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On the dislocation core structures associated to point defect cluster formation in diamond and silicon

Jacques Rabier*, Frédéric Pailloux, and Laurent Pizzagalli

Institut Pprime, Département de Physique et Mécanique des Matériaux, UPR 3346 CNRS, Université de Poitiers, ENSMA, SP2MI, BP 30179, 86962 Chasseneuil Futuroscope Cedex, France

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* Corresponding author: e-mail Jacques.rabier@univ-poitiers.fr, Phone: +33 549 496 732, Fax: +33 549 496 692

This paper focuses on the dislocation configurations that show up during the annihilation of a perfect dislocation vacancy dipole. Indeed unexpected transient dislocation core structures can be evidenced out of the atomistic structures computed during this annihilation process. Using the Geometric Phase Analysis these dislocation configurations can be analysed as partial dislocations, resulting from the dissociation of a perfect dislocation with ½[110] Burgers vector, bounding a nano crack (or a point defect cluster) along a (111) shuffle plane. Those partial dislocations appear as to be associated with an incipient dissociation/crack present in the core of perfect shuffle dislocations.

1 Introduction Since a long time dislocation glide in semiconductors with diamond structures have been thought to be convoluted with the emission of point defects [1]. This appears feasible when considering the different core structures available for dislocations [2]. Owing to the different sets where dislocations can glide in the (111) glide plane under different core structures, dislocation movement by glide was described by some shuffling between the glide set and the shuffle set associated to the possible emission of point defects [3]. This point was somehow clarified since it has been shown, for example in silicon, that perfect shuffle dislocations control plasticity at low temperature and high stress and dissociated glide dislocations the usual plastic regime [2]. However, some questions remain that are relevant to the cohabitation of point defects and dislocations. Indeed point defect clusters related to dislocation movements have been found to impact the physical properties of diamond and silicon. In diamond, point defect clusters associated to some dislocation mechanisms have been though to be responsible for the brown colour of plastically deformed diamond [4]. Trails have been evidenced in the wake of gliding dislocations in silicon [5], which have been attributed to some signature of point defects emitted by dislocations. In this context it is of interest to investigate the mechanisms involving point defects and perfect shuffle dislocations. We have recently investigated by atomistic computations the annihilation of perfect shuffle dislocation vacancy dipoles in diamond and silicon [6]. The results of these computations shed some light on a possible mechanism of point defect cluster formation related to dislocations. Indeed rather than annihilating without leaving any by-product, it was shown that below a certain distance (h_c) between the two parent dislocations of the vacancy dipole, the configuration of lowest energy is built with a cluster of vacancies that erases completely the deformation strain field of the dislocation dipole. This vacancy cluster can be also described as two internal (111) free surfaces or a nano crack. In this paper, the dislocation mechanism involved in such annihilation process is investigated in relation with the particular dislocation core structure that shows up during this annihilation process.

2 The calculation The starting configuration is a vacancy dipole built with two perfect shuffle dislocations. The two parent dislocations with ± ½ [110] Burgers vec-

tors glide on $(1\bar{1}1)$ plane and the dipole plane is (111). Those dislocations aligned along $[\bar{1}01]$ are 60° dislocations with S_1 core [7].

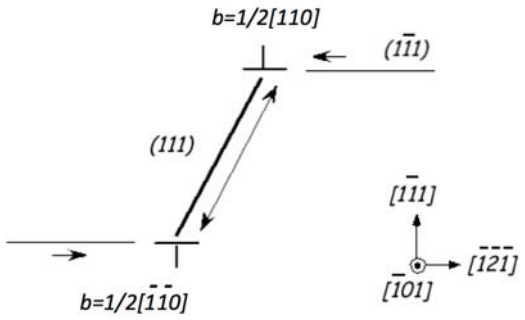

Figure 1 Dipole geometry.

The result of the calculations (in the case of diamond and using the Tersoff potential) is shown in Fig. 2 for a dislocation dipole whose height is such as to obtain a debris as the relaxed configuration with minimum energy. Starting from a perfect dislocation dipole configuration a debris having no strain field is obtained which can be seen as two internal (111) free surfaces. During such a relaxation process intermediate dislocation configurations are obtained. One of those intermediate configurations is shown in Fig. 2b.

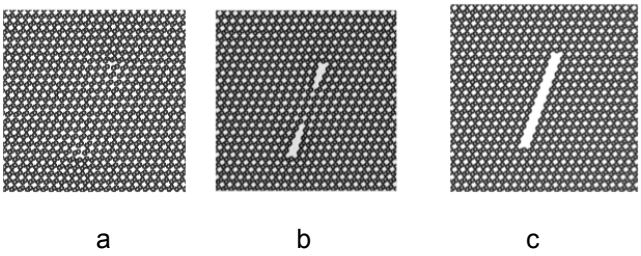

Figure 2 Dislocation configurations obtained in the course of the relaxation process of a dislocation vacancy dipole in diamond (Tersoff potential, h=2.6 nm < h_c). (a) Starting configuration, (b) intermediate configuration, (c) the fully relaxed configuration.

It appears that in the transient configuration the perfect dislocations building the dipole evolve into two dislocations showing a hollow core. This initiates the two internal free surfaces building the relaxed configuration of the dipole.

3 Results In order to understand the formation of the final relaxed configuration of the dipole and the transient core structure of the dislocations, the atomic configurations issued from the simulation were analysed using the Geometric Phase Analysis image-processing routine [8]. This image processing technique is currently used for quantifying lattice distortions in experimentally obtained High Resolution Transmission Electron Microscopy (HRTEM) images. Applied to the analysis of dislocations viewed edge-on [9], this technique has been shown to provide quantitative measurement of the strain field surrounding the dislocation core with an accuracy of 3 pm; the dislocation core showing up as a discontinuity in the phase-shift images (sharp phase-shift variation of 2π clockwise or counter-clockwise). Based on a Fourier Transform analysis of the contrast, this approach can however be applied to any image presenting a nearly periodic pattern. In our study we restrict the use of GPA to the localization of discontinuities (i.e. dislocation cores) in the patterns obtained from atomistic calculations.

The data processing is as follows. A numerical Fourier transform is applied to an atomistic configuration. Then using a Bragg filter, i.e. imaging with a xyz-diffracted beam, g, a xyz plane lattice fringe image of the configuration is obtained. The GPA analysis is applied to this last configuration. Using different g beams allows getting the Burgers vectors of the dislocations building the configuration.

Examples of such analyses are depicted in Fig. 3, where images have been built using, respectively, $\bar{2}42$ and 111 diffraction vectors. The first set of images shows two discontinuities whose separation distance diminishes during the annihilation process and these discontinuities finally disappear when the dipole is annihilated. In the second set of images, the positions of two discontinuities are quite stable up to they also disappear. Such discontinuities are consistent with the occurrence of two different types of dislocations, one type being mobile in the dipole plane. The final configuration is consistent with a perfect crystal with a significantly reduced residual stress field (discontinuities have vanished), the intermediate dipole configuration being built with two "dissociated" dislocations.

Consistent with the images of Fig. 3, it is proposed that in the intermediate configuration, each of the two perfect shuffle dislocations "dissociate" into a Frank partial and a Shockley partial following the reaction:

$$1/2\,[110] \rightarrow 1/3\,[111] + 1/6\,[11\bar{2}]\,.$$

The Shockley partial can glide in the plane of the dipole and these two partials bound a vacancy cluster or a crack of atomic dimension.

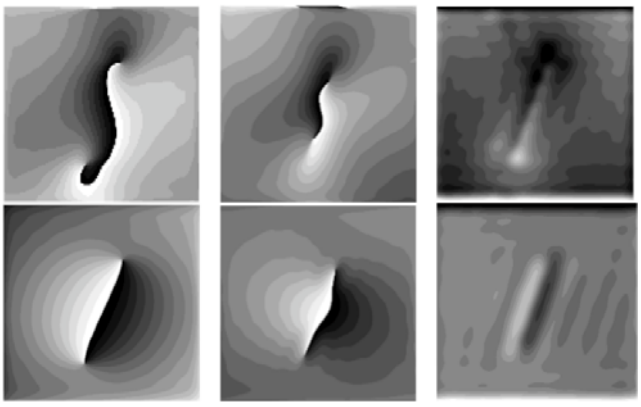

Figure 3 GPA analysis of the configurations of Fig. 2a, b, c using $\bar{2}42$ (upper figures) and 111 diffraction vector (lower figures). Phase-shift varies from 0 (black) to 2π (white).

The strain energy of each of these dissociated configurations has to be compared to the energy of the parent ½ [110] perfect dislocations. There is no gain in self energy (the partials have perpendicular Burgers vectors) and two "free" surfaces contribute to the energy. A gain in energy comes from the removal of the distorted crystal in the dislocation core and the associated modification of the strain field of the dislocations. These two partial dislocations are respectively a Frank partial and a Shockley partial. The first one cannot glide in the initial glide plane as well as in the dipole plane. The second one can glide in the dipole plane, a (111) shuffle plane. This "dissociation" in a shuffle set plane is somehow a paradoxical feature. However, such a "dissociation" does not yield to the creation of a stacking fault like in the glide set plane, but to a crack (or point defect cluster) in the shuffle plane.

Owing to the existence of this transient dissociated configuration, the formation of the debris can be re examined (cf. Fig. 4):

- The two parent dislocations dissociate as following:

$$1/2\,[110] \rightarrow 1/3\,[111] + 1/6\,[11\bar{2}]\,,$$
$$1/2\,[\bar{1}\bar{1}0] \rightarrow 1/3\,[\bar{1}\bar{1}\bar{1}] + 1/6\,[\bar{1}\bar{1}2]\,.$$

The two Shockley partials belonging to each parent dislocations are attractive and glide in the dipole plane where they can finally annihilate. During this process the crystal expands perpendicularly to the dipole plane yielding to the formation of a nano crack, which erases the strain field of the two Frank partials with opposite Burgers vectors. Such a mechanism is supported by the results of the GPA analysis on the evolution of the dipole configuration. Note that the sweeping of the dipole plane by Shockley partials is quite similar to what happen in the transformation mechanism of perfect loops into faulted loops in FCC metals (Saada [10]).

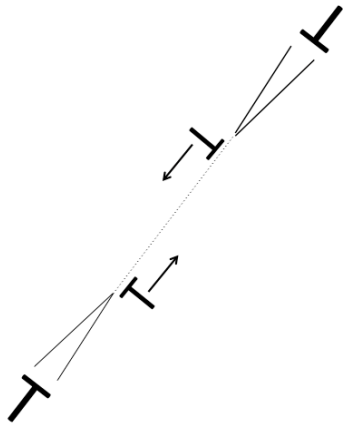

Figure 4 Scheme of the intermediate configuration of Fig. 2b. Each of the two parent dislocations dissociate into a Frank partial and a Shockley partial bounding a nanocrack (or a vacancy cluster). The two Shockley partials attract each other and annihilate.

4 Discussion It has been shown that transient cores appear in the dynamical process of the annihilation of vacancy dipole of perfect dislocations. Such core configurations are hollow and can be seen as being associated to a crack of atomic dimension or a cluster of vacancies. These metastable core configurations occur owing to the strain field of another dislocation at close distance. Such a core configuration is relevant to some incipient dissociation present in the core of each of the two perfect parent dislocations. This incipient dissociation expresses and get functional in the stress conditions of dipole annihilation. This behaviour has been already described for the dislocation cores of other materials such as MgO and alkali halides [11].

From the above analysis, the core structure of a perfect shuffle dislocation can be seen as being built with two supplementary (112) and (111) half planes. However, since when blowing up this configuration appears to be associated with the nucleation of a nanocrack, it is of interest to focus on the presence of an incipient crack in the core of perfect shuffle dislocations. Indeed, single cores with incipient nanocrack do exist in Si and diamond when the outputs of dislocation core computations [7, 12] are considered. This is shown in the case of diamond in Fig. 5.

This has to be brought together with the seminal paper of Haasen [13]. In this paper, Haasen is concerned with the thermal activation mechanism that controls dislocation glide of perfect shuffle dislocations. For this purpose the dislocation core is described using the nanocrack model: the configuration of a perfect shuffle dislocation is associated to a crack of atomic dimension which results from the directionality of the bonds and the fact that some bonds

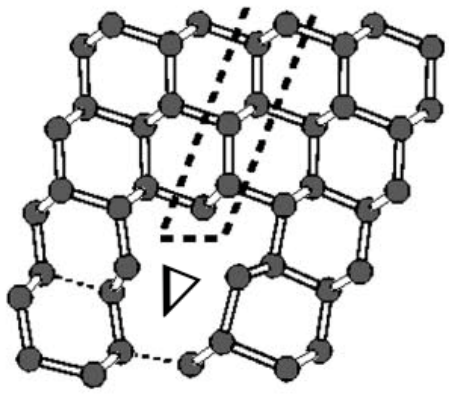

Figure 5 The core structure of 60° shuffle dislocation in diamond from [12], together with the indication of the incipient nanocrack.

undergo elongation more than 60% in the dislocation core. Consequently the movement of the dislocation in the glide plane involves the diffusion of the crack so that the dislocation glide is stress as well as diffusion assisted.

From these results, it is shown that dislocation core configurations of perfect shuffle dislocations in the diamond structure can be seen as being convoluted with some incipient nanocrack. Such nanocracks can propagate along a shuffle plane yielding to some dissociation of a perfect shuffle dislocation. The core of perfect shuffle dislocation convoluted to a nanocrack can evolve following two different ways: stay a perfect dislocation or behave as the nucleus for a nanocrack (or a point defect cluster). The evolution toward a nanocrack (or a point defect cluster) is expected to occur, not only in the course of dipole annihilation but also in the course of other dislocation mechanisms such as, for example, those related to the nucleation of dislocations and cracks in nanostructures [14, 15].

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