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A step associated with the $\Sigma = 19\ (2\bar{5}30)$ tilt boundary in GaN

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Abstract

We have investigated the atomic structure of the $\Sigma = 19\ (2\bar{5}30)$ tilt boundary with a step at the interface by combining high-resolution electron microscopy and simulated images from the relaxed structures obtained using an empirical potential of Stillinger–Weber type. Two relaxed structures composed of two parts adjacent to the step were obtained. Each part can be formed either of a mixture of six-atom and five/seven-atom rings (5/7-interface) or a mixture of six-atom and four-atom rings (4-interface). The energetic calculations show that the atomic structure of the grain boundary made up of a 5/7-interface and a 4-interface to the step is more favourable. Comparison with the experimental image is proposed.

1. Introduction

Inside gallium nitride layers the density of threading dislocations can be higher than 10^{10} cm^{-2} except in more sophisticated growth modes such as ELO (epitaxial lateral overgrowth) characterized by a density in the range of 10^5–10^6 cm^2 [1]. The properties of the materials depend strongly on the nature and density of defects. It is then important to understand theoretically the atomic structure of the defects in order to get information on their electronic characteristics. The atomic structure of $(1/3)\langle 11\bar{2}0\rangle$ edge dislocations was analysed by high-resolution electron microscopy [2]. Three configurations were found corresponding to cores with 4-, 8- and 5/7-atom cycles. The 4-atom ring structure was only detected in high-angle grain boundaries. The 8- and 5/7-atom structures were found with at least the same frequency in good quality layers. The occurrence of these different cores was explained by considering the position of the dislocation line in the unit cell of the wurtzite structure [3].

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In this work, we extend our analysis of interfacial defects on periodic tilt boundaries. On the basis of experimental and simulated images, it is shown that these grain boundaries may be described in terms of structural units corresponding to 4-, 8-and 5/7-atom cycles. The connection between energetically degenerate interfaces formed by such structural units and the formation of associated defects such as steps is discussed. The analysis is applied to a $\Sigma = 19\ (2\bar{5}30)$ grain boundary generated from a tilt around the [0001] axis.

2. Computational methods

Extended details of the computational methods can be found in [4] for the tilt boundary modelling and in [3] for the interatomic potential for force calculations; here we recall the main lines of the procedure.

The starting configuration of tilt boundary is obtained on the basis of the dichromatic complex and coincidence site lattice (CSL). The former can be viewed as an interpenetrating network of two crystals, white (λ) and black (μ), one being rotated by an angle α around [0001]. The interface plane of the bicrystal can be chosen among the planes of the CSL. In the present work, we only study the interface plane of shortest period and we have considered all possible cells of non-identical displacements (CNID) to ensure that all possible starting configurations were taken into account [5]. For a structure with a multiple-atom basis these configurations depend on the atom types in relation to the upper (λ) and lower (μ) crystal along the interface [6]. In the case of the hexagonal structure with a two-atom basis (a-type and b-type), the number of CNIDs for each interface is 4. The individual cells, in the four CNID sets, can be designated by a(λ)/a(μ), b(λ)/b(μ), a(λ)/b(μ) and b(λ)/a(μ). As regards the $\Sigma = 19\ (2\bar{5}30)$ tilt boundary, for symmetry reasons, the a(λ)/a(μ) and b(λ)/b(μ) CNIDs are identical and so are the a(λ)/b(μ) and b(λ)/a(μ) ones. For a given CNID, the starting atomic structure is obtained by discarding the white crystal (λ) below the interface and the black crystal above (μ).

The potential model used is one of the more suitable empirical potentials (Stillinger–Weber) for calculating atomic structures in semiconductors [7–9], modified to take into account the different possible interactions in GaN, namely Ga–N, Ga–Ga and N–N [3, 9]. Previous calculations of dislocation cores in silicon have shown that this potential may artificially favour overcoordination [10].

The structure of minimum energy of the interface was found by calculating the corresponding γ-surface by applying relative displacements parallel to the boundary. The relaxation procedure is a combination of the conjugate gradient method and the quench–molecular dynamics method. The relaxation finished when the temperature was smaller than 10^{-6} K.

3. Results and discussion

In recent reports [4, 11, 12], the atomic structure of several tilt boundaries with misorientation angles from 9.4° to 44.8°, including the $\Sigma = 19\ (2\bar{5}30)$ tilt boundary, have been analysed.

The relaxed structures of lowest energy are shown in figures 1(a) and (c). We point out that the starting configuration from the a(λ)/b(μ) CNID gives rise to an interface with 5/7-coordinated rings (5/7-interface; figure 1(a)),whereas the b(λ)/b(μ) CNID gives rise to an interface with 4-coordinated cycles (4-interface; figure 1(c)). Similar results have been obtained for $\Sigma 37\ (3\bar{7}40)$ and $\Sigma 7\ (1\bar{3}20)$ [11]. The connection between energetically degenerate interfaces formed by these structural units results in the formation of a step at the interface. The energy calculations indicate that the 5/7-interface ($\Delta E = 1518$ mJ m^{-2}) is energetically

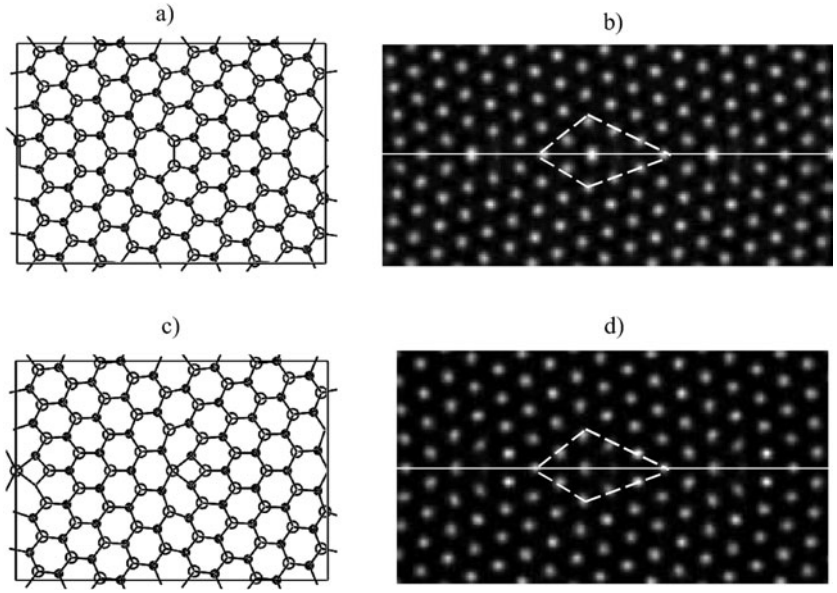

Figure 1. Atomic structures of the $\Sigma = 19$ ($\theta = 13.4°$) $(3\bar{5}20)$ tilt boundary. The structure in (a) is obtained from a starting configuration formed by the a(λ)/b(μ) CNID whereas the structure in (c) is obtained from b(λ)/b(μ). (c) The simulated image of the structure in (a). (d) The simulated image of the structure in (b). For all the figures, the full circles represent N atoms and the open circles the Ga atoms. A unit cell corresponding to one period is shown in the simulated image.

more favourable than the 4-interface ($\Delta E = 1806$ mJ m^{-2}) in agreement with the $\vec{a}$ edge dislocation core energies [3, 13]. Note that another core of the $\vec{a}$ edge dislocation, the 8-core, has been found and it is related to the 4-core by a small shift parallel to the glide plane. Both are related to the 5/7-core by a climb of the dislocation line [3].

The simulated images of these atomic configurations are shown in figures 1(b) and (d). For a given microscope, the projection of the atomic columns is black or white depending on the defocus and the thickness of the observed area. In the following, the thickness of the specimen is close to 6 nm and the defocus value is equal to -24 nm. For our microscope, Topcon 0002B, with 0.18 nm point resolution, each dark spot is the projection of two atomic columns and each white spot corresponds to empty tunnels of the structure. It is clearly shown that the 4-atom and 5/7-atom rings exhibit different contrasts. When considering one period of the 5/7-interface such as $6_1 6_2 7 5 6_2$, the simulated image shows that the unit cell (dashed lines; see figure 1(b)) contains two white spots of different contrast corresponding to the 5/7-atom rings. The notation 6_1 and 6_2 indicates the localization of the 6-atom cycle at the boundary: the interface plane crosses 6_1 (figure 1(a)) whereas it passes symmetrically between two 6_2s. As regards the 4-interface, the interface also contains two white spots inside the unit cell of one period denoted as $6_1 6_2 6_1 6'_2 4 6_2$. One of them, with a very weak contrast, corresponds to the 4-atom ring. It is worth noting that the two adjacent 6-atom rings, $6'_2$, one from the upper crystal and the other from the lower crystal, are imaged as deformed white spots.

The experimental image (EI) presented in figure 2 shows a $\Sigma = 19$ $(2\bar{5}30)$ tilt boundary that exhibits a step at the interface. A full description of this image can be found in [2, 14] where it was described as involving 8-atom and 5/7-atom rings. The Burgers vector associated with this defect has been calculated to be $(1/57)[8\bar{7}\bar{1}0]_\lambda$ which is an interfacial edge dislocation; its angle with the interface plane is 60°. The step heights were calculated to be $h_{(\lambda)} = 2d(2\bar{5}30)$

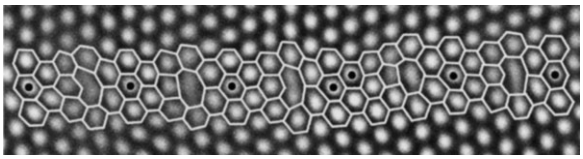

Figure 2. A micrograph of the $\Sigma = 19$ ($\theta = 13.4°$) $(3\bar{5}20)$ tilt boundary.

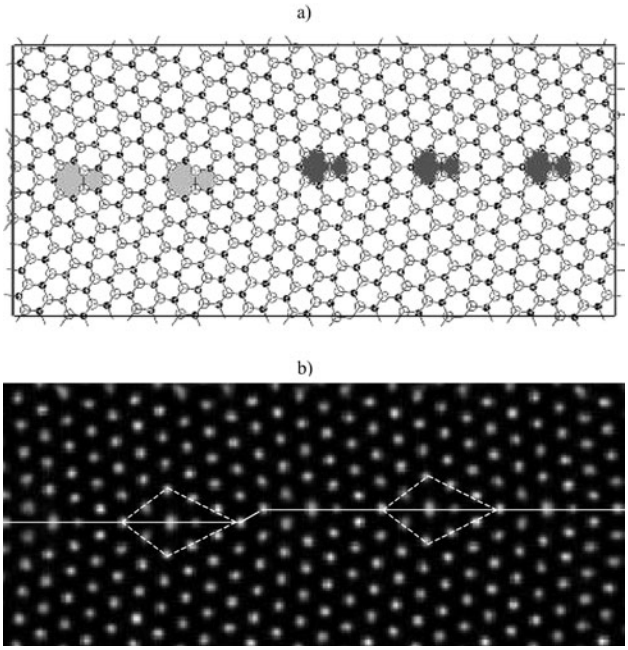

Figure 3. (a) The relaxed structure of the $\Sigma = 19$ $(3\bar{5}20)$ boundary with a step at the interface made up only of 5/7-cores; (b) the corresponding simulated image: thickness, 6 nm; defocus, −24 nm.

and $h_{(\mu)} = 3d(2\bar{5}30)$, where $d(2\bar{5}30)$ is the $(2\bar{5}30)$ interplanar spacing. Taking into account that the interface without a step can only be described in terms of one type of core, we can consider that the boundary with a step can be formed either by 5/7-cores on both sides or 5/7-cores at one side and 4-cores at the other side. As previously mentioned, the 8- and 4-cores are equivalent; they are related to a small shift along the glide plane causing a switching of one bond from one position to another. Thus, we consider the 5/7 versus 8 boundary included in the latter case. Since it is not easy to identify the core structures on the EI, we have simulated the two above-mentioned possibilities and generated the calculated images.

The relaxed structures are shown in figures 3(a) and 4(a) and the calculated images in figures 3(b) and 4(b). The former, denoted as S_1, is only formed of 7/5-cores (figure 3(a)) whereas the second, designated as S_2, contains both 7/5- and 4-cores (figure 4(a)). As clearly shown, the simulated images are able to show the fine details of the dislocation cores and dislocation positions relative to the interface. Comparing with the EI, we notice that the boundary with the 5/7-core (on the left-hand side of the step in the simulation and on the right-hand side in the EI) has a very good match. The other side of the step seems to be closer to the 4-core, although it is not clear for all the units. The calculations of the energy associated with the step formation show that the structure S_2 has an energy (0.21 eV Å^{-1})

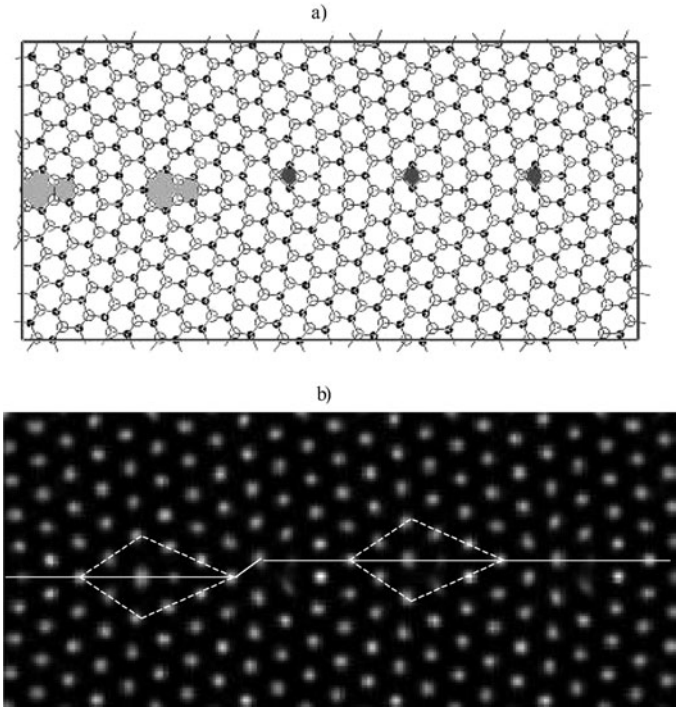

Figure 4. (a) The relaxed structure of the $\Sigma = 19$ $(3\bar{5}20)$ boundary with a step at the interface made up of 5/7- and 4-cores; (b) the corresponding simulated image.

smaller than that of the structure S_1 (0.34 eV $Å^{-1}$); thus, it seems to confirm the interpretation. However, the energy is not the only crucial parameter because the geometrical surroundings of the boundary, impurities and/or external stress fields, may influence the occurrence of the resulting configuration.

4. Conclusions

The atomic structure of the $\Sigma = 19$ $(2\bar{5}30)$ tilt boundary with a step at the interface is simulated using an empirical potential of Stillinger–Weber type and a multislice technique. We found two possible configurations, S_1 and S_2, geometrically feasible and stable under relaxation. Comparison with the EI seems to favour the configuration S_2 were the step has 5/7-cores on one side and 4-cores on the other. This result is in agreement with the energy calculations associated with the step formation, although the geometrical surroundings of the boundary, impurities and/or external stress fields may also influence which configuration occurs.

Acknowledgment

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References

[1] Beaumont B, Vennéguès P and Gibart P 2001 *Phys. Status Solidi* b **227** 1
[2] Potin V, Ruterana P, Nouet G, Pond R C and Morkoç H 2000 *Phys. Rev.* B **61** 5587

[3] Béré A and Serra A 2002 *Phys. Rev.* B **65** 205323
[4] Béré A and Serra A 2001 *Interface Sci.* **9** 149
[5] Vitek V, Sutton A P, Smith D A and Pond R C 1980 *Grain Boundary Structure and Kinetics* ed R W Balluffi (Metals Park, OH: ASM International) p 115
[6] Pond R C, Bacon D J, Serra A and Sutton A P 1991 *Metall. Trans.* A **22** 1185
[7] Stillinger F H and Weber T A 1985 *Phys. Rev.* B **38** 1537
[8] Ichimura M 1996 *Phys. Status Solidi* a **153** 431
[9] Aïchoune N, Potin V, Ruterana P, Hairie A, Nouet G and Paumier E 2000 *Comput. Mater. Sci.* **17** 380
[10] Duesbery M S, Joos B and Michel D J 1991 *Phys. Rev.* B **43** 5143
[11] Béré A and Serra A 2002 *Phys. Rev.* B **66** 085330
[12] Chen J, Ruterana P and Nouet G 2002 at press
[13] Chen J, Ruterana P and Nouet G 2001 *Mater. Sci. Eng.* B **82** 117
[14] Ruterana P and Nouet G 2001 *Phys. Status Solidi* b **227** 177