Image Simulation of Partial Dislocation Lines Plan-viewed by High Resolution Electron Microscopy

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High resolution electron microscopic (HREM) images were simulated for dissociated dislocations in GaAs observed with an electron beam incident normal to the stacking fault (SF) plane. Model structures containing two types of Shockley partial dislocations (30° and 90°) were constructed according to the elastic strain field, and atomistically relaxed with a Keating-type potential. Systematic calculations varying the film thickness, the depth of the dislocation in the film, and the defocus values revealed that the image of SF represented by a superlattice contrast with $\sqrt{3}\times\sqrt{3}$ -R 30° two-dimensional periodicity can be obtained for film thicknesses smaller than $\sim 5\text{nm}$ in the best contrast at a defocus value shorter than the Scherzer focus. Along the dislocation line, a superperiodic modulation arising from reconstruction of 30° partial dislocation core is discernible in weak contrast.

Keyword: GaAs, zincblende, stacking fault, kink, reconstruction, dangling bond, superlattice, forbidden spots.

I. Introduction

High resolution electron microscopy (HREM) is a powerful tool to investigate atomic structures of dislocations. Conventionally HREM observations of dislocations are conducted in the edge-on configuration with the electron beam incident in parallel to the dislocation line (Fig. 1). In the edge-on geometry, however, defects on dislocations, such as kinks, only blur the image of dislocation and can not be studied directly. The first attempt to image kinks on dislocations was made by Bursill and Blanchin⁽¹⁾ who used a plan-view geometry to observe dislocations in TiO_2 with an electron beam normal to the slip plane. The plan-view geometry was used also by Alexander and his coworkers⁽²⁾ to investigate the dislocation line shape in Si on an atomic scale. More recently the same technique, which we call the plan-view HREM to differentiate it from the conventional edge-on HREM, was successfully used by Suzuki and his coworkers⁽³⁾ to get good images of kinks in Si.

Fig. 1 The edge-on configuration and the plan-view configuration.

The plan-view HREM method is applicable when dislocations in diamond or zinc-blende structures are dissociated to partial dislocations that are separated by a stacking fault (SF) the local structure of which yields a characteristic contrast in the HREM image. The sublattices of these crystals are face-centered cubic (fcc) but the SF separating the two Shockley partials locally introduces a hexagonal close packed (hcp) stacking structure embedded in the fcc matrix. Atomic projection of the hcp lattice to a plane normal to the c-axis (Fig. 2 (b)) has a $\sqrt{3}\times\sqrt{3}$ superlattice pattern with a unit cell rotated by 30° from that of the fcc (Fig. 2 (a)). Under appropriate conditions, HREM yields images that approximate such projections. Therefore the plan-view HREM possibly allows us to delineate partial dislocation lines as the boundary of the SF imaged in the $\sqrt{3}\times\sqrt{3}$ -R 30° superlattice contrast.

Fig. 2 The atomic projections onto a (111) plane normal to the c-axis of the fcc lattice (a) and the hcp lattice (b).

The dislocation glide in semiconductors is controlled by the Peierls mechanism which involves two elementary processes, kink-pair formation and kink migration. The dislocation glides in semiconductors exhibit peculiar behaviors which are not observed in metals: The dislocation mobility is in most cases very sensitive to the position of the Fermi level (doping effect) and in many cases strongly enhanced by electronic excitation (radiation enhanced dislocation glide = REDG effect)⁽⁴⁾. These effects are considered to be due to the electronic activity of dislocations, though the microscopic origin is not yet completely identified. Although it was proposed that the electronically active centers originate in dangling bonds along the dislocation lines⁽⁵⁾, theoretical calculations showed that they are probably reconstructed⁽⁶⁾⁽⁷⁾. Hirsch⁽⁸⁾ then claimed that the active centers are associated with kinks but Heggie and Jones⁽⁹⁾⁽¹⁰⁾ pointed out that solitons, anti-phase defects on reconstructed bonds, are responsible for the centers.

This paper describes detailed computer simulations of plan-view HREM images of partial dislocations in GaAs which have been carried out in order to elucidate the best condition for imaging kinks, core reconstruction, and ultimately solitons in an atomic resolution. The results are compared with the previous calculations performed on Si⁽³⁾, and discussed with a particular attention to physical reasons for the best imaging conditions.

II. Model construction

To simulate images of 30°- and 90°- partial dislocations in GaAs that is to be observed by plan-view HREM, atomic model structures containing a partial dislocation were constructed in the following way: At first a 30°- or a 90°- partial dislocation was introduced into a perfect zinc-blende model lattice along the $[1\bar{1}0]$ direction according to the strain field calculated by the anisotropic elasticity theory⁽¹¹⁾⁽¹²⁾. Here we assumed that the dislocations are of the glide set; i.e., the partial dislocations are located between the narrowly spaced (111) planes. Then to introduce core reconstruction, dangling bonds of neighboring atoms along the 30°- partial dislocation were paired and subjected to relaxation by using a simple Keating-type potential⁽¹³⁾,

$$\phi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) = \frac{3\alpha}{10r_0^2} \sum_{i=1}^4 (\mathbf{r}_i \cdot \mathbf{r}_i - r_0^2)^2 + \frac{3b}{8r_0^2} \sum_{i,j>i} \left(\mathbf{r}_i \cdot \mathbf{r}_j + \frac{1}{3} r_0^2 \right)^2, \quad (1)$$

where $\mathbf{r}_i$ is the coordination vector of the i -th neighboring atom, r_0 is the bond length in the perfect lattice, and the parameters α and β represent rigidity to bond-stretching and bond-bending, respectively. Models of dislocation core reconstructed to different degrees were obtained by artificially varying the rigidity parameters α and β . The model were 7.96nm×17.29nm in the $[11\bar{2}]$ and $[111]$ directions, respectively and periodical along the $[1\bar{1}0]$ direction. A fixed boundary condition was used in the structural relax-

ation in the $[11\bar{2}]$ and $[111]$ directions. Model films were cut out from thus relaxed structures. The surface relaxation that possibly occurs in real crystals was not considered.

The electron-diffraction process was simulated by the multi-slice method using the slice thickness of $1/3 a[111] \sim 0.326$ nm and the supercell size of 4.80nm×4.15nm in the $[1\bar{1}0]$ and $[11\bar{2}]$ directions, respectively. The film thickness was varied from 2.94nm to 5.88nm. Other parameters used for computation were, the lattice constant = 0.565nm, the atomic scattering factor given by Doyle and Turner⁽¹⁴⁾, and the accelerating voltage $V = 300$ kV or 100kV. The image simulation was conducted with H-9000 (Hitachi) in mind using the spherical aberration constant $C_s = 0.90$ mm, the chromatic aberration constant $C_c = 6.18$ nm, the aperture radius of objective lens $D_1 = 6.8$ nm⁻¹ which passes 3441 diffraction spots. The defocus value DF was varied around the Scherzer focus, the usual optimum condition for lattice image: For systematic study, however, most of the simulations were performed for the Scherzer focus $((1.5C_s\lambda)^{1/2} = 50$ nm for 300kV) on unreconstructed and reconstructed 30°- partials, and unreconstructed 90°- partials. We examined the dependence of the SF contrast on the film thickness, the depth of partial dislocation in the film, the defocus value, and that of the reconstruction contrast of 30°- partials on the film thickness, the defocus value and the degree of core reconstruction which is quantified by the length of the paired dangling bonds along the dislocation core.

To quantify the visibility of the SF, the magnitude of the SF contrast was defined. The two-dimensional Fourier transform of the SF region of the image yields forbidden $\{422\}/3$ reflection spots in addition to the allowed $\{220\}$ spots in the perfect crystal. The forbidden reflection spots, however, could arise even in the perfect region from the finiteness of the film thickness (for more detail, see IV). To remove this thickness effect, the SF contrast was defined as

$$SF \text{ contrast} \equiv I_{1, SF} / I_{2, SF} - I_{1, PL} / I_{2, PL}, \quad (2)$$

where $I_{1, SF}$ and $I_{1, PL}$ represent the average intensity of forbidden spots in the diffraction from the SF region and that from the perfect region, respectively. Similarly $I_{2, SF}$ and $I_{2, PL}$ respectively represent the average intensity of the allowed spots in the diffraction from the SF region and that from the perfect region.

III. Results

Figure 3 shows simulated images of a 60° dislocation dissociated to a 30°- partial dislocation (left) and a 90°- partial dislocation (right) calculated for the film thickness of 2.94nm and the defocus value of 50nm (the Scherzer focus). The white circles superimposed on the images illustrate the position of atoms in the two (111) net planes adjacent to the glide plane. We can recognize the $\sqrt{3} \times \sqrt{3}$ -R30° superlattice periodicity corresponding to the SF whose peripheral boundary coincides with the position of the partial dislocations.

When the SF is in good contrast, the 30°- partial can be

Fig. 3 Typical lattice image of a 60° dislocation dissociated to a 30° -partial dislocation and a 90° -partial dislocation calculated for the film thickness 2.94nm (9 atomic layers), defocus value = 50nm, aperture radius = 6.8nm^{-1} .

easily distinguished from the 90° -partial by the difference in the atomic alignment along the $[11\bar{2}]$ direction crossing the dislocation line. As pointed out by Suzuki et al.⁽³⁾, while the $[11\bar{2}]$ atomic arrays are displaced at their crossing points with the 30° -partial by nearly half the atomic distance along the dislocation line, those across the 90° -partial have no shift. This can be used for experimental identification of the partial type. In the following, we focus our attention only to the 30° -partial dislocation which is considered to control the dislocation mobility.

The dependence of images on the defocus value is shown in Fig. 4 (a). Although the $\sqrt{3}\times\sqrt{3}$ -R 30° pattern in the SF is visible at the Scherzer focus (50nm), the image at the defocus of 25nm yields a more distinct superlattice contrast which is rather closer to the image that was actually observed in experiments⁽¹⁵⁾. However, most of the following simulations were carried out for the Scherzer focus (50nm).

Fig. 4 (a) Simulated images of the 30° -partial dislocations obtained by varying the defocus value on a film thickness of 2.94nm, (b) the film thickness dependence for the defocus value of 50nm (the Scherzer focus), (c) the dependence on the dislocation position in the film in film thickness of 2.94nm at the defocus value of 50nm. The arrows indicate the positions of the 30° -partial dislocations.

The variation of the lattice images with the film thickness is shown in Fig. 4 (b). The position of the dislocation line was fixed between the 4th and 5th layers from the top (the beam-incident side) surface. Naturally the SF contrast becomes less distinct with increasing film thickness. The largest film thickness for which the $\sqrt{3}\times\sqrt{3}$ -R30° periodicity representing the SF can be obtained in good contrast is $\sim 5\text{nm}$.

The effect of the position of the dislocation line in the film is exemplified by a series of images shown in Fig. 4 (c) that were calculated for the film thickness of 2.94nm (9 atomic layers). The lattice images near the dislocation line becomes blurred when the dislocation is located deeply in the film. This is considered to be due to the strain field localized near the dislocation line which should affect the image most strongly when the dislocation is at the center of the film.

The depth of the dislocation line in the film was found to be critical to get a good SF contrast. A set of Figs. 5 show the SF contrast evaluated as a function of the depth of dislocation line in the film of a specific thickness of 2.94nm (9 atomic layers). The variation of the SF contrast exhibits an oscillatory dependence on the dislocation position in the film independent of the defocus value and the accelerating voltage. The reduction of SF contrast occurs in every three layers for an intrinsic reason which will be discussed in IV. Actually such cases in which the SF is intrinsically invisible had been excluded from images shown in Fig. 4.

The dependence of SF contrast on the film thickness is summarized in Fig. 6 (a) and that on the position of the dislocation in the film in Fig. 6 (b), where SF-invisible cases

Fig. 5 The evaluated stacking fault contrast as a function of the dislocation position in the film whose thickness is 2.94nm. The figures in the parenthesis are, from left to right, the spherical aberration (mm), the accelerating voltage (kV), and the defocus value (nm).

are excluded. A notable fact is that, as pointed out above, the optimum condition for the strongest SF contrast is achieved not necessarily at the Scherzer focus but at a somewhat smaller defocus value.

The SF contrast for Si is much larger than GaAs: For example, the contrast of SF located between 4th and 5th layers in thickness of 9 atomic layers is, at the Scherzer focus, about two times larger than in GaAs obtained under the same conditions. Thus, HREM images in GaAs will be less clear than in Si.

The effect of core reconstruction on the lattice image is demonstrated in Fig. 7 (a) (unreconstructed) and (b) (reconstructed) 30°-partial dislocations. One may recognize in the reconstructed partial that the dark spots along the dislocation core exhibit an intensity modulation with a periodicity which doubles that in the unreconstructed partial. This is more clearly seen in the intensity profiles (Fig. 7 (c)) taken along the dislocation line. The reconstruction contrast is defined by the ratio

$$\text{reconstruction contrast} \equiv X/Y = (Y - Z)/Y, \quad (3)$$

(a)

(b)

Fig. 6 The dependence of stacking fault contrast on the film thickness (a), on the dislocation position in the film (b), the film thickness is 4.90nm.

where Y and Z are respectively the maximum amplitude and the minimum amplitude of the profile, $X \equiv (Y - Z)$ is the reduction of the amplitude which occurs in every two atomic distances in the reconstruction case. Figure 8 (a) shows the dependence of reconstruction contrast on the degree of reconstruction, which was varied by changing the rigidity parameter α and β in the Keating potential (eq. (1)). Here the measure of reconstruction degree in the abscissa is given by the bond-length between the neighboring atoms that were reconstructed. As expected, with increasing the degree of reconstruction, the reconstruction contrast becomes stronger. The contrast is slightly different between Ga-dislocation (Ga atoms in the core) and As-dislocation (As atoms in the core). In Fig. 8 (a) is also shown the reconstruction contrast of Ga-dislocation and N-dislocation in a model GaN crystal which was obtained by simply substituting the As atoms in the model GaAs with N atoms. The reconstruction contrast is higher in Ga-dislocation than N-dislocation in GaN and also than As-dislocation in GaAs. Figure 8 (b) shows that the reconstruction contrast does not depend systematically on the dislocation position in the film but is generally greater at the Scherzer focus (50nm) than at the smaller defocus (25nm) for which the SF contrast is rather stronger.

Fig. 7 Typical lattice images of an unreconstructed 30°- partial dislocation (a), and a reconstructed 30°- partial (b) located between 4th and 5th layers in a film whose thickness is 2.94nm. The intensity profiles along the dislocation line are shown in (c).

IV. Discussion

Although it was stated in I that the $\sqrt{3} \times \sqrt{3}$ -R30° superlattice contrast arises from the local hcp structure in the SF. More precisely, however, it should be stated that the superlattice contrast arises when the numbers of the three stacking layers, conventionally denoted by A, B and C, are different from each other. This has two consequences. The $\{422\}/3$ spots are forbidden in the perfect lattice of infinite size, but they are forbidden also when the thickness of the lattice is finite and the numbers of the three layers are accidentally identical so as to allow the complete cancellation in the structure factor. In other words, the forbidden spots appear in films whose thicknesses are not multiples of three stacking layers ($1/3a[111]$); as a consequence, the $\sqrt{3} \times \sqrt{3}$ -R30° superlattice contrast in such films spreads over the whole image even in the absence of SF.

Fig. 8 The dependence of reconstruction contrast on the degree of reconstruction (a), and on the dislocation position in the film (b). In (a) As/GaAs denotes As-dislocation in GaAs and so on. The film thickness is 2.94nm and the dislocation position in (a) is between 4th and 5th layers.

In dislocated films containing SF, if the number of layers above the slip plane and that below it are both multiples of three, the superlattice contrast from the SF region becomes weak. This is because the $\{422\}/3$ spots are nearly forbidden due to the partial cancellation in the structure factor for the same reason as discussed above. For an example, when the dislocation and hence the SF is located between 3rd and 4th layers in the film of thickness of 9 layers, the layers are stacked as ABCBCABCA. Since in this case the numbers of A, B and C layers are all three, the $\{422\}/3$ spots that represent the SF are apparently forbidden. This is the reason for the reduction of SF contrast observed in Fig. 5 for the specific positions of the dislocation in the film. The fact that the defocus value and the accelerating voltage have no essential effect on the curves in Fig. 5 is consistent with this reasoning.

Figures 6 (a) and (b) show that the optimum condition for the strongest SF contrast to be achieved is at a defocus value somewhat smaller than the Scherzer focus. In fact this is in agreement with experimental observations of dislocations in GaAs performed recently by the present authors⁽¹⁵⁾. The obvious reason is, however, not known at present. Either is not known the reason why the SF contrasts at the optimum defocus are enhanced for dislocations located near the center of the film.

Calculations showed that reconstruction of 30°-partial dislocation, if sufficiently strong, can be detected by the plan-view HREM method. The optimum defocus is the Scherzer focus, which is not the case in SF imaging. The reconstruction contrast does not exceed 30% for GaAs under the optimum condition, and may be difficult to be detected experimentally if the image is degraded by noise. Detection of solitons, anti-phase defects along the reconstructed core, will require further noise reduction and hence be more difficult. Nevertheless, the reconstruction contrast depends on the type of atoms in the core of the partial. In GaAs, the atomic numbers of Ga and As are similar and hence their atomic scattering factors are close to each other. In GaN, the atomic scattering factor of Ga is ~ 4 times larger than that of N, which leads to the higher reconstruction contrast in Ga-partials whose core is occupied by Ga atoms which mainly diffract the electron beam. Similarly to the SF contrast, the reconstruction contrast in Si is larger than in GaAs. For example, the reconstruction contrast in Si (the film thickness = 9 atomic layers, defocus value = 50nm, the dislocation between 4th and 5th layers) is about 1.5 times

stronger than that for GaAs. Therefore, experimental detection of reconstruction contrasts and hence solitons may be possible if one uses same crystals other than GaAs.

V. Conclusions

HREM lattice images in the plan-view geometry have been simulated for dissociated dislocations in GaAs. Partial dislocations can be identified as the boundary of the superlattice contrast arising from the SF which separates the partials. For good SF contrasts to be obtained, the film thickness must be smaller than ~ 5nm, and the defocus value should be set at a position shorter than the Scherzer focus.

Reconstruction in the core of 30°-partial dislocations can be detected by contrast profile along the dislocation line. The largest contrast is only about 30% for GaAs but can be greater for other crystals. The best contrast is obtained at the Scherzer focus.

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REFERENCES

- (1) L. A. Bursill and M. G. Blanchin: *Phil. Mag. A*, **49** (1984), 365.
- (2) H. Alexander, J. C. H. Spence, D. Shindo, H. Gottschalk and N. Long: *Phil. Mag. A*, **53** (1986), 627.
- (3) K. Suzuki, N. Maeda and S. Takeuchi, *Phil. Mag. A*, in press.
- (4) K. Maeda, Y. Yamashita, N. Maeda and S. Takeuchi: *Mat. Res. Symp. Proc.*, **184** (1990), 69.
- (5) H. Alexander and H. Teichler: *Material Science and Technology vol. 4*, ed. by R. W. Cahn, P. Hassen, and E. J. Kramer, VCH Weinheim, Cambridge (1993), p. 251.
- (6) S. Marklund: *Phys. Stat. Sol. (b)* **100** (1980), 77.
- (7) H. Alexander: *Dislocations in Solids vol. 7*, ed. by F. R. N. Nabarro, North-Holland, Amsterdam (1986), p. 113.
- (8) P. B. Hirsch: *Mater. Sci. Tech.* **1** (1985), 666.
- (9) M. Heggie and R. Jones: *Phil. Mag. B*, **48** (1983), 365.
- (10) M. Heggie and R. Jones: *Phil. Mag. B*, **48** (1983), 379.
- (11) I. W. Steeds: *Introduction to Anisotropic Elasticity Theory of Dislocations*, Clarendon Press, Oxford (1973).
- (12) J. P. Hirth and J. Lothe: *Theory of Dislocations*, McGraw-Hill, New York, (1968).
- (13) S. Marklund: *J. Physique* **44** (1983), C4-25.
- (14) P. A. Doyle and P. S. Turner: *Acta Cryst. A* **24** (1968), 390.
- (15) M. Inoue, K. Suzuki, E. Kanematsu, S. Takeuchi and K. Maeda: submitted to *Phil. Mag. A*.