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Dislocation cores in semiconductors. From the « shuffle or glide » dispute to the « glide and shuffle » partnership

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Overview article

Résumé. — Les structures géométriques possibles du cœur des dislocations dans les semi-conducteurs élémentaires et composés sont envisagées et discutées à la lumière des résultats de travaux en MEHR et de calculs d'énergie de cœur. Il apparaît que le cœur des partielles a une structure complexe avec un caractère moyen « glide » mais contient un certain nombre de sites « shuffle » dont la nature dépend du caractère de la dislocation. On montre que les structures de cœur peuvent rendre compte qualitativement d'un certain nombre de résultats expérimentaux sur la mobilité des dislocations et les propriétés électriques.

Abstract. — Possible geometrical structures for dislocation cores in elementary and compound semiconductors are shown and discussed in the light of a review of recent work in HREM and core energy calculations. It appears that partial dislocations have complex cores, with an average glide character, but containing a number of shuffle sites, the nature of which depends on the character of the dislocations. These core structures are shown to account qualitatively for a number of experimental results on dislocations mobility and electrical properties.

1. Introduction.

The diamond cubic structure of elementary semiconductors (ESC) (Si, Ge, diamond C) consists of two interpenetrating f.c.c. lattices, displaced from one another by one quarter of the length of the cube diagonal. This structure can be regarded as a f.c.c. lattice with a two-atom basis. In compound semiconductors (CSC) of the III-V or II-VI families, the two atoms of the basis are of different natures, which gives in the case of the cubic symmetry the so-called sphalerite structure. An hexagonal structure is also found in CSC, where the stacking of close packed planes is ABAB... instead of ABCABC (wurtzite structure). This latter structure will not be discussed in this paper for the sake of simplicity. However results similar to those discussed here could be derived easily since the tetrahedral symmetry of the sp^3 bonding is the same in both structures.

Due to their f.c.c. lattices, the diamond cubic and the sphalerite structures have the same dislocation Burgers vectors $a/2 \langle 110 \rangle$ and the same slip planes $\{111\}$ as f.c.c. crystals [1].

Lang topographs and transmission electron microscopy (TEM) observations show that dislocations induced by deformation (except at high temperatures) are straight and aligned along the three $\langle 110 \rangle$ directions of the $\langle 111 \rangle$ slip planes, which is an indication of a high Peierls stress, and leads to hexagonal shaped loops, with two opposite screw segments, and four 60° segments. Both types have been shown to be dissociated into Shockley partials (two 30° partials for the screws, and one 30° and one 90° partial for the 60° dislocation).

Such a simplicity can lead to the idea that the core structure is as well defined as the dislocation structure. Several geometrical models have been propos-

ed and discussed, in particular by Hornstra [2], and by Hirth and Lothe [1], both for perfect and for dissociated dislocations. However, images in high resolution electron microscopy (HREM) are not fully consistent with any of these simple models, while measurements of dislocation mobilities and of electrical activity of deformed crystals [3, 4] give results of increasing and confusing complexity. A number of them leads to the feeling that, in spite of their « well defined » appearance, « pure » dislocations are difficult to isolate, the question whether the invoked impurities are actually foreign atoms [5] or intrinsic point defects being open [6].

Rather than an exhaustive review, this paper is more an attempt in taking most of these informations together, in order to give a critical and prospective look on the state of the art.

2. Geometrical models.

Due to the double layer atomic arrangement of the diamond cubic structure, two sets of dislocations with identical Burgers vectors can exist, depending whether the extra half plane ends between widely spaced (shuffle) or narrowly spaced (glide) pairs of $\{111\}$ planes. Hirth and Lothe [1] pointed out that dislocations belonging to one set can be transformed into the other set by absorption or emission of a row of point defects. A glide dislocation (G) can then transform either into a shuffle vacancy (S_v) or into a shuffle interstitial (S_i) dislocation by climb.

Mainly perfect dislocations have been discussed in this respect in the literature, since it is usually asserted that an eventual dissociation of shuffle (S) dislocations would lead to a high energy stacking fault, except if one of the partials belongs to the G set [7]. Some authors have pushed forward this argument to claim that observations of dissociated (and sometimes mobile) dislocations was a proof of their G character. This is probably why partial dislocations have been investigated under the implicit assumption that they were of the G type (atomic models, core energy calculations, ...).

Moreover, the usual terminology (glide, shuffle) lies upon the remark that the motion of the *perfect* S_i dislocation, called « shuffling », seems more difficult than that of the perfect G [1].

However, there is no reason to believe that dissociated dislocations are generated from perfect dislocations, usually and implicitly considered as a « reference state ». Dislocation sources can (and probably *do*!) produce directly dissociated dislocations, since dislocations have been shown to move in the dissociated state [7], and the argument that S dislocations are less mobile than G ones has to be reconsidered for partial dislocations. Shuffle partials can then in principle exist independently of an eventual initial perfect shuffle dislocation, and will be discussed here, as well as glide partials.

In addition, it is rather obvious that a *perfect* S_v dislocation does not differ from a perfect S_i one, lying on the adjacent parallel $\{111\}$ plane, as noticed by Hirth and Lothe [1] and discussed by Blanc [8]. One can transform indeed the latter into the former by addition of a *double* row of vacancies, which does not change the perfect dislocation core (this is equivalent to a climb of the dislocation onto the neighbouring slip plane) if relaxation and bond reconstruction is allowed. This equivalence does not hold any more in the dissociated state, since the positions of the partials with respect to the fault plane will change by climb. S_i and S_v partials will then be discussed separately here.

The 60° partial dislocation is sometimes invoked in the literature. Apart from the fact that long segments of this character are not observed, it can be described as a combination of 90° and 30° segments of atomic lengths, i.e. as a « completely kinked » 30° or 90° partial. Consequently it will not be examined here.

Figure 1 shows part of a dissociated dislocation loop, both partials belonging to the G set. The arms of the loop are along the three low energy $\langle 110 \rangle$ directions of the $\{111\}$ slip plane. As in the following figures, white and black atoms belong respectively to the two interpenetrating f.c.c. lattices and will be labelled A and B. This figure shows that, in CSC, core atoms of partial dislocations are always of the same chemical nature (A or B) along a given G partial. This chemical nature is opposite for the two 30° partials which make up the dissociated screw, but is identical for the 30° and the 90° partials of a dissociated 60° dislocation. The 60° dislocations lying on the opposite sides of the loop (i.e. separated by a screw dislocation) have opposite characters. 60° dislocations with core atoms of type A are referred to as β dislocations, or better A dislocations (and similarly for core atoms of type B). For details on this nomenclature formerly defined on shuffle perfect dislocations, the reader is referred to the introduction of the Hünfeld conference [9].

Fig. 1. — Dissociated hexagonal loop belonging to the « glide » set, in its $\{111\}$ glide plane. White and black atoms refer to the two interpenetrating f.c.c. lattices respectively.

We shall discuss now the different possible cores of the 30° and 90° partials which are schematized in figures 1 to 5, as part of a dissociated 60° dislocation. The Lomer dislocations which can be formed by reactions between 60° dislocations will be discussed further.

• 30° partial. — The core of a 30° G partial (Figs. 1 and 2) contains dangling bonds (d.b.) approximately parallel to the dislocation line (1 d.b. per site). The associated shuffle vacancy core S_v is obtained by removal of the « white » atoms A in the core (Fig. 3) which leads to a hollow core with 3 d.b. per site. A shuffle interstitial core S_i can be obtained from the G core by addition of interstitials B on the d.b.'s. of figure 2. This leads also to 3 d.b. per period, but it is remarkable that there is very little space left for such an insertion of interstitial atoms in a 30° G core, except if a strong distortion of the bonds between atoms A and B is allowed. If such a structure can be retained for a single S_i site on a G core, we propose an alternative and much more favourable configuration for a pure S_i 30° partial, or for a rather long

segment of S_i character on a 30° G dislocation. This structure is characterized by a zig-zag chain of AB atoms in the core, and illustrated in figure 4. This structure can exist in principle in three different and nearly equivalent orientations (Figs. 4a, b, c). In contrast with the single S_i site, this type of core does not need any noticeable distortion nor variation of bond length, but contains the same number of d.b.'s per period (three). If S_i sites have to exist along a 30° G core, as pointed out further in this paper, they would have a strong tendency to agglomerate in rather long S_i segments.

Fig. 2. — Dissociated « glide » (G) 60° dislocation. The stacking fault is intrinsic, and separates a 90° G partial (on the left) from a 30° G partial (on the right). The partial dislocations shown here are non reconstructed, and the cores contain dangling bonds (d.b.). The 90° core contains 2 d.b.'s per period ($a/2 \langle 011 \rangle$) along the line, instead of one d.b. for the 30° core.

Fig. 3. — Non reconstructed « vacancy shuffle » (S_v) partial dislocations, obtained from those of figure 2 by removal of a row of atoms in each of them. The row A of figure 2 has been removed from the 90° partial, but the row A' could have been removed as well. In contrast, only one possibility exists in the 30° core. The 90° partial contains 4 d.b.'s per site, instead of 3 for the 30° .

a

b

c

Fig. 4. — « Interstitial shuffle » (S_i) partial dislocations, obtained from those of figure 2 by addition of a row of atoms in each of them. The 90° core is overcrowded, but the three different zig-zag arrangements of the « semi-reconstructed » 30° S_i core (Figs. 4a, b, c) allow an easy insertion of the row of additional atoms without noticeable distortions of the tetrahedral bonding.

A possibility of rearrangement of the core can be obtained by bond reconstruction in some cases. This seems rather easy in the case of the 30° G partial (Fig. 5). The pairing of atoms resulting from this reconstruction doubles the periodicity of the dislocation core, which is of importance in calculations of the electronic energy of the structure (see § 3). The reconstruction of such a G core can exhibit some « antiphase » sites, called « solitons », each of them with a single d.b. (Fig. 6). These solitons have been invoked by Heggie and Jones [10] as preferential sites for double-kink (d.k.) nucleation. It is obvious from figures 3 and 4 that such a complete reconstruction is impossible for a shuffle core. However, a partial resonant reconstruction of d.b.'s in the 30° S_v core could be considered.

Fig. 5. — Reconstructed « glide » partial dislocations. The reconstruction of the 90° G core can be achieved by pairing the d.b. of atom (1) with those in (2) or in (3) (see also Fig. 6). Reconstruction does not change the period in the core of the 90° dislocation, whereas it doubles it in the 30° core.

Fig. 6. — $\{111\}$ projection of a dissociated reconstructed 60° G dislocation, showing a soliton on each reconstructed partial.

In the case of CSC, the core atoms of the 30° G configuration are of the same chemical nature (A for instance). For this simple reason, reconstruction is probably much less favourable in this case, unless some periodic distortions are allowed along the core, which have been shown to induce charge transfers, and could therefore favour some extent of reconstruction. In the two possible shuffle structures, in addition to the geometrical difficulty of reconstructing a 30° shuffle core, the core atoms are also of the same chemical nature (B in this case), which makes any reconstruction very unlikely.

● **90° partial.** — The core of the 90° G partial (Figs. 1 and 2) has a « double comb » structure, with d.b.'s on sites A and A', i.e. with two d.b.'s per period. The addition or the removal of a row of atoms also leads to a shuffle core, but the situation is more intricate than for the 30° partial. A S_v core can be obtained by removal of one of the two rows of core atoms A or A' (Fig. 3), leading again to two hollow cores, with 4 d.b.'s per period. A « super shuffle vacancy » dislocation, corresponding to the simultaneous removal of rows A and A' cannot be excluded, but seems very unlikely since it has 6 d.b.'s per period, and a very hollow core. However, a mixture of the two S_v types A and A' seems at all possible. Similarly, the addition of a

row of interstitials B bonded either to atoms A or to atoms A' leads to two S_i cores, each with 4 d.b.'s per period. As for the 30° partial, if no bond distortion is allowed, there is very little space for the extra atoms. If some distortion of A-B bonds can take place (Fig. 4a), B atoms can find more space in one of 3 equivalent sites around A'. But a less distorted configuration like that proposed in figures 4a, b, c, for the 30° S_i core cannot exist here. From this crude geometrical argument, it follows that a 90° S_i core is much less likely than a 30° S_i core. Again, a « super shuffle interstitial » 90° dislocation with 6 d.b. per period could be obtained in principle by addition of 2 rows of interstitials, one of them linked to atoms A, and the other to atoms A', but this structure is even more unlikely.

A reconstructed 90° G core is sketched in figures 5 and 6, where it appears that two equivalent types of reconstructions are possible, separated by solitons. In contrast with the 30° G core, the reconstruction does not modify here the periodicity along the dislocation line. From figures 3 and 4, it is clear that a complete reconstruction of a 90° shuffle core is impossible. However, a partial reconstruction of the 90° S_v can be imagined as in figure 7a, which gives a core somewhat similar to that of the unreconstructed 30° G partial (Fig. 2) with the exception of an extra d.b. out of the glide plane in the case of the 90° S_v core. This similarity with a 30° G core suggests a further reconstruction which doubles the periodicity along the dislocation line, as seen in figure 7b.

In the case of CSC the reconstruction of figure 7a still holds, but that of figure 7b in which atoms of equal nature would be bound together is less likely, except if a periodic distortion along the dislocation induces a charge redistribution between core atoms.

Fig. 7. — a) A possible partial reconstruction of the 90° S_v partial dislocation of figure 3. Due to the large distance between upper and lower d.b.'s a vertical reconstruction seems unlikely.

b) A further reconstruction can be achieved by pairing the d.b.'s in the glide plane shown in figure 7(a). This gives a configuration similar to a reconstructed 30° G core, shown in its $\{111\}$ plane, except that no shear is visible here due to the pure edge character of the partial, and that an extra non reconstructed d.b. is still present, out of the glide plane, and visible in figure 7(a).

Reconstruction of the $90^\circ S_i$ core seems even more unlikely for CSC than it was for ESC.

It must be noticed at this point that if a dissociated dislocation made of S_v (or S_i) partials of the types described above recombines, the resulting perfect dislocation will significantly differ from a shuffle S_v (or S_i) perfect dislocation of the type described for instance by Hirth and Lothe [1]. The S_v (or S_i) partials are indeed obtained from the G partials by addition of *one* vacancy (or *one* interstitial) per site. Consequently, after recombination, the perfect dislocation obtained will contain two vacancies (or interstitials) per site, instead of one for the shuffle dislocation described in [1]. Conversely, a perfect S_v (or S_i) dislocation in the sense of Hirth and Lothe cannot dissociate directly into two S_v (or S_i) partials, but only into one S_v (or S_i) partial and one G partial, but this does not preclude the direct formation of dissociated dislocations made of two pure shuffle partials, as already mentioned.

The reaction between two perfect dislocations can give a number of junctions among which the well known Lomer-Cottrell (LC) barrier. For instance, two perfect dislocations with Burgers vectors $\mathbf{AB}$ and $\mathbf{BD}$ (Thompson's notation, Fig. 8f) gliding in the same plane, can lead to an attractive glissile junction according to the reaction $\mathbf{AB} + \mathbf{BD} = \mathbf{AD}$ (1), but dislocations $\mathbf{AB}$ and $\mathbf{DB}$ would lead to the repulsive reaction $\mathbf{AB} + \mathbf{DB} = \mathbf{AD}/\mathbf{BB}$ according to Hirth and Lothe's notation [1] which is a $1/2 \langle 112 \rangle$ Burgers vector. An other repulsive reaction $\mathbf{BA} + \mathbf{CD}$ can take place. This leads to a $\langle 100 \rangle$ Burgers vector. These latter dislocations have been observed in subboundaries [11] but have never been mentioned within the grains of a deformed crystal. We shall focus our attention only on the Lomer-Cottrell lock, which forms by reaction (1), with a dislocation line along the intersection $\mathbf{BC}$ of the glide planes $\mathbf{ABC}$ and $\mathbf{BDC}$. Different possibilities of symmetrical and asymmetrical dissociations are schematized in figure 8, under the assumption that stacking faults are intrinsic. A symmetrical model for the non dissociated core has been first proposed by Hornstra [2], based on an association of a 5-atom ring and of a 7-atom ring. However, if we assume that the LC dislocation is the result of a reaction between two perfect glide dislocations, its core must contain an extra atomic column (Fig. 9a) as also proposed by Hornstra [2]. Some dissociated configurations of the LC dislocations are sketched in figures 8b to 8e according whether the reacting leading partials of the incoming dissociated dislocations are of 90° or of 30° character (see also Hirth and Lothe [1] p. 305). A possible core structure for the asymmetrical configuration of figure 8b is shown in figure 9b, and corresponds rather to an extended core than to a dissociation into a Frank and a 90° Shockley partials.

Possible cores for the dissociated configurations of

Fig. 8. — Different possible configurations of a Lomer dislocation of Burgers vector $\mathbf{AD}$, formed by reaction of dislocations $\mathbf{AB}$ and $\mathbf{BD}$, and lying along $\mathbf{BC}$.

The corresponding Thompson tetrahedron is shown in f. The stacking faults are always supposed to be intrinsic :

- a) non dissociated configuration,
- b) dissociated on one $\{111\}$ plane,
- c) acute angle dissociated configuration where two leading 30° partials have combined into a $\delta\alpha$ stair rod dislocation.
- d) acute angle dissociated configuration, where two leading 90° partials have reacted to give the $\mathbf{A}\delta + \alpha\mathbf{D} = 2\delta\mathbf{a}$ stair rod dislocation,
- e) obtuse angle dissociated configuration, where the leading $30^\circ \delta\mathbf{B}$ dislocation has reacted with the leading $90^\circ \alpha\mathbf{D}$ dislocation, giving the $\alpha\delta/\mathbf{DB}$ stair rod dislocation, which is not pure edge, in contrast with the previous ones.

figures 8c, d, e are shown respectively in figures 10a, b, c. Figures 8c and 10a correspond to a reaction between two leading 30° partials, resulting in a stair-rod dislocation $\delta\alpha = 1/6 \langle 011 \rangle$. If the 30° partials belong to the glide set the core of the stair rod dislocation contains the two extra atomic columns in dashed lines, and is then quite overcrowded. It would be even more forbiddingly compact in the case of two $30^\circ S_i$ partials. If the reacting partials have a 90° character, the resulting stair rod dislocation has a Burgers vector $\mathbf{A}\delta + \alpha\mathbf{D} = \mathbf{A}\alpha/\delta\mathbf{D} = 2\delta\alpha = 1/3 \langle 011 \rangle$ (Fig. 8d), and the corresponding core is shown in figure 10b (the atoms in dashed lines in the trailing 30° partials correspond to the glide set). In contrast with the above cases of figures 8c and d, where the angle between the stacking faults is acute, the reaction between a 30° and a 90° partial gives an obtuse angle between intrinsic stacking faults, separated by a $\alpha\mathbf{D} + \delta\mathbf{B} = \alpha\delta/\mathbf{DB} = 1/6 \langle 013 \rangle$ stair rod partial, the core of which is sketched in figure 10c.

This geometrical approach, although very rough, shows that a lot of different cores can be imagined as

Fig. 9. — a) Symmetrical core for a non-dissociated Lomer dislocation, shown non-reconstructed. The number of atoms in the core corresponds to a reaction between two 60° dislocations of the *glide* set. A decoration with bivalent oxygen atoms would reconstruct the d.b.'s into a zig-zag chain perpendicular to the plane of the figure. b) Asymmetrical extended core for the same dislocation. Again, oxygen atoms can saturate all the d.b.'s in the core.

well for the 30° as for the 90° partials. The simplest configurations are the glide ones, which can reconstruct at least in ESC. S_i cores are rather « overcrowded » and would be likely to exist only if distortions of d.b.'s are allowed, of the same magnitude than those necessitated for reconstruction of the 90° G partial, except for the 30° S_i partial for which 3 low distorted chain-shaped core structures can be imagined. S_v cores are rather hollow, and some relaxation of surrounding atoms has to be expected. The 90° partial has the particularity that two different S_i or S_v sites are possible. A mixture of all these configurations can be found in principle along the dislocation line, leading to quite a complex core structure, as it will be discussed below. Cores of perfect or dissociated Lomer Cottrell dislocations result from the shuffle or glide character of the reacting dislocations from which they are formed, which leads to a number of possibilities.

3. Observations in high resolution electron microscopy : core structure.

High resolution lattice imaging seems to be a fascinating technique to answer the question whether dislocations belong to the glide or to the shuffle set. However, in order to get reasonably safe con-

Fig. 10. — Cores of the Lomer dislocation dissociated in two $\{111\}$ planes, corresponding respectively to figure 8c (a), to figure 8d (b), and to figure 8e (c). Bonds shown in dashed lines correspond to stair rod dislocations formed by reaction between two leading *glide* partials.

clusions, results must be compared to simulations computed from geometrical models. Up to now, the 30° partial has been simulated in the G, S_i and S_v configurations, whereas the 90° partial has been simulated only in the glide case.

Although the first HREM images of the 30° partial given in the literature were in favour of a G core for ESC, a more detailed analysis leads to less straightforward conclusions [14]. The density of core atoms is found between 0.5 to 1.5 core sites. Furthermore, the core image (Fig. 11) is blurred, and cannot be simulated by rows of atoms perfectly parallel to the dislocation line. The contrasts obtained on different 30° partials also differ slightly from one another.

This suggests a complex core where parts of G , S_i and S_v cores alternate along the dislocation line.

In contrast, the images of 90° cores (Fig. 11) are remarkably reproducible and fit simulations made from the glide model computed by Marklund [15]. However, it must be emphasized that some S_v sites or segments distributed along the core are certainly not detectable.

Fig. 11. — HREM image of a 60° dislocation in Silicon. Close pairs of atomic columns appear in white.

These conclusions have been obtained on 60° dissociated dislocations in subgrain boundaries and in grains of deformed Si, and in subgrain boundaries in Ge. HREM has also been used to image dissociated 60° dislocations in compound semiconductors. In GaAs, the interpretation of the results obtained by Tanaka and Jouffrey [16] on the 30° partials remains delicate. Though the contrast in their « dark atoms images » is rather insensitive to extra atomic columns in the core, the images resemble those of a glide or of a shuffle core depending on the observed dislocation. Other images of dissociated dislocations have also been obtained in CdS [17], but for lack of focal series no interpretation could be achieved.

Lomer Cottrell dislocations have been found in subboundaries, and imaged in HREM [14, 18]. In this case, the images (Fig. 12a) are consistent with the asymmetrical structure shown in figures 8b and 9b, where the « stacking fault » extends only on one lattice period, rather than with the symmetrical core. In deformed crystals, the dissociated configurations shown in figures 8c (or 10a) and 8d (or 10b) have been evidenced (Fig. 12b). If the former one is stable as far as the elastic energy is concerned, the energy of the latter is larger. However, in order to transform into the former one it must pass through the recombined symmetrical core which is a saddle point between the stable configuration of figure 8c and the metastable configuration of figures 8d or 10b, which explains that both of them have been observed.

a

b

Fig. 12. — a) HREM image of a Lomer dislocation in a subboundary, in silicon (micrograph A. Bourret, CEN-G).

b) HREM image of a Lomer dislocation in deformed silicon where the two interacting partial dislocations were of the 90° type (see Fig. 8d) (micrograph M. Elkajbaji, CEN-G).

4. Energy calculations.

The structure and the energy of a dislocation core can be in principle computed if the interatomic potential is known. In the case of covalently bonded atoms, the potential most frequently used is the Keating's potential [19] which is governed by two parameters α and β . The former is related to bond elongation, and the latter to bond bending. Two sets of values have been used for α and β . The smaller value of β used in the so called modified Keating potential [20] leads to a less rigid potential (easiest bond bending) than in the other one, and fits better the experimental phonon spectra.

The two principal weaknesses of these potentials for this kind of application are (i) that the atoms are supposed to be tetracovalently bonded (this is not actually the case in a dislocation core) and (ii) that the absolute values of the computed strain energies and of the angular bond distortions depend strongly on the values chosen for α and β .

Nevertheless, Marklund [22] used these potentials to estimate the strain energy and to determine the atomic positions in the reconstructed and non reconstructed glide cores in ESC. These atomic positions were then used to compute the energies of the occupied electronic states in both types of cores. The bond distortions due to reconstruction increase the core energy, whereas the suppression of dangling bonds due to bond coupling decreases the energy. The balance between these two effects gives an indication on whether the core does reconstruct or not.

In the case of $30^\circ G$ and $90^\circ G$ partial in Si and Ge, the increase of strain energy due to reconstruction is obviously lower for the « softer » potential (modified Keating). In this case, the increase of strain energy due to reconstruction is found to be 0.3 eV and 0.1 eV per core atom for the 90° and 30° partials respectively [22], which is less than the energy of a dangling bond calculated as the difference in electronic energy between non reconstructed and reconstructed states, and found around 0.5 eV for both partials [23]. This is in favour of a reconstructed $90^\circ G$ core, and more definitely yet of a $30^\circ G$ reconstructed core. This stronger tendency of the $30^\circ G$ core for reconstruction is due (i) to a lower increase of strain energy, and (ii) to the fact that the Peierls transition which doubles the period along the line upon reconstruction changes a broad half filled electronic band covering the whole gap into a narrow filled band close to the valence band edge, and a narrow empty band close to the conduction band. The resulting electronic energy is then lower in the reconstructed case than in the unreconstructed one. In contrast the $90^\circ G$ core does not change its period upon reconstruction, but has twice as much unpaired electrons than the $30^\circ G$ core. Therefore, there are already one filled band and one empty band in the non reconstructed core. The slight shift of these bands upon reconstruction gives a gain in electronic energy lower than in the case of the $30^\circ G$ partial.

In the case of diamond, an attempt has been made to calculate the energy of a 90° partial [24]. In this case the bond bending parameter β is larger than in silicon, and an eventual reconstruction increases the strain energy, but this is balanced by the dangling bond energy which is about 2.4 eV, and reconstruction is again likely.

In the case of CSC, where the identical chemical nature of atoms in the core does not favour bond

reconstruction, Jones and Oberg [25] have shown that small alternate distortions, which increase (« out ») or decrease (« in ») the angles between the « broken bonds » and the back bonds, strongly affect the energy band positions, and can lead to some charge transfer between « in » and « out » core atoms, and consequently to a decrease of the electronic energy. Such a relaxation can be considered as a partial reconstruction of the core in the sense defined above. However, these conclusions are derived from total energy calculations on non-optimized core structures, and are tremendously sensitive to the parameters used in the tight-binding Hamiltonian. They must be considered more as general tendencies than as conclusive results.

The only estimate of the core energy of the Lomer dislocation was performed by Bourret *et al.* [14], using a modified Keating potential, to compare relaxed core configurations to HREM images obtained for subboundary Lomer dislocations. The asymmetrical configuration which is most often observed is found to have a much higher energy than the non-dissociated symmetrical core proposed by Hornstra [2], but it can be stabilized by impurities, all the more as Lomer dislocations in subboundaries are always found to be decorated.

The results summarized in this chapter must be used carefully, since either the electronic energies are computed on atomic configurations already optimized, or the whole energy is considered, but without any optimization. Up to now, no self consistent computation has been performed to derive both atomic positions and electronic states which minimize the total energy of a dislocation core.

5. Discussion.

5.1 STRUCTURE. — In the case of the 30° partial, it has been shown in section 1 that a G core, a S_v core and three equivalent S_i cores can be imagined without prohibitive bond distortions. Image simulations show that the presence of a number of S_v sites along the core is necessary to account for the weak contrast of the central row in HREM images. In the same way, the presence of S_i sites is necessary to explain the blurred core. The HREM images are indeed consistent with an occupation of core sites between 0.5 and 1.5 as compared to the G core (occupation 1). Although the presence of impurities in the core cannot be excluded, it is likely that the 30° core contains at least a mixture of S_i and S_v sites as previously predicted by Blanc for perfect dislocations [8], and also probably a number of more stable G sites produced by mutual annihilation of S_i and S_v sites migrating along the line. The blurring observed in HREM is concentrated in the slip plane which means that among the three possible S_i configurations those in the slip plane are favoured,

probably due to the details of slip mechanisms. S_i sites have a strong tendency to agglomerate into rather long segments, in order to give the structure in figures 4a, c. The gain in energy associated to the reconstruction of the remaining G core, at least in ESC, is also in favour of an agglomeration of G sites into segments in accordance with the high migration energy found for kinks : $W_m \approx 1.2$ eV [26, 27]. The S_v sites can be either dispersed on G segments (if the concentration of agglomerated G sites is high enough compared to S_i ones) or arranged in S_v rows.

Such a complex structure explains the observed contrasts in HREM and the difference observed between HREM images of different dislocation segments. The presence of reconstructed 30° G segments, leading to a band splitting, is in agreement with the large gap observed in Ge [28]. The S_v sites and S_i segments account for EPR results obtained by Alexander [29] and Weber [30] attributed by these authors to d.b., and by Marklund [22] to S_v site on G dislocations, but which could arise from S_i sites as well. The d.b. associated to these shuffle sites are also in accordance with the EBIC contrasts of partials dislocations observed by Ourmazd *et al.* [31].

Contrary to the previous case the 90° images are well defined and consistent with a G core. Interstitial atoms in the distorted sites mentioned in figure 4a would be detectable in HREM if their concentration were high enough. In contrast some S_v sites would not affect significantly the image. The 90° core is probably of G character, reconstructed on belief of Marklund calculations [22], and of the high values of kink migration energies, but containing probably some S_v sites. However if there is a thermodynamical equilibrium between point defects in the bulk and the G, S_v and S_i sites on the dislocation line as discussed by Blanc [8], the S_i sites which seem to exist in the 30° core in appreciable concentration might exist as well to some extent in the 90° core. We conclude then to a 90° G core with a number of S_v sites, but with very few S_i sites.

In CSC the few available HREM images do not disagree with a 30° core structure containing S_i segments and non reconstructed G and S_v sites, and with a 90° core structure with a non reconstructed G core and a few S_v sites, although the interpretation of the pictures is often delicate. If such a core has to exist, the dislocation charge would alternate along the dislocation line, according to whether the core is glide or shuffle. The experiments performed by Petrenko and Whitworth [32] on the charge carried through the crystal by dislocations in II-VI compounds give circumstantial evidence that moving dislocations belong to the glide set in the sphalerite structure. If the core were of shuffle character (S_i or S_v) the charge transfer would have the

opposite sign to that observed. This remark means that if the conclusions of Petrenko and Whitworth are correct, the concentration of G site in partials is larger than that of shuffle ones as well for the 30° as for the 90° partials.

5.2 MOBILITY. — The experimental results obtained on mobility can now be reexamined in terms of the above conclusion that dislocations have variable cores. Dislocation mobilities are governed, at least at low and intermediate temperatures, by nucleation and propagation of d.k.'s. Most of the models given up to now to account for the mobility of perfect or dissociated dislocations assumed that they have a unique core structure all along the line. We shall discuss here the influence of S_v or S_i sites on d.k. nucleation and on kink migration on both types of partial dislocations.

Fig. 13. — Nucleation and expansion of a double kink at a S_v site on a reconstructed 30° G partial, which can be analysed as elementary steps of diffusion of the vacancy in the core. One of the kinks migrates with the vacancy (111 projection).

Jones and Heggie [10] have shown that solitons can be preferential sites for d.k. nucleation on a G partial, since some bonds are already cut. This is also realized on shuffle sites, as can be seen for a S_v site on a 30° G partial in figure 13 : a d.k. is nucleated on a S_v site, and one of the kinks propagates by simple core diffusion of the vacancy. A double S_v site is even more favourable as can be seen in figure 14.

In the case of a 90° reconstructed G core, the d.k. nucleation is even more easy than in the 30° case since a single S_v site is already an elementary d.k. (Fig. 15). The d.k. is in the forward or in the backward direction of motion, depending on whether

Fig. 14. — Nucleation and expansion of a double kink at a double S_v site on a reconstructed 30° G partial. The dislocation moves in the « glide » plane by zipping of « shuffle » kinks (see text) (111 projection).

Fig. 15. — Nucleation and expansion of a double kink at a S_v site on a reconstructed 90° G partial. In this case, the S_v site is *already* an elementary double kink, which can be in the « forward » or in the « backward » direction according whether the S_v site is on one of the two rows labelled A and A' in figure 2 (111 projection).

the S_v site lies on sites labelled A or A' in figure 2. The kink propagation takes place here also by diffusion of the vacancy along the core, in a similar way than in the 30° core.

However, some difficulties arise in the case of a 30° partial, since we have seen that some S_i segments might exist along the line. A d.k. formed on a S_v site of a G segment is made of one 30° kink and one 90° kink. If the vacancy is carried by the 30° kink, the 90° kink will stop as soon as it meets a S_i segment (of 30° character), failing which it would transform into a high energy 90° S_i kink. In contrast,

if the vacancy is carried by the 90° kink, the kink will stop as soon as its vacancy annihilates with the first S_i site it meets, or it will eventually propagate with its vacancy through the S_i segment. But the eventual pinning of 90° kinks on S_i segments cannot impede the motion of the 30° partial, which can proceed by migration of 30° kinks, as shown in figure 16.

Fig. 16. — Propagation of a double kink along a 30° partial containing G (or G + S_v) segments (—), and S_i segments (=). The 90° kinks stop at the extremities of the S_i segments, whereas the 30° kinks can zip along them.

Now, if a d.k. was to be nucleated directly on a S_i segment, a vacancy (i.e. a G site) would be necessary to facilitate the nucleation of the 90° kink which cannot be of 90° S_i type. This kink will then migrate with its vacancy along the S_i segment.

The existence of S_v sites on 90° partials and on 30° partials appears then to be favourable to d.k. nucleation (probably more on the 90° partial than on the 30° one, in agreement with TEM observations which show that 30° partials are straighter than 90° ones [33]), and also favourable to kink migration.

This conclusion can be supported by a very simple physical argument. Dislocation glide tends indeed to satisfy two contradictory criteria :

(i) The ratio b/d_{hkl} (which measures the « lattice friction ») must be a minimum. This is realized in semiconductors for glide on the widely spaced « shuffle » planes, rather than on the narrowly spaced « glide » planes.

(ii) Partial dislocations cannot extend stacking faults in « shuffle » planes, which would lead to high energy faults, but only in « glide » planes.

This contradiction could lead to the conclusion that dislocations move in the shuffle non dissociated state, which is not verified by experiment, or that criterion (i) is not verified for glide of dissociated dislocations. In fact, it can be noticed immediately that glide of a dissociated G dislocation by nucleation and migration of shuffle kinks satisfies both criteria, since partial dislocations actually move on the low energy stacking fault plane (criterion ii), but through a step by step motion of a kink in the shuffle plane which minimizes the b/d_{hkl} ratio (criterion i). This argument shows why there is such a strong interaction between point defects and dislocation mobility in semiconductors.

In addition several features of dislocation mobilities reported recently can be explained at least qualitatively on the basis of this assumption, such as the slowing-down of 60° dislocations, the mobilities of the different partials as a function of their 30° or 90° character and of their leading or trailing position, the deviation from Schmid's law, the asymmetry of the velocities at reversal of the applied stress etc.

Two phenomena can modify the concentration of S_i and S_v sites in the core of partials :

(1) If d.k. nucleation is helped by S_v sites and if kinks migrate essentially by S_v diffusion along the core, then the S_i and S_v sites on the 30° partial annihilate during motion and the 30° core tends to have an increasing G character. In contrast and for the same reason, in the 90° core, which is assumed to contain very few S_i sites, the initial number of S_v sites is approximately conserved during motion.

(2) We shall assume, in addition, that a concentration c^B of vacancies is present in the bulk. This concentration can be much larger than that of thermal vacancies. Indeed a simple estimate of the vacancy concentration induced by deformation can be obtained by considering the number of vacancies produced by forest cutting and subsequent jog dragging. With a total dislocation density of about 10^8 cm^{-2} , and a strain corresponding to the displacement of a dislocation between two adjacent forest trees ($\epsilon \approx 4 \times 10^{-4}$), one obtains $c^B \approx 4 \times 10^{-4}$, instead of $c_{th}^B \approx 10^{-14}$ for the thermal concentration of vacancies in silicon at 900 K with a formation energy of 2.5 eV [34]. These point defects can be absorbed by the leading partial of the dislocation but not by the trailing one, if their mobility is low enough.

In the 90° *leading partial* the effects (1) and (2) lead to an increase of the number of S_v sites which first increases the mobility since they are nucleation and migration sites for d.k. But after a while, their concentration becomes so high that the dislocation turns into a S_v dislocation with some G sites. A motion of a shuffle partial by means of S kinks violates criterion (ii) and by means of G kinks violates both (i) and (ii) criteria. The velocity of the 90° partial then decreases.

In the 30° *trailing partial* only effect (1) is efficient and leads gradually to a G core with very few S_v (and S_i) sites. The mobility decreases moderately. The resulting 90/30 dislocation has then a mobility given by

$$\frac{1}{\mu} = \frac{1}{\mu_{90}} + \frac{1}{\mu_{30}}.$$

Its velocity decreases when it moves along x and the stacking fault is rather wide (6) as long as $\mu_{90} > \mu_{30}$.

In the 30° *leading partial*, S_i and S_v concentrations decrease due to effect (1), but the decrease of

S_v sites is more or less balanced by the bulk vacancies collected during motion (effect 2). The mobility of the 30° leading partial is expected to be stationary.

In the 90° *trailing partial* effect (1) does not change S_v concentration. The mobility is constant.

The resulting 30/90 dislocation has then a mobility which does not change drastically with the displacement x , which agrees qualitatively with the results obtained by Alexander *et al.* [6].

The effect on mobilities of the non-shear component of the stress tensor, or in other words the deviation from Schmid's law [6], could be attributed to an increase of the concentration of S_v sites and a decrease of that of S_i sites in tension, and conversely in compression, with obvious consequences on mobilities according to the above discussion. The stress exponent of the velocity law should be reexamined in terms of conservative point defect diffusion in the core.

Nikitenko *et al.* [35] mentioned a strong increase of 60° dislocation velocities caused by an inversion of the applied stress. They proposed an explanation based on a breaking away of the dislocation from impurity atoms which have been swept up during the initial motion in the glide plane. This explanation still holds if impurity atoms are replaced by a large amount of vacancies swept up during motion. At the stress reversal, the bends on both sides of the dislocation become unstable and catch up suddenly, leaving a row of vacancies at the place where the dislocation stopped. The dislocation is restored from a nearly shuffle into a nearly glide configuration, and moves back much faster on a slip plane free from vacancies.

In addition, the mechanism of vacancy enhanced dislocation mobility discussed above could be used to explain some results on electrical activity observed after deformation. It can be noticed that when a dislocation loop expands and sweeps up vacancies lying in its slip plane, the collected vacancies must be redistributed on the dislocation length, which leads sooner or later to a saturation, whatever the bulk vacancy concentration might be. The resulting S_v sites migrate with kinks along the dislocations, and accumulate at bends where kinks from different straight dislocations annihilate with one another [36]. This seems to agree with the particularly high electrical activity mentioned for 60° *partial* dislocations found in bends [22, 37]. The bends get readily saturated with vacancies and must eject the extra ones in the bulk, which is a possible mechanism of point defects agglomeration by plastic deformation [6].

In the above discussion, point defects were assumed to be already present in dislocation cores, which accounts for HREM images and mobility behaviour. However, it is perhaps more reasonable

to imagine that dislocations at rest tend to minimize their energy by core reconstruction, which can take place extensively only in a G core. Under stress, a 30° G partial will then create shuffle sites in its core following the reaction.

$$2 G = S_i + S_v$$

and this will lead to a mobile 30° core, with an average G character, but with a number of shuffle sites. A similar reaction could take place in a 90° core, but there is very little place for S_i sites. S_v sites can then be nucleated in the 90° G core only by a simultaneous injection of interstitials in the bulk. This could be a possible explanation for the point defects creation due to plastic deformation mentioned for instance in [6], although an extensive creation of point defects by jog dragging for instance remains quite likely (see § 2, mobility).

In non doped CSC, it is known that the velocities of dislocations depend strongly on their types ($V(\alpha) > V(\text{screw}) > V(\beta)$) [38-41]. This could be accounted for in a similar way: the vapour pressure of the B element is usually larger than that of the A one (at least in III-V A-B compounds), which leads to a tendency for understoichiometry of B. If dislocations belong preferentially to the glide set, α dislocations are split into two glide partials with B cores (see Fig. 1). These B core are understoichiometric, i.e. can contain a number of S_v sites. This is not the case for β dislocations which have a A core, the situation for screws being intermediate since they are split into a A partial and a B one. α dislocations (with B cores) are then much more mobile than the others, according to the previous assertions.

Dislocations in CSC are also known to move very easily during observation in an electron microscope operating at a voltage which is in most cases larger than the radiation damage threshold [38, 41]. This is also in agreement with the model.

Finally, it must be noticed that the mechanism of core diffusion invoked above might be responsible of the creation of antisite defects in CSC.

6. Conclusion.

To conclude, we would like to unsettle a number of more or less « well established » assertions, to summarize some original conclusions deduced from the above analysis, and to suggest further investigations.

(i) In contrast with what was assumed so far, shuffle partials must be considered without any reference to an hypothetic perfect (shuffle) dislocation from which they would have been formed. This means for instance that the two partials of a dissociated dislocation are allowed to collect (or nucleate) in their cores a number of point defects (or shuffle sites) much larger than that could be contained in the core of the corresponding recombined perfect dislocation.

(ii) In a same way, dissociation is not synonymous with glide set. A stacking fault lying between narrowly spaced planes, i.e. in a « glide set » plane, can be bounded either by glide or by shuffle partials, or by any mixture of these two types.

(iii) There is a reasonable evidence that the core structure is not unique along a given partial. « Glide » segments predomine, which are probably reconstructed in the case of elementary semiconductors, but in association with a number of shuffle vacancy sites (on 90° partials), and of shuffle vacancy and shuffle interstitial sites (on the 30° partials).

(iv) Glide is not necessarily easier for a « glide set » dislocation than for a « shuffle set » one. Glide on a « shuffle » plane minimizes the « distortion ratio » b/d_{hkl} , while glide of dissociated dislocations must take place in a way which keeps the stacking fault in the « glide » plane. This apparent contradiction can be removed by a double kink mechanism, in which the « shuffle » character is localized on kinks which zip along a « glide » core, in agreement with (iii). The migration energy of kinks should be related in this case to the pipe diffusion energy of point defects. This mechanism is fundamentally different from climb, since point defects are not used up here, but travel to and fro in the dislocation core in a conservative way.

(v) There is a lot of possible mechanisms for nucleation and absorption of point defects at the dislocation core, which can account for a number of experimental facts, both on dislocation mobilities and on the strain dependence of some electrical properties of semiconductors. The double kink nucleation energy should be related to the characteristic saddle point energies of these processes.

However the situation is still far from being clear, and further high resolution imaging of dislocation cores would be desirable. In particular, some new high resolution microscopes operating at high voltages (300, 400 or 1 000 kV) could give crucial informations on dislocation core structures, mainly in Ge which is less sensitive than Si to radiation damage. More detailed core images of the different types of stair rod dislocations would be quite interesting, since their core occupancy is fairly sensitive to the glide or shuffle nature of the leading partial dislocation from which they have formed. Compound semiconductors are very sensitive to high energy electrons. However, a better control of defocus conditions can help in obtaining images easier to analyse (in particular « white atoms » images).

Core energy calculations which have been focussed so far on glide set dislocations should be extended to shuffle cores of partial dislocations, to stair rod dislocations, and to shuffle kinks on glide dislocations.

Velocity models should be reconsidered in terms of point defect nucleation or collection in the core, and of core diffusion of kink-vacancy (or perhaps kink-interstitial) complexes, and interpretations of electrical measurements on deformed crystals should be reconsidered under this point of view.

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