Propagation of stacking faults from "composite" dislocation cores at low temperature in silicon nanostructures.

Julien Godet and Jacques Rabier
Institut Pprime, Département Physique et Mécanique des Matériaux, CNRS-Université de Poitiers, ENSMA, BP 30179, 86962 Futuroscope-Chasseneuil, Cedex 05, France
E-mail: jacques.rabier@univ-poitiers.fr

Abstract. The unexpected occurrence of extended stacking faults in silicon nanostructures at high stress and low temperature is discussed. It is shown that those stacking faults result from the operation of “composite” dislocation core structures. It is demonstrated that such cores allow for the propagation of partial dislocations in the shuffle set with the benefit of a low Peierls stress. A classical atomistic calculation confirms indeed that shuffle partial dislocations can move under a shear stress of about 3.3 GPa (5.5% shear strain) at room temperature.

1. Introduction

Silicon appears as quite a complex material owing the multiplicity of the dislocation core structures appearing from computations and high stress mechanical experiments [1]. The complexity arises already from the diamond lattice structure where two kinds of (111) slip planes appear having very different properties, as soon as the movement of dislocations is concerned. Indeed the shuffle set (widely separated atomic plane) sustains perfect dislocation with low Peierls stress, whereas the glide set (narrowly separated atomic planes) can host Shockley partial dislocations associated to high Peierls stress (figure 1). This frustration between perfect dislocation with large strain energy and low Peierls stress, and dissociated dislocation with lower strain energy but having high Peierls stress has prompted numerous discussions about core structures [1]. Among attempts trying to reconcile shuffle set and glide set properties, “composite” models were proposed [2,3] in which partial dislocation -with small Burgers vector and low strain energy- move in the shuffle set taking advantage of a low Peierls stress. These models were left behind when it was demonstrated that the dislocations were dissociated when moving at high temperature (>~700K) and consequently located in the glide set [4]. More recently, the evidence that perfect shuffle dislocations at low temperature were controlling the brittle regime does not bring any other argument favoring the existence of composite cores [1]. However, the recent unexpected observations at room temperature of stacking faults (SFs), dissociated dislocations together with perfect dislocations at high stress in low dimensions specimens [5-7] bear witness that this picture is oversimplified and different mechanisms should be operative in these deformation conditions. Indeed, new evidences of “composite” core structures distributed over glide and shuffle sets have been put forward [7,8]. The occurrence of these dislocation cores leads to the propagation of SFs in the glide set in stress and temperature conditions where they are not usually expected. After a short presentation of the early theoretical composite models, this paper discusses how composite cores promote the formation of extended SFs and a preliminary classical molecular dynamics simulation is performed to confirm the low Peierls stress associated to the movement of shuffle partials.
2. Early models of composite core theoretically predicted

Although looking for the dissociation of a shuffle dislocation seems unrealistic since no stable SF exists in this set, a dissociation associated to shuffle dislocations was looked for [2,3,9]. This dissociation leads to a SF in the glide set, bounded at one end by a Shockley dislocation and at the other end by a shuffle partial dislocation. The formation of this last partial requires a non-conservative atomic rearrangement. This dissociated shuffle dislocation or ‘extended shuffle dislocation’ [9], was described in two ways: either as a stacking-fault ribbon bounded by two Shockley dislocations of opposite sign associated with a perfect shuffle dislocation (figure 1.c), or as a dissociated glide dislocation in which one of the partials has emitted or absorbed a row of interstitials or vacancies (figure 1.d). In this paper, the terminology “composite core” was preferred being more general than extended shuffle dislocation and refers to a core structure which extents in several different sets.

Figure 1. Different types of dislocations: (a) perfect dislocation dissociated into two Shockley partials in the glide set (g plane); b: perfect dislocation in the shuffle set (s plane); (c,d) different construction models of composite core of 90° partial dislocation also named “extended partial shuffle dislocations”.

3. Composite cores resulting from high stress and low dimension plasticity

Evidences of composite core at high stress and low dimensions were given from atomistic computations. They have been found under two types: resulting from the occurrence of a zonal dislocation [8] or from the dissociation of a perfect shuffle dislocation into two partials belonging to two different sets [7]. Both mechanisms result in the formation of SFs at low temperature.

3.1. Zonal dislocation

This type of core is nucleated from a surface step when the crystal is solicited in compression and composed of two partial dislocations affecting two shuffle sets as well as the glide set in between [8]. It appears in very specific conditions: when the applied mechanical stress results in a local shear stress in the anti twinning sense. The movement of such a dislocation is achieved through cooperative atomic movements in two shuffle sets associated to a flattening of the glide set situated in between. This results in the apparent propagation of a partial dislocation with a 1/3<112> Burgers vector, a Burgers vector two times larger than that of the usual Shockley partial, but surprisingly leading to the extension of a unique extended SF in the glide set.

Affecting dynamically three planes and built with two partials dislocation gliding in two consecutive shuffle sets, this dislocation core can be seen as the core of a zonal dislocation [10]. It can be noted that the Burgers vector of this leading (“super”) partial can be decomposed in a perfect and a partial as follows: 1/3 $[211] \rightarrow \frac{1}{2}[101] + \frac{1}{6}[121]$. In that way, it can be viewed quite similarly as a “composite core dislocation” of one of the models describing an extended shuffle dislocation (see figure 1.c). However, as both dislocations do not elastically interact, once the movement of the zonal dislocation is interrupted, a perfect shuffle dislocation should be emitted under large apply stress, leaving behind a SF bounded by a Shockley partial despite the low temperature. This mechanism could explain why such zonal dislocations have never been experimentally observed.
Figure 2. Composite cores observed in simulations and their hypothetical dissociations. (a) zonal dislocation built with two $1/6<11\bar{2}>$ partials dislocation in the shuffle set (noted 1 and 2) associated with a rearrangement of the glide set (noted 3) [8]; (b) dissociation of a zonal dislocation in a shuffle perfect and a glide partial. (c) core of shuffle perfect dislocation that has been spread out on 3 shuffle and 2 glide planes (labeled S3) [11]. (d) S$_3$ core can be understood as a composite core formed by a shuffle partial and a glide partial [7]. (e) SF extension when one of the partials is emitted.

3.2. The dissociation of S$_3$ dislocation core

Shuffle perfect dislocations (at least the 60°) are known to carry the deformation but are unstable. When they stopped they can be converted in a core of lower energy that is sessile, called S$_3$ (figure 2.c) [11]. This dislocation can be viewed as a composite dislocation with incipient partials in the shuffle and one in the glide set (figure 2.d). Applying a larger stress on the S$_3$ dislocation leads usually to crack nucleation [12]. However, as the fracture stress $\sigma_F$ in nano-objects varies with the size (d), as $d^{-1/2}$ [13], this shows that a dissociation mechanism is favored over crack nucleation for low dimensions. Consequently, in nanostructures under large compressive stress and low temperature, perfect S$_3$ dislocations can dissociate into two partials with Burgers vector of the type $1/6<11\bar{2}>$, one of them belonging to the glide set, the other one to the shuffle set (figure 2.e). This results in the formation of an extended SF from a S$_3$ core at low temperature, the extension of the SF being performed by the displacement of the shuffle partial [7].

Here, two different dissociation mechanisms of composite core dislocations have been shown at the origin of SF extension at low temperature. The mechanisms do not require the movement of glide partial dislocations but only the mobility of perfect and/or partial shuffle dislocation. This result allows reconciling the presence of SF at low temperature in a domain on which the glide partials (known to extend SFs) have a very low mobility. Although a shuffle partial dislocation has been expected already to be involved in the formation of extended SFs [7], the Peierls stress on one kind of shuffle partial dislocation is investigated in the following section to check whether it can move at low temperature.

4. Peierls stress estimation at 300K

Atomistic computations were performed using a modified version of the Stillinger-Weber potential (see [7] for simulation set up). A composite shuffle partial dislocation was introduced in a periodic simulation box along $z$, by introducing a 60° perfect dislocation in the shuffle plane stacked on a 90° partial dislocation located in a glide set plane (figure 3). The movement of the partial in the shuffle set was evidenced under a shear stress as low as 3.3 GPa applied in the anti twinning sense at room temperature. This preliminary result proved that one time created this shuffle partial is much more mobile at low temperature than a glide one. Furthermore the atomic displacements found during the dislocation movement leading to the formation of extended SF bear witness of a shuffle mechanism occurring between the glide and the shuffle sets as it was assumed before [10].
5. Concluding remarks

While the extension of SF at high temperature in bulk silicon is associated to the mobility of glide partial dislocations, composite core dislocations spread out in glide and shuffle set planes, appear to be required to explain the presence of SF at low temperature. Indeed, in such low temperature range in which the glide partial dislocations exhibit a very low mobility, large stresses promote the displacement of perfect as well as partial dislocation in the shuffle set, provided those partials are issued from some composite dislocation core structures. The occurrence of composite cores comforts some of the early hypotheses about core structures of dislocation in silicon [2,3] leading to partial dislocations moving in the shuffle set. Two propagation modes have been reported in this paper: through the fusion of the planes of the glide set or by a shuffling between the two planes of the glide set. However, the formation of composite core structures reported here asks for specific conditions: a local anti twinning shear stress and a large compressive component in the applied stress. Those conditions are required for helping to the fusion of the glide set for the propagation of the zonal dislocation, and to favor the dissociation of the $S_3$ core. All these features (high stress, low dimensions, surface effects) suggest that composite core structures are likely to be efficient, beside other deformation mechanisms, in silicon nanostructures encountering large compressive stresses at low temperature, such as MEMS or NEMS devices.

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