Interaction of Dislocations on Crossed Glide Planes in a Strained Epitaxial Layer

K. W. Schwarz
IBM Watson Research Center, P.O. Box 218, Yorktown Heights, New York 10598
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The full three-dimensional Peach-Koehler formalism is implemented numerically and used to investigate encounters between threading and misfit dislocations in a strained epitaxial layer. The possible outcomes of such interactions are found to include blocking, binding, repulsive passage, and attractive instabilities. We show that blocking is a weak effect, and that the peculiar substrate pileup structures previously attributed to a "modified Frank-Read mechanism" are actually a natural consequence of having sources operating on intersecting glide planes. [S0031-9007(97)03439-X]

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The movement and interaction of dislocations over mesoscopic distances are fundamental to many phenomena in crystalline materials, ranging from the work hardening and fracture of bulk solids to strain relaxation processes in semiconductor heterostructures. Although the study of dislocations has been actively pursued for many decades, with both theory and experiment reaching a high degree of sophistication, quantitative comparisons between theory and experiment are often lacking, and even many qualitative observations are not well understood. This gap is due to the complicated nature of dislocation dynamics, which makes both analytical prediction and intuitive reasoning difficult.

A promising tool for establishing the desired qualitative and quantitative links between theory and experiment is numerical simulation. While considerable computational effort has been devoted to studying, e.g., dislocation core structures at the atomic level, attempts to calculate the behavior of dislocations on the micron scale have been surprisingly few [1–3], and have been confined to the simplest of problems. This has motivated us to develop a much more ambitious computational approach capable of dealing with arbitrarily configured, interacting dislocations characterized by any allowed Burgers vector and moving on any allowed glide plane [4]. In the present paper, we apply this approach to a problem of both fundamental and technological interest, namely, the dynamics of dislocations in a strained epitaxial layer. Although the discussion here emphasizes the fundamental problem of how to predict the evolution of a pair of interacting dislocations, we also obtain two specific results that are of immediate interest in that they call into question previous ideas of how a strained epitaxial layer relaxes.

The program in its present form implements the full three-dimensional Peach-Koehler formalism [5] to simulate glide of perfect dislocations described by isotropic, linear elasticity theory. Such a generic model is widely applicable and can be modified to apply more quantitatively to any particular system. For the special case of SiGe layers it is, for example, possible to take account of anisotropy and of the Peierls stress. These are expected to lead to relatively uninteresting corrections, however, and in particular there is no experimental evidence of Peierls stress effects at the high stress and temperature levels characteristic of this system. Similarly, although Gosling and Willis [6] have recently shown how one can in principle account for the effect of a free surface, we avoid this very complicated formalism either by treating capped layers, or by using an approximate image construction. On the other hand, once the core regions of dislocations in SiGe come very close to each other, the fact that they are substantially dissociated is likely to have a strong effect on their behavior. Thus, a more complete treatment of the attractive instabilities discussed below will require an extension of the program to include dissociation [3]. Similarly, an expansion to include the effects of intrinsic point defects on the dislocation motion is planned to enable us to address issues involving climb.

An elementary calculation [7] of dislocations moving in a strained layer on an unstrained substrate is displayed in Fig. 1. In general, dislocations can move easily only on the crystal planes of closest packing (*glide planes*), and can have only one of a small set of Burgers vectors, corresponding to the shortest lattice vectors in the glide plane. To orient the reader, the Burgers vectors and glide planes appropriate to the particular problem we will discuss are shown in Fig. 1(a). The behavior of a single Frank-Read source on a particular glide plane is then as shown in Fig. 1(b). As expected, a short segment of dislocation, pinned between two points [8] and under applied stress, grows around until it reconnects to itself, leaving an outwardly propagating loop and the original pinned segment. This process repeats to produce a series of propagating dislocations. The particular features that arise in the strained-layer environment include generation of a *misfit dislocation pileup* (M) as new loops push the earlier ones into the unstrained substrate, and the formation of the characteristic outwardly propagating *threading dislocations* (T) as the loops reconnect to the free surface.

The circumstances which lead us to investigate this type of problem are as follows. Layers of $Si_{1-x}Ge_x$ grown

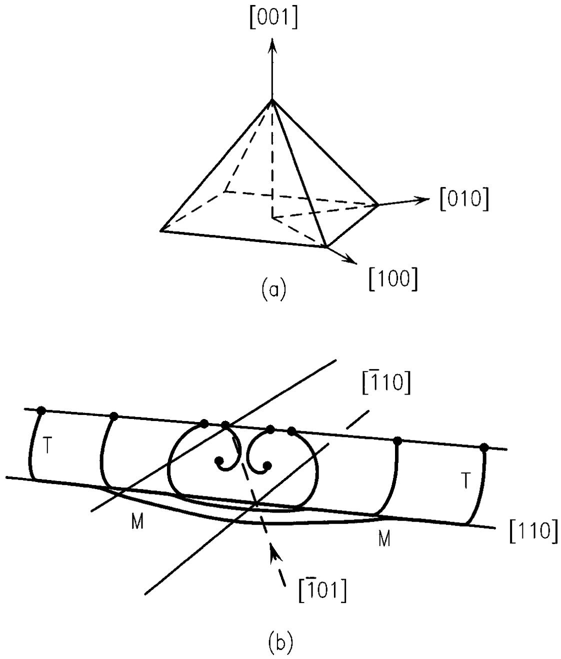

FIG. 1. (a) The pyramid shows the crystallographic directions appropriate to the fcc structure of Si. The base of the pyramid is parallel to the plane of the layer, which coincides with the [001] plane of the crystal. The faces of the pyramid define the {111} set of glide planes, while the edges coincide with the ⟨011⟩ set of allowed Burgers vectors. (b) Same-perspective view of a particular calculation showing the dislocation pattern generated by a Frank-Read source on the [$1\bar{1}1$] glide plane. The source generates threading dislocations which travel away, leaving behind misfit dislocations in the substrate. Dots mark where the source ends are pinned, and where the dislocations terminate on the free surface at the top of the layer. Also shown for later reference is the intersecting [111] glide plane, and the glide plane edge (dashed line) formed by the intersection.

epitaxially on a crystalline Si substrate (and other similarly mismatched epitaxial layers) are rapidly increasing in technological importance, and are currently the object of intense study [9–11]. $Si_{1-x}Ge_x$ having a different lattice constant from pure Si, such a layer will grow under strain if deposited on a Si substrate. When the mismatch is sufficiently great and the layer sufficiently thick, this strain will in general give rise to dislocations which move so as to reduce the strain. Ideally, dislocations such as those shown in Fig. 1(b) would be nucleated individually and travel to the edge of the sample along the various glide planes, leaving behind a two-dimensional array of misfit dislocations in the interface, and relaxing the strain in the SiGe layer without significantly degrading its electronic properties. In practice, large numbers of dislocations tend to be nucleated at once all over the sample, travel a relatively short distance, and become immobilized by various mechanisms which at present are only poorly understood. The result is a technologically useless layer filled with threading dislocations, with areal densities reaching 10^{12} cm^{-2}. In recent years, however, the idea of grading the Ge concentration has led to relaxed layers with threading densities below 10^6 cm^{-2}. This remarkable result has been produced both by a process in which weakly graded layers are grown at high (≈900 °C) temperatures [12], and by a process in which more strongly graded layers are grown at much lower (≈500 °C) temperatures [13,14]. In either case, it is not really clear what happens in the layers, and why such a remarkable improvement in layer quality is obtained. To our knowledge, the program described here is the first which allows one to study the interactions between threading dislocations and between threading and misfit dislocations on the various glide planes, and thus to approach this kind of problem from a fundamental point of view.

The present paper reflects our initial focus on the interaction between dislocations moving on intersecting glide planes, like the two shown in Fig. 1(b). Such dislocations will interact strongly only in the neighborhood of the edge formed by the intersection of the glide planes, with the situation most likely to occur being that in which a threading arm tries to propagate across a misfit dislocation left behind in the substrate by a threading arm that has previously passed by on the other glide plane. Even assuming that only stress-relieving 60° dislocations are involved, there are still sixteen possible encounters of this type, depending on which glide plane the misfit line is on, on the Burgers vectors of the two dislocations, and on the direction from which the threading arm is approaching the glide plane edge. Each case differs in detail, and there are a variety of possible outcomes. These are not obvious, and can be analyzed only in terms of the kind of calculations that are presented here.

One possibility that has been extensively discussed in the literature is the *blocking* of the threading arm motion by the misfit line [15,16]. Half of the encounters are characterized by a repulsive long-range interaction, so that it requires a strain greater than the critical strain [17] for the threading arm to approach the misfit line. If a fixed misfit line and a constant shape for the approaching threading dislocation are assumed, one finds that it requires a strain two or three times the critical strain to overcome this repulsion. This has led to the general impression that such blocking is a significant impediment to the movement of threading dislocations, and hence to the relaxation of strained layers. Our results indicate that this is never the case. The misfit line is readily pushed down into the strain-free substrate, and there is in fact no blocking effect at all unless a restoring force is applied to prevent this from happening. Since there is usually some small restoring force, e.g., from image effects, blocked stationary states can occur. However, even if the misfit line is held fixed, the approaching threading arm deforms readily in order to pass over it. This result was obtained previously [4] by means of the two-dimensional Brown formalism, and it provides a valuable check on the calculations to note that the results obtained with the three-dimensional formalism are in this instance identical. By calculating this deformation process for the various types of encounters, we find that blocking never occurs at strains greater than about 1.15 of the critical strain, and is thus a far weaker effect than has been estimated previously.

To see what can happen when blocking is overcome, we study the long-term outcome of the encounter $T^+[1\bar{1}1]\frac{1}{2}[\bar{1}01] \rightarrow M^+[111]\frac{1}{2}[\bar{1}01]$ at higher strain levels [18]. In this particular case, the threading arm passes over the preexisting misfit dislocation, pushing it down into the substrate [Fig. 2(a)]. Eight of the sixteen possible encounters have this general outcome, although each differs in detail. The other eight types of encounter exhibit a different behavior. To illustrate this, we discuss the important case $T^-[1\bar{1}1]\frac{1}{2}[\bar{1}01] \rightarrow M^+[111]\frac{1}{2}[\bar{1}01]$ in some detail. Here the long-range interaction is attractive, and there is no impediment at all to the incoming threading arm. Nevertheless, as one raises the stress above the critical value, one first finds that the approaching dislocation also stops in a stationary state [Fig. 2(b)]. This is now a *bound* state in which the two dislocations attract, but are kept from approaching more closely by the fact that each dislocation is constrained to move on its own glide plane. Such a state is somewhat different from a blocked state, in that the misfit line is not everywhere being pushed into the substrate, and no restoring force needs to be applied for the state to exist. Like blocked states, however, bound states are stable only up to about 20% above the critical stress. At higher stresses, the interacting threading-misfit pair experiences an *attractive instability* [Fig. 2(c)], the mutual deformation being such as to inevitably bring the two dislocations together at a point on the glide plane edge.

It is of course clear that the final stages of an attractive instability cannot be treated in terms of perfect dislocations and the continuum approximation. As the instability develops and the cores move closer together, the fact that the lines are substantially dissociated must eventually be taken into account, while the final stages of the instability must presumably be resolved at the atomistic level. What one can do in the present context, however, is to enact the allowed topological transition, and then to look at the subsequent evolution of the system. In the case of the $T^-[1\bar{1}1]\frac{1}{2}[\bar{1}01] \rightarrow M^+[111]\frac{1}{2}[\bar{1}01]$ encounter, where the two Burgers vectors are the same, the instability illustrated in Fig. 2(c) is expected to result in a reconnection. Figure 2(d) then shows that, if such a change is enacted, the subsequent effect is one of strong dynamical repulsion and the formation of *corner misfit* dislocations of various characteristic shapes. Thus, our computations predict that encounters of the type $T^-[1\bar{1}1]\frac{1}{2}[\bar{1}01] \rightarrow M^+[111]\frac{1}{2}[\bar{1}01]$, at more than about 20% above the critical stress, lead to a reconnective instability which is expected to eventually produce substrate configurations that differ drastically from simple dislocations pileups such as the one shown in Fig. 1(b).

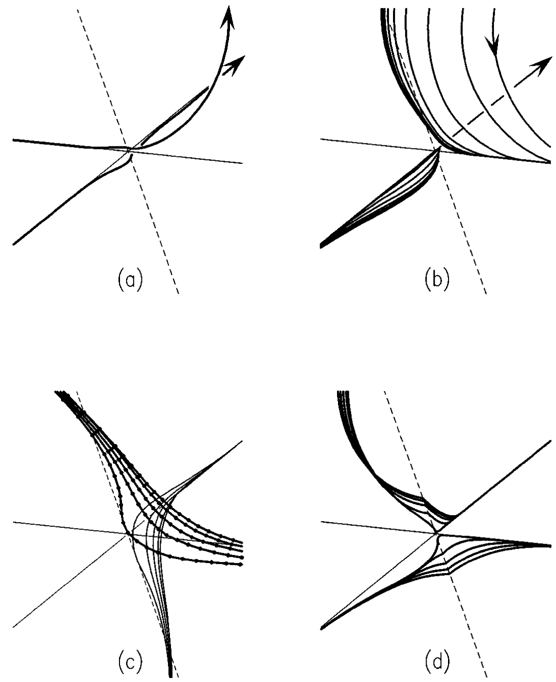

FIG. 2. Threading arm on the $[1\bar{1}1]$ plane approaching a misfit dislocation on the $[111]$ plane. For (a), (b), and (d) the region shown is a $\times 10$ magnification of the region where the $[\bar{1}10]$, $[110]$, and $[\bar{1}01]$ (glide plane edge) directions intersect at the bottom of the layer, as shown in Fig. 1(b). Figure 1(c) is magnified by a further factor of 20. This set of calculations was carried out for a symmetrically capped layer 1000 Å thick (critical strain $= 3.30 \times 10^{-3}$). (a) Repulsive passage of the threading arm over the misfit. The calculation is for a strain of 3.80×10^{-3}. Blocking (not shown) occurs only for strains below about 3.60×10^{-3}. (b) Stationary bound state formed when the threading arm approaches the misfit line from the opposite direction. The strain here is 3.60×10^{-3}. A sequence of states separated by equal time steps is shown. (c) Development of an attractive instability from the situation shown in Fig. 2(b) when the strain is increased to 4.50×10^{-3}. The two dislocations rush to meet at a point on the glide plane edge, and arrive oriented in opposite directions. The actual points representing the dislocation in the calculation are indicated for the threading arm. A sequence of states separated by equal time intervals is shown. (d) Rapid separation which occurs when a reconnection is made at the final configuration shown in 2(c). The reconnected dislocations now pass from one glide plane to the other, and form cusplike structures at the glide-plane edge as they move apart. Again, equal time steps separate the configurations shown.

Further discussion of the many different kinds of encounter is deferred to a later paper. Instead, we conclude by illustrating how the type of basic considerations illustrated in Figs. 1 and 2 are essential for understanding the more complicated phenomena that are expected to be important in strained layers. Consider two arbitrarily chosen Frank-Read sources on intersecting glide planes (Fig. 3). The dislocations emitted by such sources interact

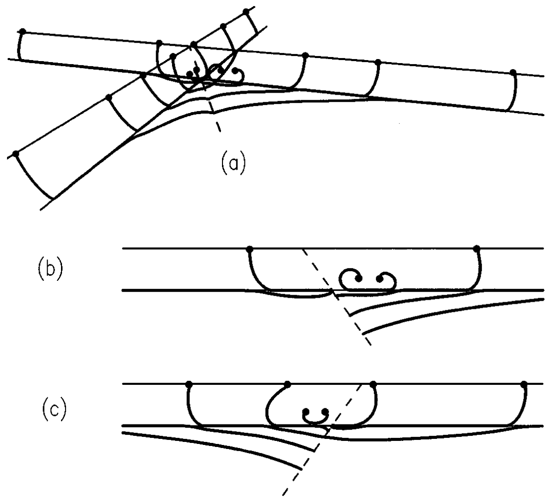

FIG. 3. Typical configuration produced by two Frank-Read sources on intersecting glide planes. The calculation was carried out for a film 5000 Å thick, under a strain of 4.00×10^{-3}. Dots denote the terminations of dislocations on the free surface of the layer or on the pinning sites defining the sources [8]. (a) Perspective view similar to Fig. 1(b). (b) View along the $[\bar{1}10]$ direction. (c) View along the $[\bar{1}\bar{1}0]$ direction.

as they pass the glide plane edge, combining the phenomena shown in Figs. 1 and 2 with other more complicated processes to form corner misfit pileups structures of various kinds. Such substrate structures have been widely observed, and have been attributed to the action of a special "modified Frank-Read mechanism" [13,14,19]. The results shown in Fig. 3 demonstrate rather strikingly that they are instead a natural consequence of having sources on intersecting glide planes.

In summary, a numerical study has brought out several new features of dislocation interactions which are expected to be important in understanding strain relaxation in epitaxial layers. We find that interacting threading arms and misfit lines can undergo a variety of fates including blocking, binding, repulsive passage, and attractive instabilities. The attractive instabilities will lead to reconnection, kink creation, and jog creation, depending on the Burgers vectors involved. Although many details will need to be sorted out to fully understand how a layer relaxes, two specific results already illustrate the usefulness of such calculations. First, we find that, contrary to previous claims, blocking effects are generally negligible. Secondly, we have computed the substrate dislocations patterns produced by two simple Frank-Read sources on intersecting glide planes, and find that they closely resemble certain experimentally observed patterns. The modified Frank-Read mechanism that had been proposed to explain such patterns is thus seen to be unnecessary.

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