

Development of Multiscale Computational Model for Carrier Mobility in GaAs Nanopillars with Twin Boundaries

Mitsumoto KAWAI*

ABSTRACT

A multiscale computational model for the calculation of the effect of (111) twin boundaries on electron mobility in GaAs nanopillars synthesized using the Selective Area Metal Organic Vapor Phase Epitaxy (SA-MOVPE) method has been developed. The Non-equilibrium Green's function method is applied in the calculation of quantum conductance in order to explicitly incorporate the effect of twin defect morphology. Quantum conductance is converted to a thermally-averaged scattering factor to connect quantum conductance to mobility. With this newly introduced factor, electron mobility can be corrected for a twin boundary scattering model. The calculated electron mobility for GaAs nanopillars synthesized under standard SA-MOVPE conditions with a mean twin spacing of 2.48 nm was 1000 cm²/V/s. In addition, the contribution of twin boundary scattering to the reduction of electron mobility was estimated to be 60% of the effect of the scattering factors overall.

1. Introduction

Nanopillar-shaped semiconductor elements of diameters of several tens to several hundreds of nm are manufactured for a variety of applications, including photovoltaic generation devices, sensors, and thermoelectric conversion devices⁽¹⁾. When heterojunction interfaces are employed in semiconductor elements, misfit dislocation can occur as a result of lattice mismatch⁽²⁾. Dislocation results in lattice vacancies, producing significant resistance to the electromigration that is important to device performance. In an attempt to avoid this issue, nanopillars are being synthesized with diameters smaller than the dislocation intervals. Broadly speaking, two methods of synthesis are employed. These are the vapor liquid solid (VLS) method and the selective-area metal-organic vapor phase epitaxy (SA-MOVPE) method⁽¹⁾. The VLS method uses Au and other catalysts. By contrast, the SA-MOVPE method does not use a catalyst, being a “bottom-up” method of film growth in which the area of deposition of the supplied gas on the substrate is restricted by the application of an amorphous film to sections of the substrate. Whichever method is employed, high-density

twin structures have been observed perpendicular to the direction of electromigration (the direction of film growth)⁽³⁾. Because these twin structures are stacking faults, they represent electromigration barriers, and this is analogous to a decline in thermal conductivity due to the influence of stacking faults⁽⁴⁾. Devices using compound semiconductors incorporating nanopillar shapes are designed on the basis of an expectation of high electron mobility. It is of concern that the reduction of electron mobility resulting from the effect of twin structures may have a significant effect on device performance. In addition, test measurement of electron mobility in nanopillars is challenging due to the miniscule nature of the parameter, and quantitative analyses are not conducted within the range surveyed in this study.

Focusing on GaAs nanopillars synthesized under standard conditions using the SA-MOVPE method, the research discussed in this paper developed a method of quantifying electron mobility able to explicitly consider the effect of high-density twin structures on mobility. Using this method, the study calculated electron mobility in nanopillars incorporating twin structures and the ratio represented by the effect of twin structures to total scattering factors.

* Fundamental Technology Research Center

2. Twin Structures in GaAs Semiconductor Nanopillars

The subjects of computation in this study, GaAs nanopillars along the $[\bar{1}\bar{1}\bar{1}]$ growth direction, were grown epitaxially on a GaAs(111)B substrate using the SA-MOVPE method. In terms of growth conditions, the substrate temperature was 750°C, hydrogen was used as the carrier gas, the Ga source was trimethylgallium, at a partial pressure of $P_{Ga} = 1 \times 10^{-6}$ atm, and the As source was arsine, at a partial pressure of $P_{As} = 1 \times 10^{-4}$ atm. These conditions will be referred to as “standard conditions” below^{(1), (3)}.

Figure 1 shows the results of observation of nanopillars using a scanning electron microscope (SEM). Hexagonal nanopillars have grown on the GaAs(111)B substrate (left), with a growth direction of $[\bar{1}\bar{1}\bar{1}]$ and a side orientation of $\{110\}$ (right).

In order to determine the morphology of the twin structures in these nanopillars, transmission electron microscope (TEM) observations were conducted, and the results were analyzed. Figure 2 shows the results of TEM observation at an incidence of $[01\bar{1}]$. The results show high-density twin faces perpendicular to the $[\bar{1}\bar{1}\bar{1}]$ growth direction (upper). A TEM photograph taken at a magnification of 500,000x was subjected to image processing to magnify it to approximately 1,000,000x, revealing rotational twins termed 3C structures (middle) and twins termed 2H structures (AB structures) (lower). However, the repeating continuous ABAB structures termed wurtzite structures were not observed. Here, A, B, and C express the positional relationship of Ga-As atom pairs to the $[\bar{1}\bar{1}\bar{1}]$ growth direction.

In order to determine the tendency of the spacing between the twin faces, measurements of spacing were conducted using the results of TEM observations, and the results were subjected to statistical processing. Figure 3 shows a section of a TEM photograph used

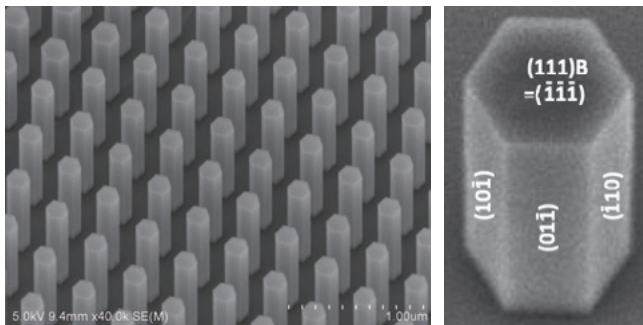


Fig. 1 Macroscopic SEM image (incidence of 30°) of synthesized GaAs nanopillars grown on (111) B GaAs substrate (left) and magnified SEM image of one nanopillar with plane directions (right)

in the measurement of twin spacing and a histogram showing the results of statistical analysis of measured values (horizontal axis: twin spacing). The mean spacing was 2.48 nm, with a standard deviation of 1.64 nm (total number of measurements: 248). More than 80% of the twins were 3C structures, with less than 20% 2H structures.

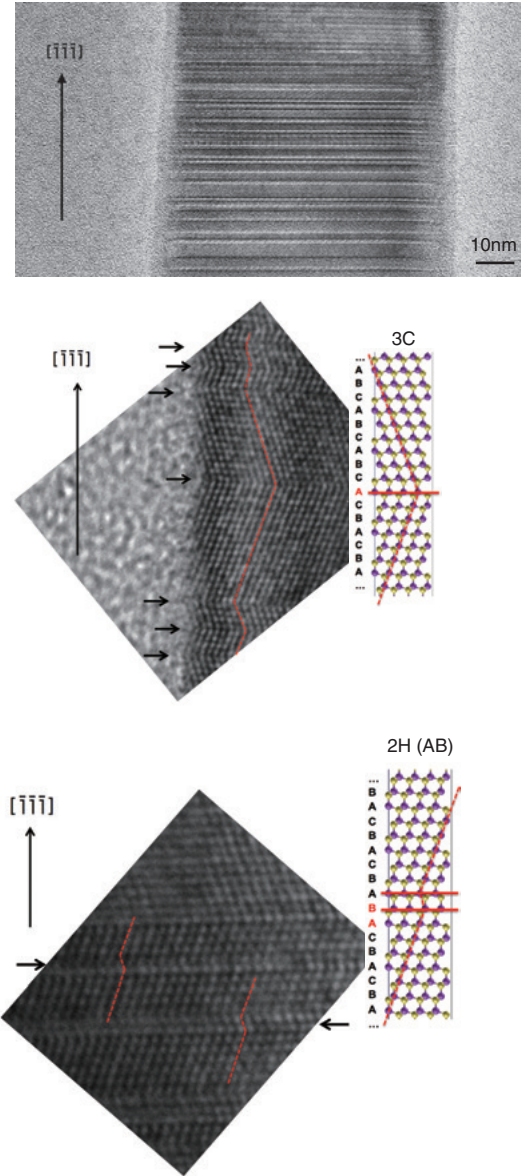


Fig. 2 Cross-sectional TEM image of multi-twinned GaAs nanopillar (upper) 3C-type twin boundaries which have so-called ABCBA stacking sequences from bottom to top (z-direction) (middle), and 2H-type (AB-stacking) twin boundaries which have so-called ABCABABC sequences (lower). Purple and yellow spheres represent Ga and As atoms, respectively.

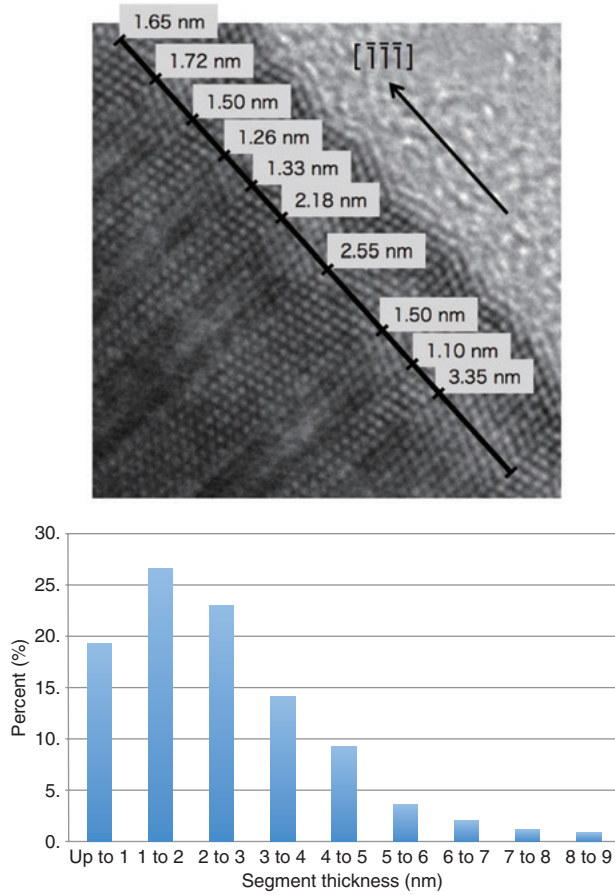


Fig. 3 TEM image of measured twin spacing along $[111]$ direction (upper), and histogram of twin spacing with 248 sampling points, average twin spacing of 2.48 nm (lower)

3. Calculation Methods

The classical picture of electron mobility is as a ratio between drift velocity, v_{drift} , and electrical field, E , defined as follows:

$$M \equiv \frac{\langle v_{drift} \rangle}{-E} \quad (1)$$

The effect of twin structures on this indicator of the ease of electron motion was quantified. In establishing the theoretical formula, it was essential to explicitly incorporate the effect of the twin structures. In order to do so, quantum conductance was first determined using first-principle calculations that did not incorporate test values (Section 3.1.), using atomic models with a variety of twin structures. In other words, electron scattering was evaluated with electrons treated as wave motion. Next, quantum conductance was converted to a scattering factor in order to multiscale by incorporating it in the equation for evaluation of mobility (the classical picture)(Section 3.2.).

In addition, Section 3.3. will discuss the relationship

between other factors that affect electron mobility and the effect of twin structures.

3.1. Method of Calculation of Quantum Conductance

The non-equilibrium Green's function (NEGF⁽⁵⁾) method based on the density-functional approach was employed in the calculation of quantum conductance. SIESTA⁽⁶⁾⁻⁽⁸⁾ was used as the computation code. In this code, inner shell electrons are treated as norm-conserving pseudopotentials, and the linear combination of the numerical atomic orbital (LCAO) method is used as the basis function. GGA-PBE⁽⁹⁾ was used as the exchange-correlation functional, energy cutoff was 300 Rydberg, and the k-point (coordinates on the reciprocal lattice space) division was $31 \times 31 \times 1$, based on the Monkhorst-Pack method⁽¹⁰⁾. The values calculated directly using the NEGF method represent transmittance $T(k, \epsilon)$, a function of the k-points and energy, ϵ . The following relationship holds between transmittance and quantum conductance, $G(k, \epsilon)$ ⁽¹¹⁾:

$$G(k, \epsilon) \equiv \frac{I}{V} \int_k \int_\epsilon T(k, \epsilon) d\epsilon dk \quad (2)$$

As an example of the set-ups employed in the computations, Fig. 4 shows a model with a stacking fault in the first layer (a 3C twin structure). In the NEGF method, electrodes are set as sources of electron influx and efflux, and the effects of these phenomena are considered in the form of self-energy in Green's function. Because of this, the atomic models that form the subject of the computations are broadly divided into three sections. These are sections regarded as left and right electrodes, and a section to which the electrons from the electrodes are sent (the section in which the electrons scatter). The difference in electrical potential

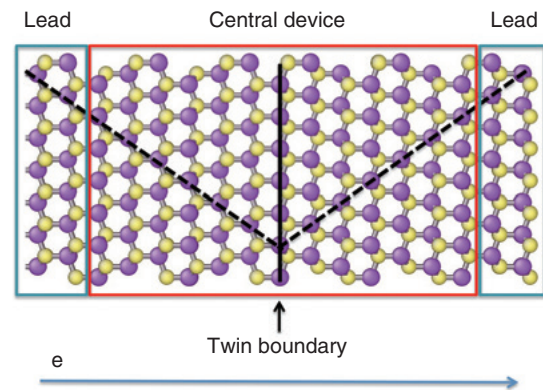


Fig. 4 Configuration of system treated by NEGF method with left and right leads along z-axis (electron transfer direction: $[111]$), under two-dimensional periodic boundary conditions on xy plane. Yellow spheres indicate arsenic, and purple spheres indicate gallium

between these electrodes is considered as a difference in chemical potential between the electrodes. In other words, with ε_f as Fermi energy, a potential difference of $\varepsilon_f \pm eV/2$ is imparted to the left and right electrodes.

In this model, in which the twin faces under consideration are in one layer, an atomic model incorporating 13 layers of Ga-As as single pairs in the electron scattering section (the twin section) and two layers of Ga-As in each of the left and right electrode sections, in contact with the 13 layers, was employed. The total number of atoms was 136 (2x2x(13+2+2)x2).

3.2. Method of Conversion of Quantum Conductance to Mobility

This section will first provide an overview of the understanding of the scattering of electrons by twin faces in the classical picture, and next discuss the method of linking it to quantum conductance (multiscaling), the quantum picture.

In the classical picture, twin structures are considered the sole scattering factor, and electrons are temporally accelerated over time, τ from one twin face to the next twin face by the electrical field, E . If the electrical field is assumed to be small, the electron drift velocity, v_{drift} , can be evaluated using the following equation:

$$\langle v_{drift} \rangle = -\frac{1}{2} \cdot \frac{eE\tau}{m} \quad (3)$$

e : Elementary charge

E : Electrical field

m : Mass of electrons

τ : Time between scattering events

The mean is expressed as 1/2 of the coefficients. This is because all of the electrons conducted to the nanopillars necessarily arrive at and are scattered by the twin faces, the scattering sources, and the electron drift velocity immediately following scattering by twin faces can be regarded as basically zero and the electrons can be regarded as accelerating linearly at $v_{drift} \propto E$ until reaching the next scattering body.

Next, time between scattering events, τ , was modeled. Because drift velocity is extremely small compared to heat velocity, time between scattering events is independent of the electrical field, and if time between scattering events is assumed to be rate-controlled by heat velocity, it can be expressed using the following equation:

$$\tau = \frac{\lambda}{\sqrt{\langle v \cdot v \rangle}} = \frac{\lambda \sqrt{m}}{\sqrt{\langle mv \cdot v \rangle}} = \frac{\lambda \sqrt{m}}{\sqrt{k_B T}} \quad (4)$$

λ : Distance between scattering events

k_B : Boltzmann constant

T : Temperature

Here, the nanopillars are regarded as one-dimensional.

Given this, from Eq. (1), (3) and (4), mobility, $M[m^2/Vs]$, can be expressed as follows:

$$M \equiv \frac{\langle v_{drift} \rangle}{-E} = \frac{e\lambda}{2\sqrt{mk_B T}} \quad (5)$$

In addition, terming electron density n , current density, J , can be expressed as follows:

$$J = -en \langle v_{drift} \rangle = \frac{e^2 n \lambda E}{2\sqrt{mk_B T}} \quad (6)$$

Using Eq. (6), electron conductance in the classical picture, $\sigma[\Omega^{-1}m^{-1}]$, can be expressed by Eq. (7), demonstrating that the relationship between mobility and conductance is maintained.

$$\sigma \equiv \frac{J}{E} = \frac{e^2 n \lambda}{2\sqrt{mk_B T}} enM \quad (7)$$

Equation (5), derived as indicated above as the scattering factor for the twin structures incorporated in the nanopillars, corresponds well with the equation for evaluation of electron mobility obtained from tests⁽¹²⁾, as will be discussed below. Equation (12) in Reference (12) formularizes mobility, M_μ , as shown below, with l as the mean free path (in Reference (12), mobility is expressed as μ).

$$M_l = (4/3)el \frac{1}{\sqrt{2\pi mk_B T}} \quad (8)$$

The ratio between Eq. (5) and Eq. (8) is 1.064, as shown below (because the twin structures are the only scattering bodies, $\lambda=l$).

$$\frac{M_l}{M} = \frac{4/3 \sqrt{2\pi}}{1/2} \approx 1.064$$

The scattering coefficient $s(k_\perp, \epsilon)$, generated by quantum conductance obtained from NEGF computations, is defined by Eq. (9) below.

$$s(k_\perp, \epsilon) \equiv 1 - \frac{G(k_\perp, \epsilon)}{G_0(k_\perp, \epsilon)} \quad (9)$$

Here, G_0 , G are the quantum conductances when twin structures do not exist and do exist, respectively.

The respective quantum conduction values were employed to determine k-point and energy functions using the NEGF method (Section 3.1.). $k_\perp \equiv (k_x, k_y)$ indicates that periodic boundary conditions are maintained on the k_x - k_y plane on the reciprocal lattice space before and after scattering events, because twin faces exist perpendicular to the z-axis, the direction of electron motion. It is therefore possible to designate the state before and after scattering

events using (k_x, k_y) .

At the limits of the scattering coefficient defined by Equation (9), $s(k_{\perp}, \epsilon)=0$ indicates that there is no scattering by twin structures, and $s(k_{\perp}, \epsilon)=1$ indicates that twin structures are an extremely strong scattering factor.

In the actual computations, average thermal equilibrium was calculated for quantum conductance at each k-point and energy level within the range in which electrons existed, as shown by Eq. (10) below. Because of this, the Fermi distribution function, which expresses the probability of the existence of electrons with energy ϵ in this state of thermal equilibrium, was employed. Temperature, T , was set at 300 K.

$$\langle s \rangle = \frac{\sum_{k_{\perp}} \int_{\mu}^{+\infty} f(\epsilon) G_0(k_{\perp}, \epsilon) s(k_{\perp}, \epsilon) d\epsilon}{\sum_{k_{\perp}} \int_{\mu}^{+\infty} f(\epsilon) G_0(k_{\perp}, \epsilon) d\epsilon} \quad (10)$$

$f(\epsilon)$: Fermi distribution function

$$f(\epsilon) = \left(1 + e^{\frac{\epsilon - \mu}{k_B T}} \right)^{-1} \quad (11)$$

μ : Chemical potential

The method of introducing the scattering coefficients calculated using Eq. (10) to electron mobility and conductivity is discussed below. Because the effect of twin structures differs between structures, computations were corrected using scattering coefficients that took into consideration the effect of each structure. In concrete terms, correction was applied to the twin spacing, λ_{TB} , using the scattering factor, $\langle s \rangle$, taking into consideration quantum scattering, to create mean free paths. Equations (12) and (13) below were used for correction in relation to mobility and conductivity.

$$M = \frac{e}{2\sqrt{mk_B T}} \cdot \frac{\lambda_{TB}}{\langle s \rangle} \quad (12)$$

$$\sigma = \frac{e^2 n}{2\sqrt{mk_B T}} \cdot \frac{\lambda_{TB}}{\langle s \rangle} \quad (13)$$

By this means, the model was multiscaled by incorporating the effect of quantum conductance in twin structures in the evaluation equation (the classical picture).

3.3. Relationship with Other Factors Affecting Mobility

Section 3.2. discussed a method of computation of mobility that treated twin structures as the only scattering factor. However, in actuality there are numerous other factors that produce electron scattering. Aggregate mobility, M_{total} , which takes these other factors into consideration, is calculated using Eq. 14⁽¹³⁾. The right-hand term of the equation expresses the individual mobilities that are affected by the respective scattering

factors.

$$M_{total}^{-1} = M_{e-TB}^{-1} + M_{e-e}^{-1} + M_{e-phonon}^{-1} + M_{e-dopant}^{-1} + M_{e-surface}^{-1} + \dots \quad (14)$$

M_{e-TB}^{-1} : Twin structures

M_{e-e}^{-1} : Scattering between electrons

$M_{e-phonon}^{-1}$: Phonon scattering

$M_{e-dopant}^{-1}$: Scattering on dopant

$M_{e-surface}^{-1}$: Surface scattering

With the sum of the terms on the right-hand side, excluding the first term, as the effect of factors other than twin structures, it was possible to use measurement results for a thin GaAs film in which twin structures were not observed⁽¹⁴⁾. To determine M_{total}^{-1} , $M = M_{e-TB}$ was first obtained using Eq. (12), following which Eq. (14) was employed, using the abovementioned mobility measurement results. The ratio of the effect of the twin structures to total scattering factors was also determined, as M_{e-TB}/M_{total} .

4. Results and Considerations

This section will discuss the results of calculations conducted by incorporating the quantum conductance obtained from NEGF calculations in the developed method of quantitative analysis of electron mobility [Eq. (12)]. Section 4.1. will discuss the results of calculations of quantum conductance, and Section 4.2. will discuss the conversion of the quantum conductance results into electron mobility.

4.1. Results of Calculation of Quantum Conductance

Figures 5 and 6 show the results of calculations of quantum conductance for 3C and 2H structures, considered as the basic twin structures. In the atomic model, the z-axis ($=[\bar{1}\bar{1}\bar{1}]$) was the direction of electron motion. In the results, the vertical axis shows the ratio between these measurements and conductance when no twin structures exist and the horizontal axis shows energy. Quantum conductance was reduced by both types of twin structure, indicating an effect as a scattering source. However, no systematic effect was observed for either of the twin structures.

Figure 7 shows the results of analysis of quantum conductance for each k-point in a structure with one 3C twin face (the structure on the left in the upper figure in Fig. 5). Scattering behavior on this twin face differs depending on the k-point. Given this, the effect of twin faces on quantum conductance is dependent on the k-points and energy. In other words, even if the spacing between the twin structures is the same, if the structures themselves differ, quantum conductance differs.

Figures 8 and 9 show the results of conversion of the results shown in Figs. 5 and 6 to current-voltage characteristic (I-V characteristic) using Eq. (2). Within the scope of the twin face spacings calculated here, no systematic differences were observed in the spacings of the 3C type (Fig. 8). However, in the case of the 2H type (Fig. 9), a tendency for current flow to be retarded as the number of twin faces increases was observed at the number of faces under study [elec (no twin structures) $\rightarrow$ 3C $\rightarrow$ 2H $\rightarrow$ 2AB $\rightarrow$ 3AB].

Next, characteristics identified based on the results of the analysis of nanopillars discussed in Chapter 2 were studied with a particular focus on twin spacings, and 14 types of representative nanopillar twin structure model were formulated using two different compositions. Based on the histogram shown in Fig. 3, the ratios of spacings between twin faces were as follows: 40% were 2 nm or less (ABC and AB stacks), 20% were 2-3 nm (ABCx2), 20% were 3-5 nm (ABCx3), and 20% were 5 nm or more (ABCx5). Because AB stacks (2H) were observed in some of the nanopillars, AB stacks were incorporated in the representative models of twin spacings at the above

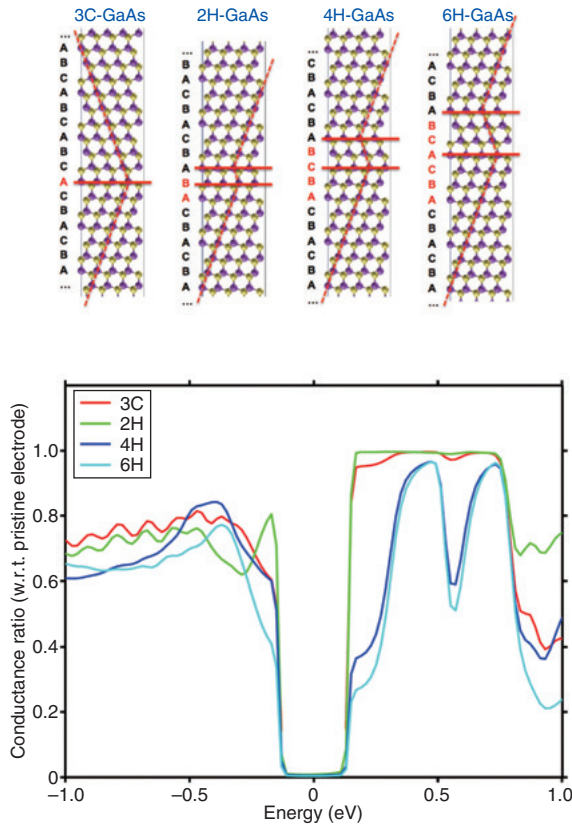


Fig. 5 Quantum conductance calculated using NEGF in different 3C-type structures. Schematic showing GaAs crystals with different types of 3C twin boundaries (upper). Calculated quantum conductance with respect to energy (lower).

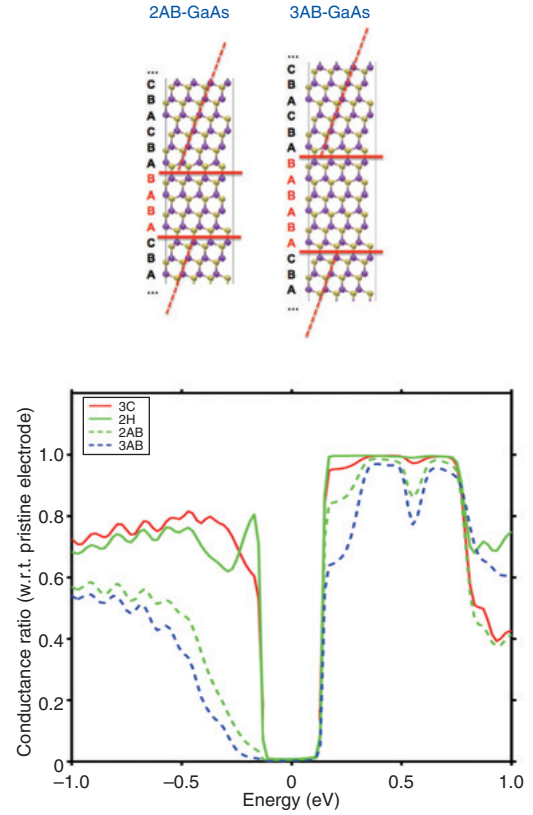


Fig. 6 Quantum conductance calculated by NEGF in different AB-type structures. Schematic showing GaAs crystals with different types of AB twin boundaries (upper). Calculated quantum conductance with respect to energy (lower).

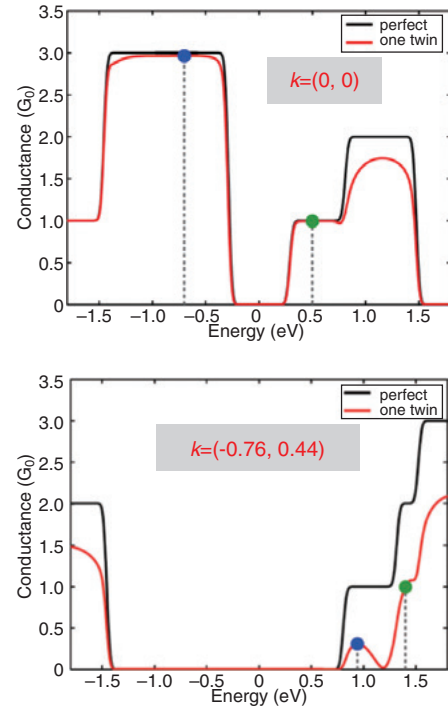


Fig. 7 Quantum conductance with respect to k-points in 3C twin morphology

ratios. The AB stacks were inserted at the respective twin boundaries in each model. Figure 10 shows an example of the representative models of twin structures. The left-hand side shows ordered twin spacings, and the right-hand side shows random twin spacings.

Figure 11 shows the results of calculation of quantum conductance for these arrangements of twin structure spacing. Valence bands were observed as an effect of the arrangement of the twin spacings (shown by the arrows in the figures), but the overall tendency was almost the same. In addition, no conspicuous difference was observed when AB structures were present or absent.

Given these results, the arrangement of the spacing of twin structures can be considered not to have a significant effect on quantum conductance within the scope of the computations conducted in this study.

4.2. Results of Conversion of Quantum Conductance to Mobility

Section 4.1. discussed the computation of quantum conductance using atomic models, with explicit consideration of the effect of twin structures. Figure 12 shows the results, including results for quantum

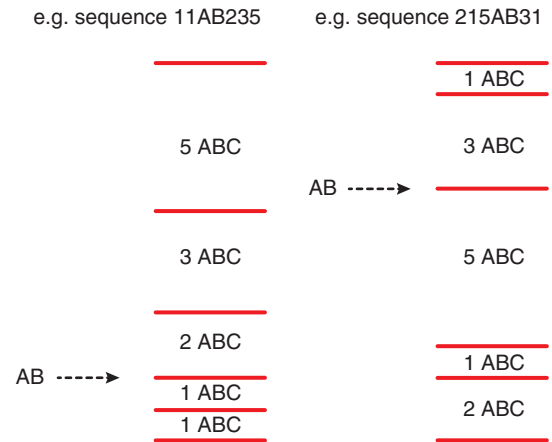


Fig. 10 Examples of representative twin sequence models AB stacks are inserted in 3C boundaries (red line) Ordered twin sequence from bottom to top with AB-stacking between “1ABC” and “2ABC” (left); Random twin sequence with AB-stacking between “5ABC” and “3ABC” (right)

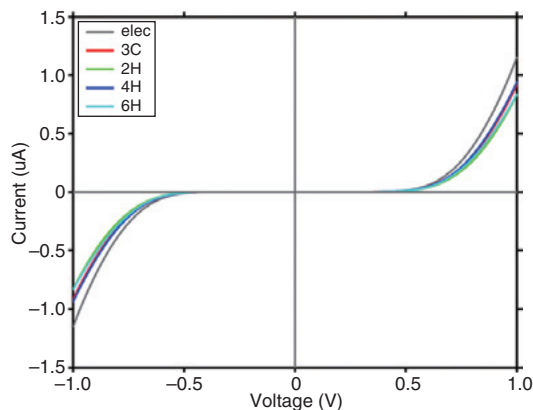


Fig. 8 I-V curve for 3C-type twin boundaries

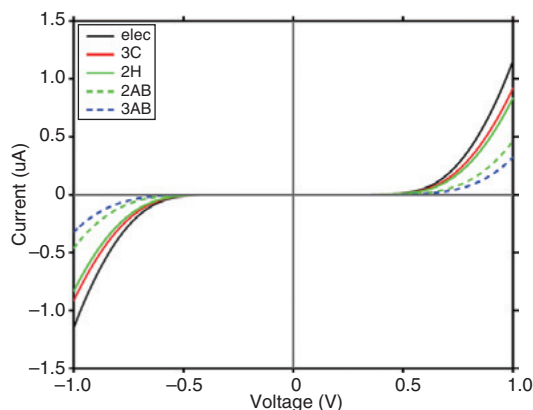


Fig. 9 I-V curve for AB-type twin boundaries

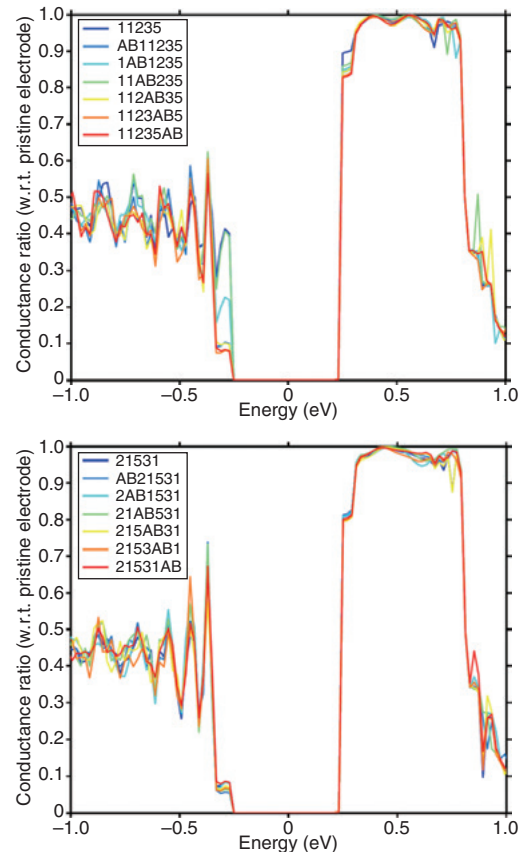


Fig. 11 Quantum conductance with respect to energy in representative models: Ordered twin sequences (upper); Random twin sequences (lower)

conductance computed using different combinations of twin spacings, converted to figures for mobility using Eq. (12). The converted figures for mobility are proportional to the mean twin spacing, matching the intuitive conclusion from the classical picture. Next, the ratio of the effect of twin structures to all scattering factors was computed using Eq. (14). Results obtained from Fig. 12 were used as the first right-hand term of the equation. The other right-hand terms were provided by the results of measurements of electron mobility in a thin GaAs film (without twin structures) ⁽¹⁴⁾. From Fig. 3, the mean twin spacing of nanopillars synthesized under standard conditions is approximately 2.48 nm, indicating from Fig. 12 that it was possible to predict $M_{e-TB} \approx 1600 \text{ cm}^2/\text{V/s}$. In Reference (14), electron mobility in a thin GaAs film without twin structures is ($n \approx 10^{18}/\text{cm}^3$, $T = 300 \text{ K}$), $M_{e-e}^{-1} + M_{e-phonon}^{-1} + M_{e-dopant}^{-1} + M_{e-surface}^{-1} + \dots \approx 2500 \text{ cm}^2/\text{V/s}$. Given this, electron mobility following the introduction of twin structures was computed as $M_{total} \approx 1000 \text{ cm}^2/\text{V/s}$. In addition, the effect of twin structures on electron mobility as a percentage of all scattering factors was computed as approximately 60%.

The results discussed above suggest that at a mean twin spacing of 2.48 nm, electron mobility declines by 60% against figures for a GaAs film with no twin structures, indicating that the existence of high-density twin structures is a factor that exerts a significant effect on electron mobility.

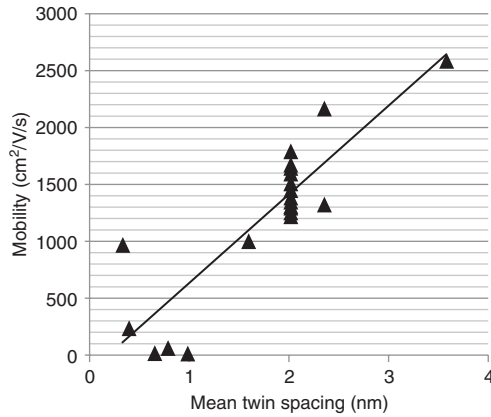


Fig. 12 Predicted mobility as a function of mean twin spacing

5. Conclusion

A method of quantitative prediction of the effect of twin structures on electron mobility has been developed. Twin structures were explicitly considered using the NEGF method based on first-principle calculations. Multiscaling was effected by converting figures for quantum conductance calculated using the NEGF method to scattering coefficients and incorporating these in an equation for evaluation of electron mobility. This made it possible to calculate electron

mobility in nanopillars in which twin structures exist.

The results of calculations using the developed method indicated that electron mobility in GaAs semiconductor nanopillars grown using the SA-MOVPE method under standard conditions (twin spacing of approximately 2.48 nm) would be $1000 \text{ cm}^2/\text{V/s}$. Given that electron mobility was measured at $2500 \text{ cm}^2/\text{V/s}$ in a thin GaAs film in which twin structures did not exist, the ratio of the effect of twin structures to the effect of total scattering factors was calculated as approximately 60%. It was therefore possible to separately evaluate the effect of scattering by twin structures.

By means of this research, computational materials science has clarified the mechanism of a phenomenon that has been challenging to study in tests, and the results obtained will find application in a variety of areas, including materials development and device design.

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■ Author ■



Mitsumoto KAWAI