APPENDIX: Electron diffraction patterns

In order to obtain theoretical patterns of electron diffraction, three factors such as the reciprocal lattice, structure factor and double diffraction should be taken into account. They are explained in order below.

All polytypes of SiC can be treated using hexagonal-type primitive cells. Usually Millar-Bravais indices such as $(hkil)$ and $(hk\cdot l)$*) are used to identify lattice planes of SiC, because this notation explicitly expresses symmetrical relationships between various faces in a hexagonal lattice. However, this notation is not benefit for vector calculation. Therefore, concerning diffraction Miller indices such as (hkl) are mainly used in this thesis. Though Miller indices for a cubic lattice are more popular for 3C-SiC, here all polytypes are treated as hexagonal lattices to keep generality of discussion. Readers should take care to avoid confusion due to interminglement of these notations.

*) Here, i must be equal to $-(h+k)$[1]. Therefore, i can be omitted and substituted by a dot. It must be remembered that $(hk\cdot l)$ is equal to $(hkil)$ and not equal to (hkl).

(i) Reciprocal lattice of SiC

A primitive cell of SiC is defined by primitive vectors of a_1, a_2 and a_3 shown in Fig.1. SiC consists of repetition of tetrahedrons shown in Fig.2. The length of edges of the tetrahedron is equal to $|a_1|$ and $|a_2|$ and its height is equal to $|a_3|/n$. Therefore, $|a_1|=|a_2|=|a_3|/(n\sqrt{6}/3)=a_0=3.08$Å. n is a number of layers in the repeat distance of a primitive cell in the [001] direction. The ‹001› direction is a so-called c-axis direction. a_1, a_2 and a_3 are expressed as follows:

$$a_1 = a_0\begin{pmatrix}\cos 30^\circ\\ \sin 30^\circ\\ 0\end{pmatrix},\quad a_2 = a_0\begin{pmatrix}\cos 150^\circ\\ \sin 150^\circ\\ 0\end{pmatrix},\quad a_3 = a_0\begin{pmatrix}0\\ 0\\ n\sqrt{6}/3\end{pmatrix}. \qquad (1)$$

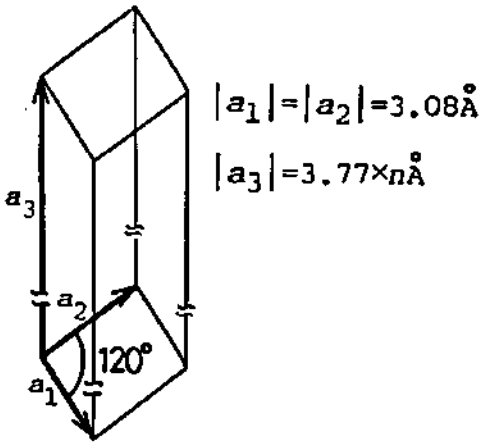

Fig.1 Primitive cell of SiC.

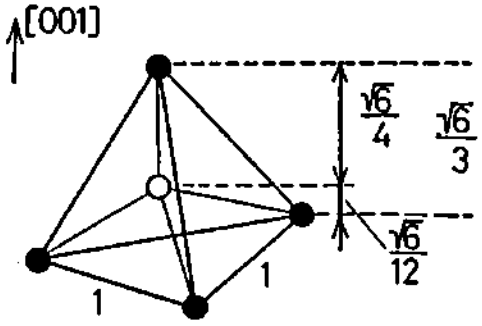

Fig.2 Tetrahedron component of SiC crystals.

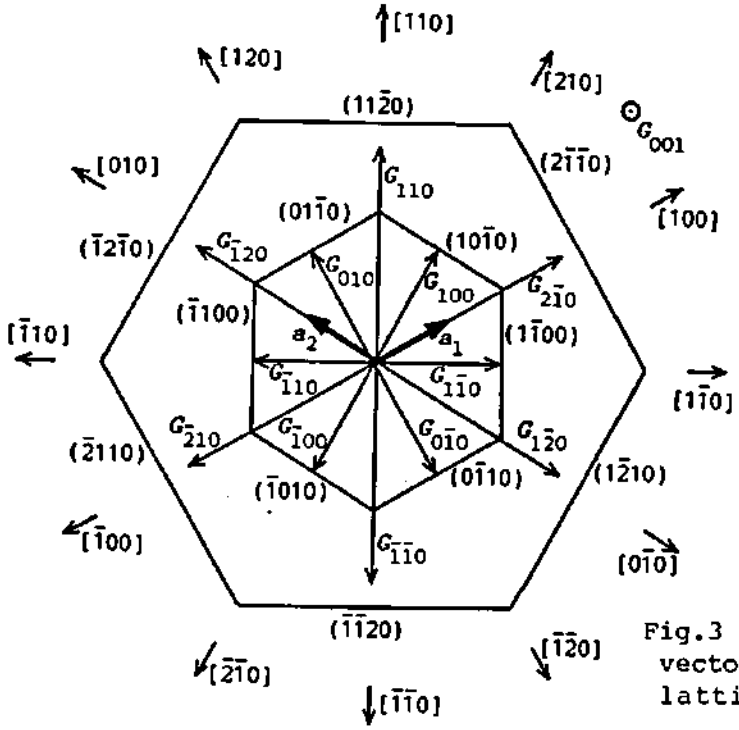

Fig.3 Orientations of reciprocal vectors, lattice directions and lattice planes.

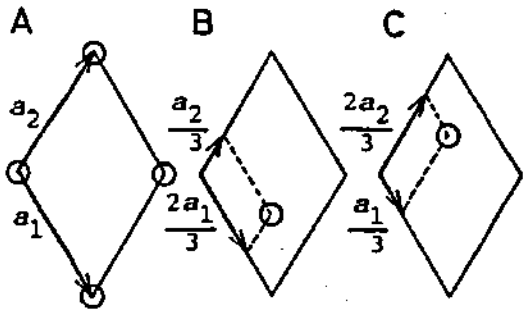

Fig.4 Positions of atoms in *A*-, *B*- and *C*-layers.

The axis vectors b_1, b_2 and b_3 of the reciprocal lattice are given as follows[2]:

$$b_1 = (2\pi/V)a_2 \times a_3 ,$$
$$b_2 = (2\pi/V)a_3 \times a_1 , \qquad (2)$$
$$b_3 = (2\pi/V)a_1 \times a_2 ,$$

where $V = a_1 \cdot a_2 \times a_3$.

Therefore, the axis vectors of the reciprocal lattice for SiC are obtained as follows:

$$b_1 = b_0 \begin{pmatrix} \cos 60^\circ \\ \sin 60^\circ \\ 0 \end{pmatrix} , \quad b_2 = b_0 \begin{pmatrix} \cos 120^\circ \\ \sin 120^\circ \\ 0 \end{pmatrix} , \quad b_3 = b_0 \begin{pmatrix} 0 \\ 0 \\ 3\sqrt{2}/4n \end{pmatrix} , \qquad (3)$$

where $b_0 = (4\pi\sqrt{3}/3)a_0$) .

In the real space the angle between a_1 and a_2 was 120°, however, in the reciprocal space the angle between b_1 and b_2 is 60°. A reciprocal lattice vector G_{hkl} is defined as follows:

$$G_{hkl} = hb_1 + kb_2 + lb_3 \quad (h,k,l: \text{ integers}) . \qquad (4)$$

G_{hkl} is perpendicular to (hkl) and $2\pi/|G_{hkl}|$ is equal to lattice spacing of (hkl). Figure 3 shows relatioships concerning orientations among the reciprocal lattice vectors, lattice directions expressed by Mirror indices and lattice planes expressed by Mirror-Bravais indices. (hkl) is perpendicular to $G_{h\underline{k}\underline{l}}$ and omitted in Fig.3. (hkl) is not perpendicular to $[hkl]$. $\{2\bar{1}\bar{1}0\}$ and $\{10\bar{1}0\}$ planes are drawn by a large and small hexagons, respectively. In the case of Mirror-Bravais indices $\{2\bar{1}\bar{1}0\}$ and $\{10\bar{1}0\}$ planes are perpendicular to $\langle 2\bar{1}\bar{1}0\rangle$ and $\langle 10\bar{1}0\rangle$ directions.

(ii) Structural factor

The condition of diffraction is given as follows using the wave vector k of an incident beam($|k| = 2\pi/\lambda$, λ: wave length of the incident beam)[2]:

$$2k \cdot G_{hkl} = G^2 , \qquad (5)$$

where G is $|G_{hkl}|$. However, even if G_{hkl} satisfies this equation, sometimes diffraction cannot be observed. For example, diffraction due to Si(100) and (200) is not observed in the case of X-ray diffraction. Such phenomena are explained by the

structure factor. The structure factor S is given as [2]

$$S(G_{hkl})=\sum_j f_j \exp(-2\pi i(hx_j+ky_j+lz_j)) \ , \qquad (6)$$

$$r_j= x_j a_1 + y_j a_2 + z_j a_3 \ , \qquad (7)$$

where r_j is the vector to the center of atom j in a primitive cell and f_j atomic form factor. The atomic form factor is common to the atoms of a kind. Scattering intensity is proportional to $S\cdot S^*$. When $S=0$, diffraction is not observed.

The structure factor of SiC is obtained by the procedure explained below. Structures of all polytypes of SiC are identified by stacking sequences of layers in <001> direction as explained in Chapter I. For example, 3C and 6H-SiC have the staking sequences of *ABC* and *ABCACB*. The primitive cell of SiC contains n Si atoms and n C atoms. The positions of atoms in the primitive cell are expressed utilizing the stacking sequence. Locations of atoms in each layer are shown in Figs.4(a)-(c). Each Si atom locates $|a_3/4n|$ away from the nearest C atom belonging to the same layer as shown in Fig.2. When a Si atom locates at the origin and belong to *A*-layer the structure factor S is given for all polytypes as follows:

$$S= (f_{Si}+\exp(-2\pi i/4n)f_C)\cdot \sum_{j=0}^{n-1} \exp(-2\pi i(g_j+il/n)) \ , \qquad (8)$$

$$g_j(\text{A-layer})=0,\ g_j(\text{B-layer})=(-h+k)/3,\ g_j(\text{C-layer})=(h-k)/3 \ , \qquad (9)$$

Where f_{Si} and f_C are the atomic form factors for Si and C. $(f_{Si}+\exp(-2\pi i/4n)f_C)$ will not be zero for any G_{hkl} and the next formula can be used to obtain G_{hkl} which makes S be zero.

$$S'=\sum_{j=0}^{n-1} \exp(-2\pi i(g_j+il/n)) \ , \qquad (10)$$

For example S' of 2H-SiC whose stacking order is *AB* is explicitly expressed as follows:

$$S'_{2H}=1+\exp(-2\pi i(-h+k)/3)\cdot\exp(-\pi il) \ . \qquad (11)$$

If l is an odd number and $(-h+k)$ is a multiple of 3, S' and S will be zero.

(iii) Prediction of diffraction pattern

When G_{hkl} satisfies eq.(5) and $S'(G_{hkl})\neq 0$, diffraction is observed as a spot on a screen. In order to obtain reciprocal vectors which satisfy eq.(5), the construction due to Ewald[3] is convenient. So-called the Ewald sphere of $|k|$ in a radius which contact with the origin of reciprocal space is drawn. Reciprocal lattice points which contact with the Ewald sphere give rise to diffraction. In the case of electron diffraction, a radius of the Ewald sphere is much larger than the axis vectors of the reciprocal lattice. Therefore, nearby the origin, the Ewald sphere is approximated by a plane normal to the incident beam. The reciprocal points which contact with the plane are given using two reciprocal vectors which are not parallel to each other and perpendicular to the incident beam. A map of these reciprocal points appears as diffraction pattern on a screen.

In the case of RHEED observation of SiC(0001), G_{001} is always perpendicular to the incident azimuth. Another vector which is perpendicular to the incident azimuth is achieved by referring Fig.3. For examples, G_{010} and $G_{1\bar{2}0}$ are perpendicular to [100] and [210] azimuths, respectively. A [100] azimuth RHEED pattern of 2H-SiC(0001) is drawn as follows. G_{010} and G_{001} are perpendicular to [100] azimuth. Grid points given by $m_1G_{010}+m_2G_{001}$ (m_1,m_2: integer) represent a observable pattern. These two vectors are perpendicular to each other and $|G_{010}|/|G_{001}|=1.89$ based on eqs.(3) and (4)*). Therefore, the pattern is drawn and indices are given to each point as shown in Fig.5. In the case of RHEED observation, spots given by negative values of m_2 cannot be observed shaded by a specimen. A spot due to G_{hkl} which makes $S'(G_{hkl})$ zero is drawn by an white circle and others are drawn by solid circles. However, spots indicated by white circles are actually observed because of the double diffraction[4]. If diffraction due to $G_{h1,k1,11}$ and $G_{h2,k2,12}$ takes place, diffraction due to $G_{h1\pm h2,k1\pm k2,11\pm 12}$ also takes place even if $S(G_{h1\pm h2,k1\pm k2,11\pm 12})$ is equal to zero. Such a phenomena is called the double diffraction. For example, G_{001} in

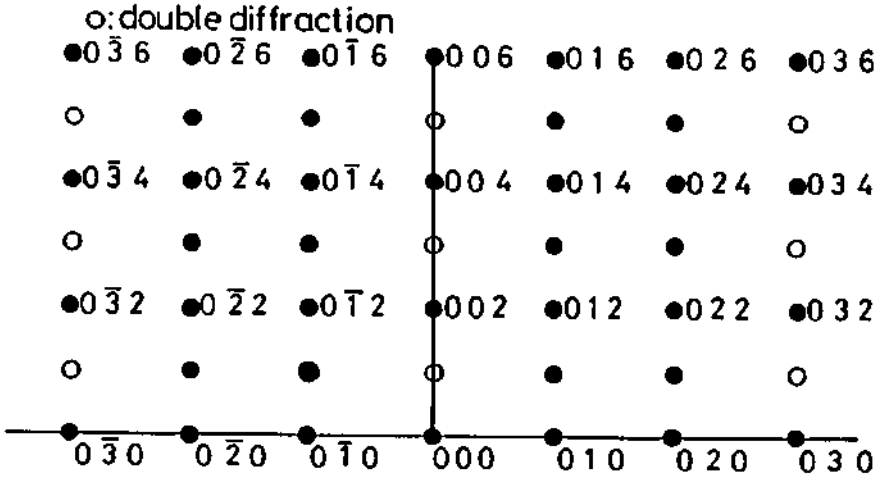

Fig.5 [100](or [2$\bar{1}\bar{1}$0]) azimuth RHEED pattern of 2H-SiC(0001).

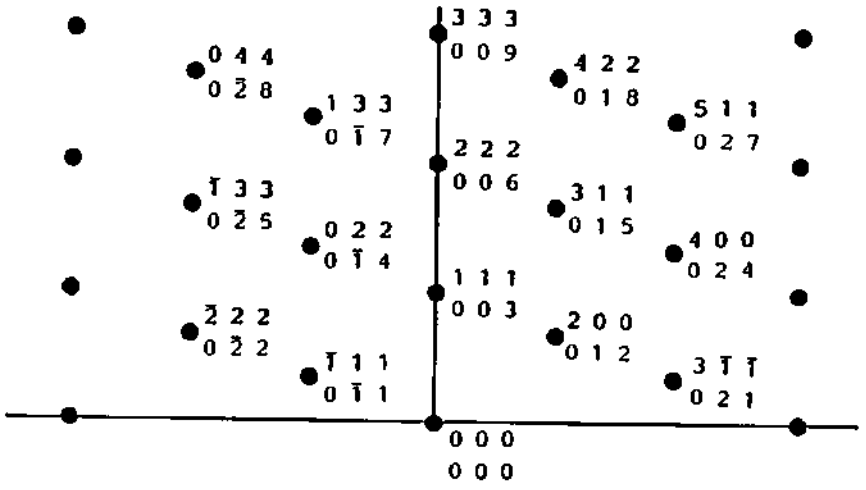

Fig.6 [100] azimuth pattern of 3C-SiC(0001). This expression is equal to "[01$\bar{1}$] azimuth pattern of 3C-SiC(111)" for cubic notation. Indicies for hexagonal and cubic notations are written in normal and bold-faced characters.

Fig.5 is synthesized by G_{100} and G_{101}.

In the discussion above, all polytypes of SiC are treated as hexagonal lattices. However, symetrical relationships peculiar to 3C-type cannot be explicitly expressed by this way. For comparison of notations for a hexagonal and a cubic lattice, A [100] azimuth pattern of 3C-SiC(0001) (or a $[01\bar{1}]$ azimuth pattern of 3C-SiC(111) in cubic notation) is shown in Fig.6. Indices are given by the both notations.

*) The lattice spacing d_{hkl} of (hkl) faces in hexagonal lattice is given by following expression.

$$d_{hkl}^{-2}=(4/3)(h^2+hk+k^2)/a+l^2/c^2 \quad (a=|a_1|=|a_2|,\ c=|a_3|)\ .$$

$|G_{hkl}|$ is also calculated utilizing this formula.

References

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[3] M.Plutton, *Surface Physics*, (Oxford Univ. Press, Oxford, 1975), Chapter 3.

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