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# Dependence of Peierls stress on lattice strains in silicon

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ABSTRACT

Several non-Schmid effects of plasticity in Si are discussed in this article. The contribution of shear strain applied in the direction of the Burgers vector and normal to it in the glide plane, and of strain applied normal to the glide plane to defining the Peierls stress are analyzed. The analysis is performed using a combination of atomistic simulations and the Peierls–Nabarro model based on generalized stacking faults. It is shown that a shear strain acting in the direction of the Burgers vector decreases the Peierls stress and the effect is due to the reduction of the shear modulus. Bonding across the glide plane has the most important contribution to the Peierls stress, but the elastic non-linearity of the surrounding material contributes to reducing the instability threshold. A shear strain acting perpendicular to the Burgers vector has no effect on the Peierls stress. A compressive strain normal to the glide plane reduces the Peierls stress for shuffle dislocations and has a weak increasing effect on the critical stress of glide-set dislocations.

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## 1. Introduction

Plastic deformation in crystalline materials takes place by the motion of dislocations on specific slip systems. The resistance dislocations face during motion is due to their interaction with the lattice and with other obstacles such as forest dislocations, solute atoms, precipitates, grain and twin boundaries. At low temperatures and in materials with strong bonding, the dominant contribution comes from the Peierls stress required to move an isolated dislocation in the perfect lattice.

Silicon has a diamond cubic lattice with strong bonding and undergoes a brittle-to-ductile transition at approximately 873 °K [1]. In this material, dislocations are strongly pinned by the Peierls barriers. The magnitude of the critical stress has been studied extensively experimentally [2,3], theoretically [4–6] and using atomistic simulations [7,8]. The main slip system is $\{111\}\langle 110\rangle$. There are two types of glide planes denoted by shuffle and glide, with the shuffle planes having an interplanar distance of 2.35 Å, and the glide planes being spaced 0.78 Å apart. A simple geometric model suggests that the density of bonds crossing the shuffle plane is smaller than that for the glide plane. It is currently accepted that the activity in the shuffle plane dominates at low temperatures and high resolved shear stresses, while at high temperatures motion in the glide system controls plasticity. As confirmed by ab initio and atomistic models, glide dislocations are dissociated in partials, while shuffle dislocations are not. This helps identifying the nature of slip in electron microscopy, as the simple observation of a compact, undissociated core indicates that the respective dislocation resides in the shuffle plane.

The interplanar potential is usually characterized by the $\gamma$-surface. The standard $\gamma$-surface is computed by separating the crystal in two parts across a glide plane and evaluating the variation of the energy per unit area associated with the relative shift of the two blocks in the selected plane. Hence, the $\gamma$-surface has minima at shifts equal to the lattice periodicity. Additional minima appear for certain configurations which correspond to stacking faults. In Si, no minimum is observed in the shuffle plane, while the glide plane $\gamma$-surface has a minimum at a relative shift of 1/6 $\langle 112\rangle$, which corresponds to the Burgers vector of a partial dislocation. The minimum energy paths on the $\gamma$-surface linking these minima indicate the preferred glide mode of the crystal and define the structure and evolution of the core of dislocations moving over the Peierls barriers. The $\gamma$-surface in Si was computed for both planes using ab initio [9] and atomistic [10] simulations.

The Peierls stress can be computed directly from atomistic simulations, by effectively forcing a dislocation to move under an applied far-field. The Peierls stress is usually computed in situations in which dislocations remain straight during motion, despite the fact that in lattices with high resistance dislocations move by the kink mechanism [11]. The critical stress is also estimated using the Peierls–Nabarro model (PN). In this semi-analytical formulation the core is represented as a continuous distribution of infinitesimal dislocations on the glide plane. The core structure is described by a distribution of infinitesimal dislocation density (slip magnitude). The solution results by requiring that the distribution is in equilibrium under the action of the mutual repulsion of the infinitesimal dislocations and the lattice rebound forces. An

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additional term appears when a resolved shear stress is applied. Under the action of this perturbation, the core distorts. The Peierls stress is evaluated as the applied stress for which no solution can be found.

In the initial literature on the subject, the rebound force was computed from the interplanar potential which was assumed to be sinusoidal [12]. An analytic solution can be obtained in this case. In later refinements, the rebound force was computed as the derivative of the $\gamma$-surface [6].

Let us return now to the central problem discussed in this article and consider an isolated, straight dislocation in an infinite crystal. When the Peierls stress is evaluated in atomistic simulations, a shear strain is applied in the direction of the Burgers vector until instability is reached and the dislocation core shifts forward by at least one inter-atomic distance. At the instability, the surrounding lattice is elastically distorted and hence the local bonding is different from that in the unloaded lattice. Nevertheless, when the Peierls stress is evaluated using the PN model and the atomistically-determined $\gamma$-surface, the interplanar potential is computed by shifting the two blocks of atoms relative to each other as rigid entities. Hence, this $\gamma$-surface includes only the contribution from the distortion of bonds in the glide plane. It is therefore more natural to consider a $\gamma$-surface in which the two blocks are allowed to deform elastically in response to the applied stress, with the relative shift being applied simultaneously. This generalized $\gamma$-surface (GGS) was used recently in the context of dislocation nucleation [13].

One may question the need to use the PN model when predicting the Peierls stress in situations in which atomistic simulations are feasible. However, atomistic models provide simply a number: the value of the critical stress. The PN model, although an approximation, provides more insight into the physics that determines the lattice resistance to dislocation motion. Specifically, one identifies the contribution of the bonds across the glide plane (when the classical $\gamma$-surface is used), that of the bond distortion elsewhere in the model (when the GGS is used), and the effect of the non-linearity of the elastic material behavior.

The present study outlines these contributions to the Peierls stress. Three strains are considered: two shear strains acting in the glide plane, one along and one perpendicular to the Burgers vector, and a normal strain acting in the direction of the glide plane normal. The model and procedures used are described in Section 2, the results are discussed in Section 3 and conclusions are presented in closure.

## 2. Model and simulation procedures

Silicon is represented with the three-body Stillinger–Weber (SW) potential which has been used extensively in atomistic simulations [14]. A large number of potentials have been developed for Si, the most broadly used being SW, Tersoff [15,16] and EDIP [17]. Each of these potentials has strengths and weaknesses. Godet et al. [18] compared the three potentials against ab initio data (density functional theory-local density approximation, DFT–LDA) specifically with respect to their performance with respect to large shear strains applied in the shuffle and glide {1 1 1} planes. They conclude that the SW potential better reproduces the ab initio results with respect to the smoothness and the amplitude of the energy variation, and the localization of shear in the shuffle set. The SW potential provides the best approximation of the maximum restoring force for the $\langle 1\,1\,0\rangle$ direction in the shuffle plane and the $\langle 1\,1\,2\rangle$ direction in the glide plane, and for the theoretical shear strength and the strain associated with this critical stress in both planes. The un-relaxed unstable stacking fault energy for traces in the Burgers vector direction is best predicted for the $\langle 1\,1\,0\rangle$ direction in the shuffle plane by the SW potential, and for the $\langle 1\,1\,2\rangle$ direction of the glide plane by the EDIP potential. The values of the relaxed unstable stacking fault energy are best predicted by the Tersoff potential in both these crystal directions. Based on these findings, we conclude that the SW potential is best suited to represent the phenomena discussed in this article.

Atomistic models are used to determine the $\gamma$-surface under specific applied strain states. The three far fields considered in this work are shown schematically in Fig. 1. Vector $s$ defines the interplanar shift in the glide plane and is always taken in the direction of the Burgers vector: $s \parallel b$, $|s|/|b| \in [0, 1]$. The far field strain, $\varepsilon$, loads the entire model, except the two atomic planes defining the glide plane, where the relative shift is entirely defined by $s$. If $\varepsilon = 0$, one recovers the configuration customarily used to evaluate the $\gamma$-surface (Fig. 1a); this situation is denoted as Case 1. Three other cases are considered: $v = \varepsilon \cdot n \parallel s \parallel b$ (Fig. 1b, Case 2), where the strain has exclusively a shear component in the glide plane and in the direction of the Burgers vector ($n$ is the normal to the glide plane), $v = \varepsilon \cdot n \perp b$ (Fig. 1c, Case 3), where the strain has a shear component in the glide plane and in the direction perpendicular to the Burgers vector, and $v = \varepsilon \cdot n \parallel n$ (Fig. 1d, Case 4), where the strain has only a component perpendicular to the glide plane. These are the three elementary distortion modes that can be applied relative to the glide plane and $b$.

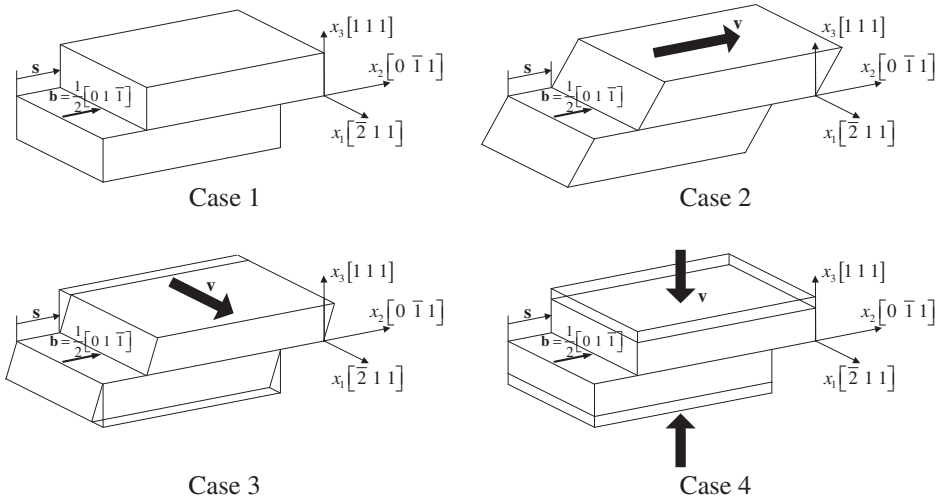


**Fig. 1.** Schematic representation of the loading conditions considered in this work.

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