Oscillator Strength of Normal-Incidence Intersubband Absorption in Conduction Bands of Si and Ge Quantum Wells Using Polarization

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Abstract

A theoretical calculation and an optical measurement method of normal-incidence absorption are proposed. By using a waveguide structure, optical interference and the problem of low level signal can be avoided in the measurement of normal-incidence absorption. The oscillator strength of intersubband absorption for a waveguide structure is calculated in Si(001), Si(110), and Ge(001) quantum wells. The polarization angle dependence of the measured and the calculated absorption strength can be obtained with the same waveguide structure, and be compared after normalization. The normal-incidence absorption in Si(110) and Ge(001) quantum wells is shown theoretically, and can be observed in the optical measurement using waveguide structures at the polarization angle of 90° .

I. Introduction

The intersubband transition, which is a carrier transition between energy states in a quantum well that absorbs a photon is direct even though the band gap is indirect. Therefore, Si-based material can be applied in the fabrication of optical devices using intersubband transitions. The first intersubband absorption has been observed in GaAs quantum wells, for which carrier transition occurs in Γ point[1]. Due to the symmetry, carriers cannot be excited by the optical field parallel to the quantum well layer, which corresponds to the normally incident light. Si(001) quantum well (Si well and $Si_{1-x}Ge_x$ barrier on Si(001) substrate) has the same problem[2,3]. However, for the conduction bands of Si(110) and Ge(001), the normal-incidence absorption is possible due the tilted energy valleys toward the growth direction[4,5]. Without normal-incidence absorption, a detector should have a grating or the light should be incident at an angle, which reduces the efficiency. Normal-incidence absorption can be measured by optical or electrical method. Though optical measurement is much easier, faster, and less expensive, it is not easy to measure the absorption strength optically in the case of normal-incidence because of the interference which is much stronger than the signal. Therefore, a waveguide structure can be used to prevent the interference and to enhance the signal strength. The signal from a waveguide structure includes intersubband absorption by both the normal incident light and parallel incident light. By changing the polarization angle of the incident light, the ratio of the perpendicular field and parallel field varies, and the two signal can be distinguished.

In order to identify the normal-incidence absorption, we need to calculate the absorption strength by normally incident light and to compare with the measurement. The calculation of the directly measurable absorption coefficient is very difficult due to the non-ideal nature of real samples. Therefore, a rather simple dimensionless quantity, the oscillator strength[1] and its polarization dependence of Si(001), Si(110) and Ge(001) are calculated in this paper. By polarizing the incident light, the polarization dependence of a structure can be measured as mentioned above and be compared with those of the normalized oscillator strength. The comparison of the normalized oscillator strength and the normalized absorption strength obtained by measurement shows good agreement for Si(001) and Ge(001)[2,5]. The result for Si(110) is not satisfactory and requires further study[4].

II. Oscillator Strength

The oscillator strength for the direct conduction band valley

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(conduction band minimum at Γ point) has been calculated for GaAs[1] and can be modified for the indirect conduction valley of Si and Ge (conduction band minimum at X and L point, respectively) with the optical electric field of the light incident at an angle[6]. The optical field of a unit magnitude can be represented by the polarization vector as shown in Fig. 1, and can be written as

$$\hat{\varepsilon} = \varepsilon_x \hat{x} + \varepsilon_y \hat{y} + \varepsilon_z \hat{z} \quad (1)$$

where $\hat{x}$, $\hat{y}$ and $\hat{z}$ represent unit direction vectors toward [100], [010], and [001] direction, respectively[6].

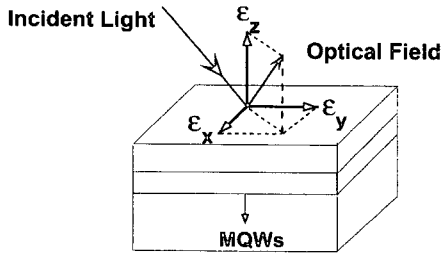

Fig. 1. The definition of a polarization vector. For incident light at an angle with a unit optical field, x, y, and z components of the polarization vector are defined as ε_x, ε_y, and ε_z.

Square potential wells are formed in $Si_{1-x}Ge_x/Si_{1-y}Ge_y$ heterostructures without doping due to the conduction band offsets. In contrast, parabolic potential wells are formed in the δ-doped layers with finite widths[7]. The heterostructures with δ-doping will be a mixture of the two. The oscillator strength for an infinite square potential well and a parabolic potential well are calculated for simplicity. For an infinite square potential well, the oscillator strength for a transition from state n to state n+1 can be written as [6,8]

$$f_{n\to n+1} = \frac{m_o}{w_{zz}} (\varepsilon_x w_{zx} + \varepsilon_y w_{yz} + \varepsilon_z w_{zz})^2 \frac{64}{\pi^2} \frac{(n+1)^2 (n+2)^2}{(2n+3)^3} \quad (2)$$

For the isotropic conduction band with an infinite square potential well, the equation above gives the same results as West's [1], assuming an isotropic mass. Due to the narrow and deep potential well, most of the transitions occur between the ground state and the first excited state, and the oscillator strength can be simplified to [6]

$$f_{0\to 1} = 0.96 \frac{m_o}{w_{zz}} (\varepsilon_x w_{zx} + \varepsilon_y w_{yz} + \varepsilon_z w_{zz})^2 \quad (3)$$

For a parabolic potential well, the oscillator strength for the transition from state n to state n+1 is

$$f_{n\to n+1} = \frac{m_o}{w_{zz}} (\varepsilon_x w_{zx} + \varepsilon_y w_{yz} + \varepsilon_z w_{zz})^2 (n+1) \quad (4)$$

For the isotropic conduction valley at the Γ point, the off-diagonal terms of the inverse mass tensor, w_{zx} and w_{yz} are zero, and the above oscillator strength reduces to that of an infinite parabolic potential for the Γ valley[7]. The oscillator strength of the transition from the ground state to the first excited state can then be simplified to

$$f_{0\to 1} = \frac{m_o}{w_{zz}} (\varepsilon_x w_{zx} + \varepsilon_y w_{yz} + \varepsilon_z w_{zz})^2 \quad (5)$$

which is almost the same as that for an infinite square potential well. Therefore, further calculations will be done under the assumption of a parabolic potential well for simplicity.

Since the effective masses of the occupied valleys determine the transition, it is necessary to analyze the occupancy of the conduction valleys. Fig. 2 shows the energy ellipsoids of Si(001), Si(110), and Ge(001), which are used in this study. Si(001) has six energy ellipsoids at the X points and they are composed of two X2 ellipsoids with a heavy effective mass and four X4 ellipsoids with a light effective mass. Si(110) has also six energy ellipsoids at the X points. However, the X4 ellipsoids are tilted toward the growth direction [110] and the effective mass is different from that of X4 ellipsoids in Si(001)[4]. Ge(001) has the halves of eight energy ellipsoids at the L points and the electrons equally occupy all of the L valleys. When the oscillator strength of each valley is different, the overall oscillator strength is the average of the contribution from each of the occupied valleys and is as follows :

$$f_{0\to 1} = \frac{1}{n^\nu} \sum_\nu \eta^\nu \frac{m_o}{w_{zz}^\nu} (\varepsilon_x w_{zx}^\nu + \varepsilon_y w_{yz}^\nu + \varepsilon_z w_{zz}^\nu)^2 \quad (6)$$

where n^ν is the number of occupied valleys and η^ν is the fractional occupancy in the νth valley. Equation (6) can be applied to quantum wells created by the heterostructures and/or the δ-doping.

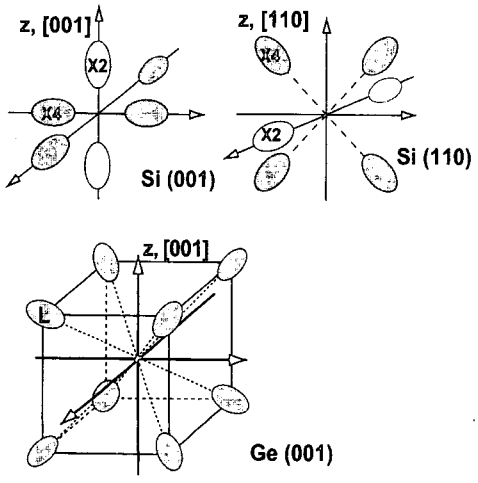

Fig. 2. The energy ellipsoids of Si(001), Si(110) and Ge(001).

III. Normal-Incidence Absorption

The polarization vector represents an IR(Infra-Red) beam which is incident to a sample from an arbitrary direction. When ε_z is non-zero, the oscillator strength cannot be zero because the diagonal element of the inverse mass tensor, w_{zz}, cannot be zero. However, when ε_z is zero, the optical field has only ε_x and/or ε_y components and the oscillator strength can be zero. For GaAs and Si(001) quantum wells, the oscillator strength reduces to

$$f_{0\to 1} = \frac{m_o}{w_{zz}^{\nu}} (\varepsilon_z w_{zz})^2 \tag{7}$$

regardless of the incident direction of the light since the off-diagonal elements of the inverse effective mass tensors are zero. Consequently, the oscillator strength is zero when ε_z is zero. For normally incident light to the surface, ε_z is zero, and there is no intersubband absorption in GaAs and Si(001).

In contrast, for the normal incident light (i.e., $\varepsilon_z = 0$), the oscillator strength for Si(110) and Ge(001) quantum wells can be written as

$$f_{0\to 1} = \frac{m_o}{w_{zz}^{\nu}} (\varepsilon_x w_{zx}^{\nu} + \varepsilon_y w_{yz}^{\nu})^2 \neq 0 \tag{8}$$

because the off-diagonal elements, w_{zx} and w_{yz} are not zero. Therefore, normal-incidence absorption is possible in Si(110) and Ge(001) quantum wells.

IV. Waveguide Structure

In actual experiments, a waveguide structure is often employed to measure the absorption spectra. The reasons for this are that a waveguide increases the absorption strength by multiple internal reflections, and therefore, gives a larger signal; and we can extract the polarization angle dependence of the absorption strength. It is very difficult to find the exact potential distribution in the quantum wells, and therefore, some uncertainty results in the theoretical values for given samples. However, the polarization angle dependence is independent of potential distribution in the z direction and determined by the effective masses (that is, a quantum well material determines them). Using a polarizer, we can easily obtain the polarization angle dependence of the absorption spectra and can compare them with the theoretical values. For convenience of comparison with experimental data, we also calculate the oscillator strength for a waveguide. Therefore, the polarization angle dependence of the measured absorption strength can be compared with calculated results.

Figure 3(a) shows the waveguide structure, and $\hat{z}$ is the growth direction of the multiple quantum well. A polarization angle θ is defined as 90° when the optical field is parallel to the surface and the waveguide edges for the propagating light incident to the side facet which has 45° angle from the growth direction as shown in Fig. 3(a). In this case, the polarization vector can be written as

$$\begin{aligned} \hat{\varepsilon} &= \varepsilon_x \hat{x} + \varepsilon_y \hat{y} + \varepsilon_z \hat{z} \\ &= \cos 45^\circ \cos\theta \hat{x} + \sin\theta \hat{y} + \sin 45^\circ \cos\theta \hat{z} \end{aligned} \tag{9}$$

for the waveguide structures, and the oscillator strength is reduced to

$$f_{0\to 1} = \frac{m_o}{w_{zz}} \left(\frac{1}{\sqrt{2}} w_{zx} \cos\theta + w_{yz} \sin\theta + \frac{1}{\sqrt{2}} w_{zz} \cos\theta \right)^2 \tag{10}$$

The 0° polarization angle can be defined accordingly. When θ is 90° it is the same as the normal incidence case because there exists the optical field parallel to the quantum well plane only.

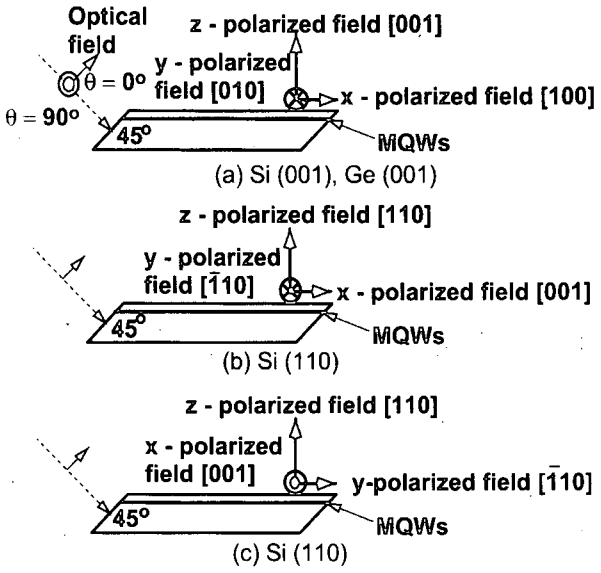

Fig. 3. The definition of x-, y-, and z-polarized fields with respect to crystallographic axes in the waveguides of Si(001), Ge(001), and Si(110). (a) Si(001) and Ge(001). (b) Si(110) when the light is incident in the [001] direction. (c) Si(110) when the light is incident in the [$\bar{1}$10] direction. The polarization angle is defined in (a). For the light incident to a waveguide at a 45° with respect to the growth direction, the polarization angle θ is defined as 90° when the optical field is parallel to the quantum well layers, and 0° is defined accordingly.

The polarization angle dependence of the oscillator strength can be calculated for the waveguide structures of Si(001), Si(110), and Ge(001) quantum wells using two equations above.

IV-1. Si (001)

First, we will discuss the Si(001) case. We define the x, y, and z component of the optical field as x-, y- and z-polarized field, respectively. For Si(001), $\hat{x}$, $\hat{y}$, and $\hat{z}$ are defined as [100], [010], and [001] direction, respectively, as shown in Fig. 3(a). Since the inverse mass tensor of Si(001) does not have any non-zero off-diagonal elements, the oscillator strength will have only one term involving w_{zz}.

Si(001) has two X2 valleys and four X4 valleys. Because they have different effective masses, the X2 valleys and the X4 valleys have different energy subbands. The inverse effective mass of X2 valleys is $1.02/m_o$ and that of X4 valleys is $5.26/m_o$. Therefore, the ground state of X2 valleys is lower than that of X4 valleys due to the heavy mass of electrons in X2 valleys. Therefore, the X2 valleys are occupied first, and the ratio of occupancy is determined by the energy difference between the ground states. Considering the contributions from each valley, the oscillator strength can be written as

$$f_{(001)}^{Si} = \frac{m_o}{2}(4w_{zz}\eta^{X4} + 2w_{zz}\eta^{X2})\cos^2\theta \tag{11}$$

where η^{X2} and η^{X4} are fractional occupancies in the X2 and the X4 valleys, respectively, such that

$$\begin{cases} 2\eta^{X2} + 4\eta^{X4} = 1 \\ \eta^{X2} = 0 \sim 0.5 \\ \eta^{X4} = 0 \sim 0.25 \end{cases} \tag{12}$$

The calculated oscillator strength is plotted as a function of the polarization angle θ in Fig. 4. The solid line and the dashed line represent the oscillator strength of the X4 valleys and the X2 valleys, respectively. The oscillator strength of the X4 valleys is much larger than that of the X2 valleys due to the larger inverse effective mass. The dotted line represents the oscillator strength when each valley is equally occupied (the X4 valleys have twice the number of electrons in this case).

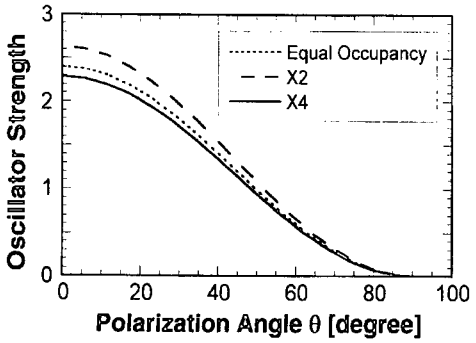

Fig. 4. The polarization angle dependence of the oscillator strength in Si(001) quantum wells.

IV-2. Si (110)

For Si(110), $\hat{x}$, $\hat{y}$, and $\hat{z}$ are chosen along the [001], [$\bar{1}$ 10], and [110] directions, respectively, and the projection of the incident light to the xy-plane is in the x direction as shown in Fig. 3(b). Although Si(110) also has four X4 valleys and two X2 valleys, the X4 valleys are tilted toward the growth direction [110], and the inverse mass tensor has non-zero off-diagonal terms. Considering the contributions from each valley, the oscillator strength can be written as

$$\begin{aligned} f_{(110)}^{Si} &= m_o\left[\frac{2w_{xx}}{2}\eta^{X2}\cos^2\theta + \frac{\eta^{X4}}{w_{zz}}\sum_{j,k=1}^{2}\left(\frac{1}{\sqrt{2}}w_{zz}\cos\theta + (-1)^{j+k}w_{yz}\sin\theta\right)^2\right] \\ &= m_o\left[(w_{xx}\eta^{X2} + 2w_{zz}\eta^{X4})\cos^2\theta + \frac{2w_{yz}^2\eta^{X4}}{w_{zz}}\sin^2\theta\right] \end{aligned} \tag{13}$$

where w_{xx}, $w_{zz}(=w_{yy})$, and w_{yz} are $5.26/m_o$, $3.14/m_o$, and $2.12/m_o$, respectively. The first two terms represent the intersubband absorption by the coupling of the z-polarized field and the diagonal terms of inverse mass tensor, and the third term represents the intersubband absorption by the coupling of x-polarized field and the off-diagonal terms of the inverse mass tensor, i.e. normal-incidence absorption. Therefore, η^{X4} should not be zero for normal-incidence absorption. The oscillator strength written in the equation above is plotted as a function of the polarization angle θ in Fig. 5. The solid line and the dashed line represent the oscillator strength of the X4 and X2 valleys, respectively. The oscillator strength of the X4 valleys is almost constant because it is obtained from a waveguide. If the light is incident parallel to the quantum well layers, the oscillator strength at the 0° polarization angle is doubled while that at the 90° polarization angle remains the same. The oscillator strength of the X2 valleys is larger than that of the X4 valley at the 0° due to its larger inverse effective mass. The dotted line represents the oscillator strength when each valley is equally occupied as in the case of Fig. 4.

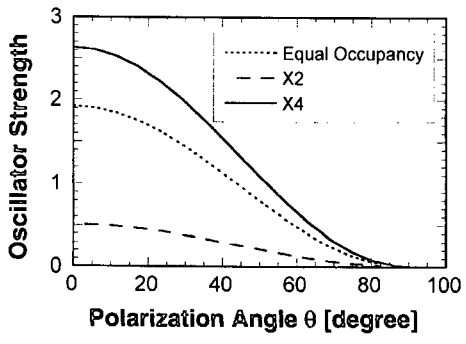

Fig. 5. The polarization angle dependence of the oscillator strength in Si(110) quantum wells when the optical field is incident along the [001] direction.

If the projection of the incident light on the xy-plane is in the y directions shown in Fig. 3(c), then the polarization angle dependence of the oscillator strength is quite different. The polarization vector is changed to

$$\hat{\varepsilon} = \sin\theta\hat{x} + \cos 45^{\circ}\cos\theta\hat{y} + \sin 45^{\circ}\cos\theta\hat{z} \tag{14}$$

and consequently, the polarization angle dependence of the oscillator strength can be written as

$$\begin{aligned} f_{(110)}^{Si} &= m_o\left[\frac{2w_{xx}}{2}\eta^{X2}\cos^2\theta + \frac{\eta^{X4}}{w_{zz}}\sum_{j,k=1}^{2}\left(\frac{1}{\sqrt{2}}w_{zz}\cos\theta\right.\right. \\ &\quad \left.\left. + \frac{(-1)^{j+k}}{\sqrt{2}}w_{yz}\cos\theta\right)^2\right] \\ &= m_o\left[\left(w_{xx}\eta^{X2} + \frac{2(w_{zz}+w_{yz}^2)}{w_{zz}}\eta^{X4}\right)\cos^2\theta\right]. \end{aligned} \tag{15}$$

In this case, the oscillator strength has a $\cos^2\theta$ dependence and normal-incidence absorption does not take place. Therefore, the incident direction of the polarized light is important for Si (110) quantum wells and normally incident unpolarized light always induces the intersubband absorption. The absorption strength is plotted in Fig. 6, which is similar to Fig. 4. However, the magnitudes of the oscillator strength are different from those of Fig. 4 due to the different inverse effective masses.

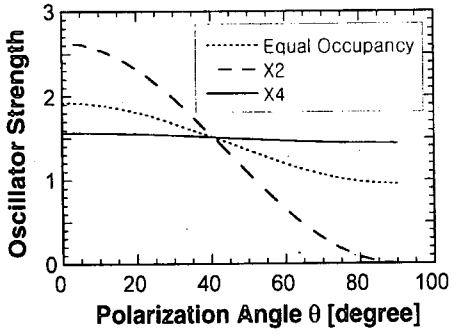

Fig. 6. The polarization angle dependence of the oscillator strength in Si(110) quantum wells when the optical field is incident along the $[\bar{1}10]$ direction.

IV-3. Ge (001)

For Ge(001), $\hat{x}$, $\hat{y}$, and $\hat{z}$ are chosen to be along the [100], [010], and [001] directions, respectively. Also, the projection of the incident light on the xy-plane is in the y direction as shown in Fig. 3(a). The total oscillator strength is averaged over all of the L valleys, and can be written as:

$$\begin{aligned} f_{(001)}^{Ge} &= \frac{m_o}{4w_{zz}}\left[\sum_{i,j=1}^{2}(-1)^i\frac{w_{zx}}{\sqrt{2}}\cos\theta\right. \\ &\quad \left. + (-1)^j w_{yz}\sin\theta + \frac{w_{zz}}{\sqrt{2}}\cos\theta\right)^2\Big] \\ &= \frac{m_o}{2}\left[\frac{w_{zx}^2}{w_{zz}}\cos^2\theta + \frac{2w_{yz}^2}{w_{zz}}\sin^2\theta + w_{zz}\cos^2\theta\right] \end{aligned} \tag{16}$$

where $w_{zx} = w_{yz} = 3.86/m_o$ and $w_{zz} = 8.33/m_o$. The first two terms are due to the coupling of the off-diagonal terms of the inverse mass tensor and the optical field, and the third term is due to the coupling of the diagonal terms and the optical field. In other words, the first, the second, and the third term are caused by x-, y-, and z-polarized fields, respectively, which were defined in Fig. 3. The z-polarized field couples with the diagonal terms, inducing the intersubband transition. This intersubband transition occurs for all carriers occupying any of the valleys. The x- and y-polarized fields couple with the off-diagonal terms of the inverse mass tensor, leading to normal-incidence intersubband absorption. This intersubband transition is possible only for those carriers in the energy ellipsoids which are not on the principal axes such as Si(110) and Ge(001). In other words, the off-diagonal terms of the inverse mass tensor should be non-zero. The oscillator strength is $m_o(w_{yz})^2/w_{zz}$ for $\theta = 90^{\circ}$, which is the normal-incidence case.

The oscillator strength of Ge(001) quantum wells is plotted in Fig. 7 as a function of the polarization angle θ. Due to the small effective mass, the oscillator strength is larger than those of Si(001) and Si(110) for both 0° and 90°. Since the energy of X valleys in Ge is not known well, there is a possibility that electrons occupy X4 valleys. In that case, the oscillator strength at 90° is smaller and the polarization angle dependence is different as shown in Fig. 7. The experiment shows that electrons occupy L valleys[6].

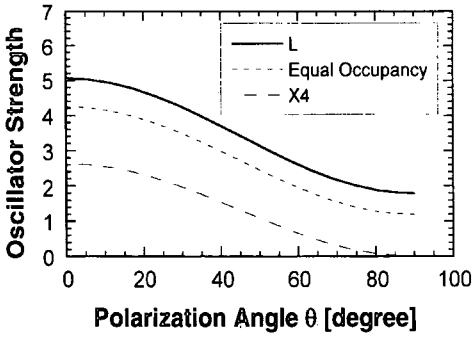

Fig. 7. The polarization angle dependence of the oscillator strength in Ge(001) quantum wells.

V. Summary

The oscillator strength is calculated for the electrons in Si(001), Si(110), and Ge(001) quantum wells where they make intersubband transition. The oscillator strength has the polarization angle dependence when a waveguide structure is used. While the polarization angle varies from 0° to 90°, two components of optical field change and so does the absorption spectra. Each quantum well has the unique

polarization dependence and the absorption spectra at $\theta = 90^{\circ}$ corresponding to the normal-incidence absorption. By measuring the absorption strength of a waveguide structure and comparing the normalized results with the normalized oscillator strength from the calculation, it is possible to identify if the signal is due to the intersubband absorption. Ge(001) has larger oscillator strength than Si(001) and Si(110) for both normal-incidence and parallel-incidence light due to the small effective mass of electrons.

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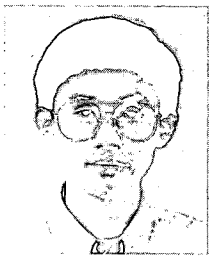

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