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The Orientation of Crystal Thin Layer with Diamond Structure Using Raman Scattered Light

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A method for determining the orientation of an arbitrarily oriented crystal thin layer using Raman scattered light has been proposed. The intensity of Raman scattered light from the diamond structure thin layer as a function of both the normal of the thin layer and the polarization direction of incident light is derived, and the orientation of the thin layer is then determined by means of four extrema of this function. The orientation results of this method for silicon wafers are compared with that determined by the X-ray method.

1. Introduction

The orientation of a semiconductor crystal thin layer, such as silicon epitaxial layer, MBE layer and SOI structure [1], is a parameter of great concern in the manufacture of semiconductor devices. The conventional used method, however, are unable to determine effectively the arbitrary orientation of the thin layer with thickness only about one micron. For example, the optical reflection method is not applicable to thin layer due to its destructive nature. It is difficult to obtain the orientation information of thin layer by X-ray method due to its large penetration depth ($\sim$25u). And the electron diffraction method is also inapplicable to any arbitrarily oriented thin layer due to the complexity of the diffraction pattern for an arbitrary orientation. Fortunately, the method of Raman scattering is useful in determining the orientation of thin layer, since the intensity of Raman scattered light is closely related to the crystal symmetry and the penetration depth of the incident light is small ($<$1u).

In the past, there existed a few studies of the orientation using Raman scattered light[2][3][4]. However, all those previous results are only applicable to a few special orientations. On the other hand, in the present study, the light intensity of vibration scattering from the diamond structure thin layer as a function of both the normal of the layer and the polarization direction of incident light is derived. So it is possible to determine the orientation of an arbitrarily oriented thin layer by means of four extrema of this function. To verify this method, the orientation results for silicon wafers by the present method have been compared with that determined by the X-ray method. The application of this method to analyse thin layers will be reported in another paper.

2. Method

Three coordinate systems are introduced. $(\vec{X}\ \vec{Y}\ \vec{Z})$ is the system of the crystal axes. $(\vec{x}\ \vec{y}\ \vec{z})$ is the system related to the thin layer with $\vec{z}$ perpendicular to the surface of the thin layer, $\vec{x}$ and $\vec{y}$ parallel to the surface of the thin layer, and the components of the unit vectors of $\vec{z}$ and $\vec{x}$ are taken respectively as (A,B,C), $(B,-A,0)/\sqrt{A^2+B^2}$ in $(\vec{X}\ \vec{Y}\ \vec{Z})$. Where $A^2+B^2+C^2=1$. $(\vec{x}'\ \vec{y}'\ \vec{z}')$ is the system used in experiment with $\vec{z}'$ parallel to $\vec{z}$,

and $\vec{x}'$ making an angle α with $\vec{x}$. If the incident and scattered rays propagate along $\vec{z}'$ and $-\vec{z}'$ respectively, and their unit electrical vectors $\vec{\varepsilon}_i$ and $\vec{\varepsilon}_s$ are parallel to each other and equal to $\vec{\varepsilon}$, and make an angle θ with $\vec{x}'$, then the components of $\vec{\varepsilon}$ in $(\vec{x}'\ \vec{y}'\ \vec{z}')$ are $(\cos\theta, \sin\theta, 0)$. From the coordinate transformation, the components of $\vec{\varepsilon}$ in $(\vec{X}\ \vec{Y}\ \vec{Z})$ are obtained to be

$$\vec{\varepsilon}: [B\cos\varphi + AC\sin\varphi, -A\cos\varphi + BC\sin\varphi, -(A^2+B^2)\sin\varphi]\frac{1}{\sqrt{A^4+B^2}}, \quad (1)$$

with $\varphi = \theta - \alpha$. (2)

According to the general theory of Raman scattering, the spectral differential cross section of vibration scattering for non polar crystal is[5]

$$\frac{d^2\sigma}{d\Omega\, d\omega_s} = A_0 \frac{\omega_i \omega_s^3}{\omega_0} \frac{n_s}{n_i}(n+1)\, g(\omega, \omega_0) \sum_h \left| \varepsilon_s^i \varepsilon_i^j (d^{ij}\xi^h) \right|^2. \quad (3)$$

Where A_0 is a constant; ω_i, ω_s and ω_0 are the frequencies of incident light, scattered light and phonon; n_i and n_s are the refractive indices of the crystal corresponding to the incident and scattered light; n is the phonon number; $g(\omega, \omega_0)$ is a function with its maximum at ω_0 and the integration of which over ω is equal to unity. $(d^{ij}\xi^h)_s$ are the tensor elements of susceptibility derivative, the matrix form of which in $(\vec{X}\ \vec{Y}\ \vec{Z})$ for diamond structure are

$$\left.\begin{aligned} |d^{ij}\xi^x| &= d\begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{vmatrix}, \\ |d^{ij}\xi^y| &= d\begin{vmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{vmatrix}, \\ |d^{ij}\xi^z| &= d\begin{vmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{vmatrix}. \end{aligned}\right\} \quad (4)$$

The scattered light intensity is proportional to the spectral differential cross section at ω_0 and the incident light intensity. Under the condition that $\vec{\varepsilon}_i = \vec{\varepsilon}_s = \vec{\varepsilon}$, and substituting (1),(4) into(3),then I,the light intensity of vibration scattering from diamond structure thin layer can be obtained as

$$I = \frac{B_0}{(A^2+B^2)^2} \sum_{i=0}^{4} C_i \cos^{4-i}\varphi \sin^i\varphi, \quad (5)$$

with $C_0 = A^2 B^2$,

$$\left.\begin{aligned} C_1 &= 2AB(A^2-B^2)C, \\ C_2 &= (A^2-B^2)^2C^2 - 2A^2B^2C^2 + (A^2+B^2)^3, \\ C_3 &= -2AB(A^2-B^2)\,C^3, \\ C_4 &= A^2B^2C^4 + (A^2+B^2)^3 C^2. \end{aligned}\right\} \quad (6)$$

And B_0 is a constant which is independent on A, B, C.

From the definition of unit vector, there are only two independent parameters which are chosen to be B/A and C/A. In general, the choice of two parameters can be quite arbitrary. However, for the sake of convenience, the following restriction is taken:

$$1 \geqslant B/A \geqslant C/A \quad (7)$$

The scattered light intensity I, expressed in (5) and (6), is a periodic function of φ with period of 180°. In the 0~180° region of φ, I has four extrema: high valley (HV), high peak (HP), low valley (LV) and low peak (LP). All the intensities of these extrema, I_{HV}, I_{HP}, I_{LV}, I_{LP} and the angles of these extrema, φ_{HV}, φ_{HP}, φ_{LV}, φ_{LP} depend on the orientation parameters B/A and C/A. From the four extreme intensities, two intensity ratios, I_{HV}/I_{HP} and I_{LV}/I_{LP}, can be obtained.

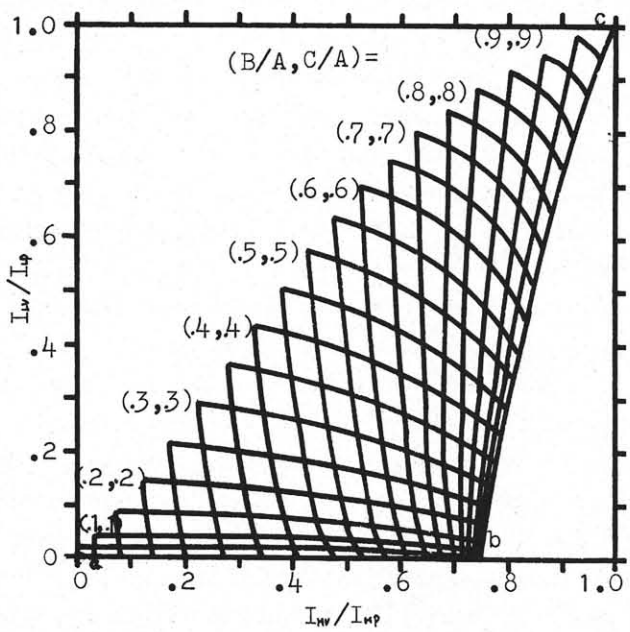

Fig. 1 Dependence of the intensity ratios I_{HV}/I_{HP} and I_{LV}/I_{LP} on the orientation parameters B/A and C/A. The vertical and horizontal lines are iso-B/A and iso-C/A lines.

The dependence of I_{HV}/I_{HP} and I_{LV}/I_{LP} on B/A and C/A is shown in Fig. 1. The

vertical and horizontal lines are iso-B/A and iso—C/A lines respectively. The values in brackets are B/A and C/A. It is obvious that the value of I_{HV}/I_{HP} depends mostly on B/A and I_{LV}/I_{LP} mostly on C/A. All iso-B/A and iso-C/A lines are in a curve-side triangle. The three vertices a, b, c correspond just to the three main orientations, namely [100], [110] and [111]. The points on the sides ab, bc and ac correspond to the orientations from [100] to [110], from [110] to [111] and from [100] to [111] respectively. And the scattered light intensities corresponding to the sides ab, bc and ac have characteristics that $I_{LV} = 0$, $I_{HP} = I_{LP}$ and $I_{HV} = I_{LV}$, respectively.

Among the extreme angles, the low valley angle φ_{LV} has the least dependence on orientation parameters. The dependence of φ_{LV} on B/A and C/A is shown in Fig. 2. It shows that φ_{LV} decreases monotonously with the increase of B/A or C/A.

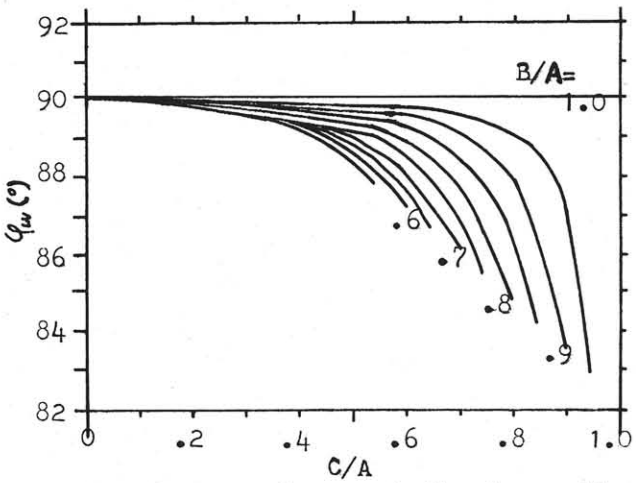

Fig. 2 Dependence of the low valley angle φ_{LV} on the orientation parameters B/A and C/A.

For an arbitrarily oriented thin layer with diamond structure, the procedure for determining the orientation is as follows: A polarized laser ray is projected perpendicularly onto the thin layer and the backscattered light with the same polarization direction as that of incident ray is chosen to be received. Then the thin layer is turned around the incident ray for varying θ, and the scattered light intensity I corresponding to each θ is measured. From the four extreme intensities in the $I \sim \theta$ relation, the B/A and C/A can be obtained using Fig. 1, and then A, B, C are known. From B/A and C/A, φ_{LV} can be found by using Fig. 2, then α is found by using formula (2) and the experimental value Θ_{LV}. Thus, the orientation of this thin layer is determined. If more accurate values are needed, then an iterative procedure can be used according to formulae (2), (5), (6) and taking above A, B, C, α as initial values.

3. Results

The specimens used in this study are surface—polished crystal silicon wafers and epitaxial silicon layers with different orientations. The instrument employed is the Raman spectrometer, Ramalog 5, made by the SPEX company, together with a specimen holder, designed and made by ourselves, from which the

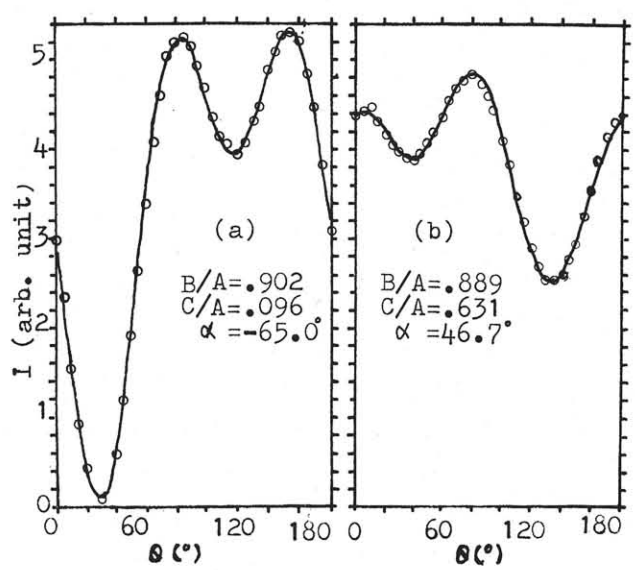

Fig. 3 Scattered light intensity I as function of turned angle θ for crystal silicon wafer (a) and epitaxial silicon layer (b). The circles are experimental results and the solid lines are theoretical results from formulae (2), (5), (6) and the values of B/A, C/A and α listed in this figure.

angle θ can be read accurately. The wavelength of the incident light is 5145Å. When the frequency shift ω_0 of the intensity peak (about 522 1/cm) and the background are determined from the Raman spectrum of silicon, the $I \sim \theta$ relation at ω_0 is then measured. The intensity I corresponding to a certain θ is obtained by averaging 40 received data and substracting the background.

In Fig. 3, the experimental $I \sim \theta$ relations for a crystal silicon wafer (a) and an epitaxial silicon layer (b) are shown by circles. From these data, the values of B/A, C/A and α can be found, which are listed in Fig. 3. Then the theoretical $I \sim \theta$ relations are calculated which are also shown in the same figure with solid lines. It can be seen that the theoretical results agree with experimental results very well for both silicon wafer and epitaxial layer.

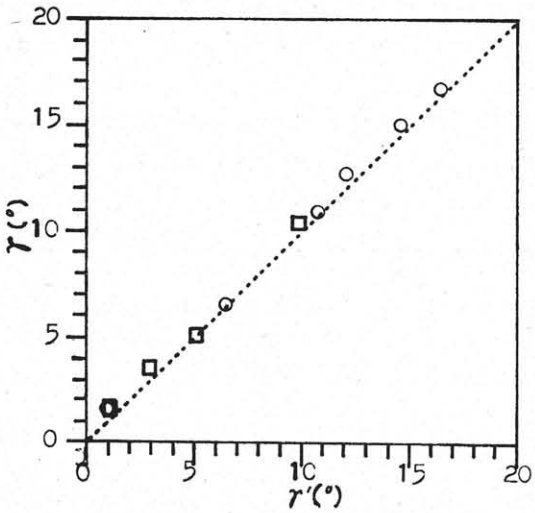

Fig. 4 Comparison of deviation angles obtained by this method (γ) and X-ray method (γ'). Squares are deviation angles from the normals of the wafers to [111] direction. And circles are that to [311] direction.

To compare the above method with X-ray method, two groups of silicon wafers are prepared with their normals close to two special directions which can be determined by X-ray method. When the values of B/A and C/A for each wafer have been determined using the present method, the deviation angle from the normal of each wafer to the special direction can be determined conveniently. In Fig. 4, the comparison of deviation angles obtained by the present method (γ) and X-ray method (γ') is shown, with the squares and circles expressing the deviation angles from the normals of the wafers to [111] and [311] directions, respectively. The agreement of orientation between results obtained by the present method and that by X-ray method is quite satisfactory.

4. Conclusions

1. The method proposed in this paper —— Extreme Raman Scattered Light Method can, with good accuracy, determine the orientation of an arbitrarily oriented crystal thin layer with diamond structure.

2. This method could be extended to another important structure of the commonly used semiconductors —— zinc blende structure.

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