model of a dislocation core contained within an FCC lattice and on a $\{1\,1\,1\}$ slip plane involves two discrete partial dislocations, each with partial Burgers vectors $\mathbf{b}_{p,1} = \frac{\sqrt{2}}{6}|\mathbf{b}|\langle 1\,2\,1\rangle$ and $\mathbf{b}_{p,2} = \frac{\sqrt{2}}{6}|\mathbf{b}|\langle 2\,1\,\bar{1}\rangle$ satisfying $\mathbf{b} = \mathbf{b}_{p,1}+\mathbf{b}_{p,2}$.

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The two partial dislocations are separated by an intrinsic stacking fault with a width of R_{eq} and energy density γ_{isf}. To maintain the equilibrated width, R_{eq}, the attractive force (γ_{isf}) provided by the stacking fault must be balanced by a repulsive force. Since the shear stress fields of each partial dislocation repel with a force of $\sim 1/R_{eq}$, equating the attractive and repulsive forces leads to a reference equilibrium spacing of [9]

$$\frac{R_{eq,ref}(\theta)}{|\mathbf{b}|} = \left(\frac{|\mathbf{b}|C_{44}}{24\pi\gamma_{isf}}\right) \times \mathscr{F}(\theta) \tag{1}$$
$$\mathscr{F}(\theta) = \left[(3\widetilde{B}_{tt} - \widetilde{B}_{mm})\cos^2(\theta) + (3\widetilde{B}_{mm} - \widetilde{B}_{tt})\sin^2(\theta)\right]$$

where the material dependence is contained within C_{44}/γ_{isf}, and the orientation dependence within θ which denotes the angle between the Burgers vector ($\mathbf{b}$) and the dislocation line direction. The elastic shear moduli $\widetilde{B}_{tt}$ and $\widetilde{B}_{mm}$ act within the slip plane along and perpendicular to the dislocation line direction, respectively, and are in units of $C_{44}/(4\pi)$. They are related to the shear moduli tensor $\mathbf{B}$ (e.g., [24]) and any material unit vector ($\mathbf{e}$) through the relation $\mathbf{Be}\cdot\mathbf{e} = \widetilde{B}_{ee}C_{44}/(4\pi)$. For the materials investigated within this study $\widetilde{B}_{tt}$ and $\widetilde{B}_{mm}$ are listed within Table 1, and are reasonably material independent.

While Eq. (1) has provided incredible insight, the underlying assumptions on which it resides are not always justified. The entire inter-planar energy surface (known as the γ-surface [25]) is represented by a single representative energy, γ_{isf}, and simultaneously the two repelling partial dislocations are represented by Dirac's delta functions separated by R_{eq}. The failure of Eq. (1) is manifest upon examination of Al dislocation cores, which are sufficiently narrow as to be amenable to computation by *ab initio* methods (DFT) [26,27]. Application of Eq. (1) (with Burgers vector $|\mathbf{b}| \approx 2.57$ Å and the parameters listed within Table 1) predicts $R_{eq,ref} \approx 0.95|\mathbf{b}|$, however, as demonstrated by both Woodward et al. [26] and Das et al. [27], employing DFT, for the same screw dislocation within Al, $R_{eq} \approx 2|\mathbf{b}|$, which is a factor of two greater than the discrete elastic prediction. Providing additional ambiguity, as reported by Woodward et al. [26] the range of $1.91 \leqslant \frac{R_{eq}}{|\mathbf{b}|} \leqslant 6.23$ is reported within the literature [28,29] for the same Al screw dislocation. As noted within [30], some of these discrepancies may be attributed to internal stresses, such as the Peierls stress. For a host of other metals with larger dislocation cores (larger C_{44}/γ_{isf}) Molecular Statics (MS) and Molecular Dynamics (MD) simulations have also been employed towards computing Eq. (1) [28,29,31–38].

One alternative class of approaches which retains a linear elastic description as within Eq. (1) yet considers the complete slip distribution across the dislocation core is that of Peierls and Nabarro [39,40] which has been extended by Vitek [25] to include the generalized stacking fault energy surface (γ-surface). Infinitesimal units of dislocation slip are mutually repulsive due to their linear elastic interactions, however are constrained by the misfit energy density provided by the γ-surface. The result is a spread dislocation core, which is both free of singularities, and also exhibits the long-ranged fields characteristic of dislocations. Within Fig. 1 we depict the relationship between (a) the displacement path across the γ-surface, (b) the displacements $(u_{\langle 1\,1\,0\rangle}(x), u_{\langle\bar{1}\,1\,2\rangle}(x))$ versus position (x) across the slip plane, and (c) the displacement gradient $(\partial u_{\langle 1\,1\,0\rangle}(x)/\partial x)$ versus position (x). For every position along the slip plane (x), the displacement vector $(u_{\langle 1\,1\,0\rangle}(x), u_{\langle\bar{1}\,1\,2\rangle}(x))$ corresponds to a misfit energy density on the γ-surface within Fig. 1a. The stacking fault width (R_{eq}) within Fig. 1c is characterized by the separation between the two peaks in the gradient of the displacement along the slip direction ($\langle 1\,1\,0\rangle$).

Within Fig. 1a and b we denote the extent of deviation with the variable ξ ($0 < \xi < 1$), indicating the maximum amount of displacement along the $\langle\bar{1}\,1\,2\rangle$ direction, where $max(u_{\langle\bar{1}\,1\,2\rangle}|_{\xi=1}) = |\mathbf{b}|\sqrt{3}/6$. The deviation which is significantly more pronounced for the screw dislocation has been noted previously by Schoeck [41,42] and more recently Szelestey et al. [32]. However, to the authors knowledge, the relationship between the deviating path across the γ-surface and corrections to the derived stacking fault width remains to be examined. The scope of this work is to develop a quantitative analytical model for the stacking fault width between FCC partial dislocations, incorporating the observed deviation across the γ-surface. Towards this pursuit, we first demonstrate the relationship between the deviation (ξ) and the equilibrium stacking fault width (R_{eq}) of the dislocation. Through a simple mechanistic model, we directly relate R_{eq} as computed through a discrete dislocation type model to the deviation ξ. Second, with the magnitude of $\xi = \xi(R_{eq})$ determining the extension of each partial Burgers vector along $\langle\bar{1}\,1\,2\rangle$ we derive an expression for R_{eq} incorporating the influence of ξ. We compare our predictions for both the magnitude of the deviation as a function of R_{eq}, as well as our corrected R_{eq} to our own simulation data, and that obtained from within the literature e.g. [26,27,31,32], and demonstrate excellent agreement.

We proceed by introducing our variational method (section two) based upon the classical Peierls-Nabarro dislocation [39,40] model to numerically solve for both ξ and R_{eq}. Within the third section, we develop our analytical model for both ξ and $R_{eq} = R_{eq}(\xi)$ which allows for a direct comparison to numerical data. Within results & discussion (section four) we directly compare our derived R_{eq} to others data found within the literature, and discuss the implications of the successful comparison between *discrete linear* elasticity and higher fidelity models. We conclude with a summary of the key findings of this work.

2. Simulation methodology

The objective of our work is to study the influence of the deviation (see Fig. 1a & b) of the displacement path across the γ-surface. Therefore, we must model the slip profile of a relaxed,

Table 1
Misfit energy densities (mJ/m^2) and elastic constants ($\widetilde{B}$ in units of $C_{44}/4\pi$ & C_{44} in units of GPa) for the materials examined within this study [45]; *The elastic constants for Al are found within Ref. [26].

	γ_{isf}	γ_{usf}	γ_T	$\widetilde{B}_{tt}$	$\widetilde{B}_{mm}$	C_{44}
Al*	140.2	151.4	334.8	0.87	1.36	30.8
Ag	17.8	100.4	298.2	0.59	1.09	37.4
Au	27.9	66.5	228.5	0.61	1.27	25.1
Cu	38.5	163.7	509.4	0.55	0.99	75.7
Ir	324.4	614.9	1207.9	0.83	1.13	254.4
Ni	144.6	289.0	785.8	0.67	1.04	128.1
Pd	138.1	197.9	459.5	0.62	1.15	60.7
Rh	184.6	454.1	962.7	0.78	1.11	182.1