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PREMONOCHROMATOR CHARACTERISTICS OF Si AND Ge CRYSTALS FOR NUCLEAR BRAGG SCATTERING

July 1990

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Premonochromator Characteristics of Si and Ge Crystals for Nuclear Bragg Scattering

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The use of monochromator plays an important role as monochromatizing the photon from a facility having an electron storage ring to a narrow band width about the wavelength determined by the Bragg condition. This paper describes the dynamical diffraction formulae and collects the characteristics data of premonochromators of Si and Ge crystals for nuclear Bragg scattering. The numerical studies show the following data.

(1) Reflectivity, Bragg reflection width, energy resolution and integral reflecting power for the various reflections of Si and Ge crystals at the photon with the resonance excitation energy of the Mössbauer nuclei of ^{181}Ta(6.21 keV), ^{169}Tm(8.42 keV), ^{57}Fe(14.41 keV), ^{119}Sn(23.87 keV) and ^{238}U(44.70 keV).

(2) Tables of susceptibilities and figures of rocking curves for the various reflections of Si and Ge crystals.

Keywords: Monochromator, Photon, Electron Storage Ring, Bragg Reflection, Dynamical Diffraction, Si and Ge, Nuclear Bragg Scattering, Reflectivity, Energy Resolution, Mössbauer Nuclei, Susceptibility, Rocking Curves

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核ブラッグ散乱用前置モノクロメータシリコン・ゲルマニウム結晶の特性

日本原子力研究所大型放射光施設計画推進室
原見　太幹

（１９９０年６月１日受理）

電子蓄積リングからの光をブラッグ条件で決まる狭いバンド幅に単色化するのに，モノクロメータが重要な役割を果たす。この論文は，動的回折を記述し核ブラッグ散乱用シリコン・ゲルマニウム結晶の特性データを収集したものである。

データは，^{181}Ta（6.21 keV），^{169}Tm（8.42 keV），^{57}Fe（14.41keV），^{119}Sn（23.87 keV），^{238}U（44.70 keV）のメスバウア核共鳴励起エネルギーの光に対するシリコン・ゲルマニウム結晶の反射率，反射幅，エネルギー分解能，積分反射パワー，分散，ロッキンギ曲線である。

日本原子力研究所：〒319－11　茨城県那珂郡東海村白方字白根２－４

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{NOMENCLATURES}

$\vec{a}, \vec{b}, \vec{c}$: unit cell vector along the principal axes,

C : polarization factor,

d : spacing between Bragg reflecting planes,

E : photon energy,

ΔE: energy width of Bragg reflection,

e^{-2M}: Debye temperature factor,

F_{hr} : structure factor defined by Eq. (8),

F_{hi} : structure factor defined by Eq. (9),

f^0 : atomic scattering factor defined by Eq. (20),

f_j : atomic scattering factor of the j-th atom,

Δf' : real part of anomalous dispersion correction,

Δf'' : imaginary part of anomalous dispersion correction,

g : function defined by Eq. (5),

h, k, l : Miller indices of Bragg reflection,

I : integral reflecting power defined by Eq.(16),

L : function defined by Eq. (3),

M : function defined by Eq. (21),

m : mass of atom,

R : reflectivity,

r_e : electron radius,

T : temperature,

V : unit cell volume,

W : function defined by Eq. (4),

x : function defined by Eq. (24),

θ_B : Bragg angle,

θ_0 : incident angle of photon on reflecting plane,

$\Delta\theta_s$: angular deviation of reflection center
from Bragg angle,

Θ_M : characteristic Debye temperature,

κ : function defined by Eq. (6),

λ : photon wavelength,

$\Delta\lambda$: wavelength width of Bragg reflection defined by (15),

μ : absorption coefficient,

$\Phi(x)$: function defined by Eq. (23),

$\Psi_{h(r,i)}$: function defined by Eq. (7),

ω_s : intrinsic width of Bragg reflection defined by (13),

1. INTRODUCTION

This preliminary report is intended to present an information on the characteristics of premonochromator for nuclear Bragg scattering. It is expected by using these informations that much closer interaction can be established between users and the beam line physicists.

The photon from bending magnets or insertion devices (undulator and wiggler) can have important application in solid-state spectroscopy, molecular physics, biology and photo chemistry. We presented the source characteristics; energy, brilliance, flux and power spectra of synchrotron photon from bending magnets and insertion devices(undulator and wiggler) in the previous papers[1,2]. The continuous spectrum of synchrotron x-rays offers a great freedom to select wavelengths and band widths most suitable to particular experiments. On the other hand, this makes installation of monochromator indispensable. The use of monochromator plays an important role as monochromatizing the photon from an electron storage ring to a narrow band width about the wavelength,λ, determined by the Bragg condition:

$$\lambda = 2d\sin\theta_B, \tag{1}$$

where d is the spacing between the Bragg reflecting planes and θ_B is the angle between the incident x-ray and the reflecting planes. Monochromator should have the following performances; (i) high intensity reflection or transmission, (ii) high peak-to-background ratio, (iii) resistivity to radiation damage, (iv) good thermal stability.

We describe the dynamical diffraction formulae of x-rays in perfect crystals Si and Ge which are common materials to build x-ray monochromators. For large perfect crystals the kinematical theory is no longer valid and the dynamical theory must be used. The dynamical theory differs from the kinematical theory in that it correctly allows for the attenuation of the incident beam of x-rays by scattering and absorption which the kinematical theory ignores. Commercially available high-quality crystals of Si and Ge are nearly perfect and their diffraction properties are satisfactorilly predictable from the dynamical theory.

In chapter 2, the dynamical diffraction theory is outlined. In chapter 3, the crystal structures of Si and Ge are described. In chapter 4, the atomic scattering factors of Si and Ge are collected. The familiar Debye Waller factor is discussed in chapter 5. Monochromator characteristics of Si and Ge for nuclear Bragg scattering are described in chapter 6. In chapter 7, conclusion is given.

2. DYNAMICAL DIFFRACTION

Suppose linear polarized x-rays in Bragg geometry (i.e.back reflection) strikes the surface of an infinitely thick crystal with center of symmetry. The reflectivity can be written[3,4,5]

$$R(W)=L-\sqrt{L^2-1}, \tag{2}$$

$$L=\frac{1}{1+\kappa^2}\left\{W^2+g^2+\left[\left(W^2-g^2-1.0+\kappa^2\right)^2+4\left(gW-\kappa\right)^2\right]^{1/2}\right\}, \tag{3}$$

$$W=\frac{\psi_{or}}{C\,|\psi_{hr}|}+\frac{\sin 2\theta_B}{C\,|\psi_{hr}|}(\theta_0-\theta_B), \tag{4}$$

$$g=\frac{\psi_{0i}}{C\,|\psi_{hr}|}, \tag{5}$$

$$\kappa=\frac{|\psi_{hi}|}{|\psi_{hr}|}. \tag{6}$$

The variation of R as a function of L is shown in Fig.2.1. Figure 2.2 shows the values of L as functions of g and κ. The formulae (2) and (3) are numerically evaluated for values of g varying from zero to -0.6 and for values of κ = 0.0, 0.1 and 0.2. The reflection curves are plotted in Figs. 2.3 ,2.4 and 2.5. The curves are symmetric about W = 0.0 only when κ = 0.0. R for all values of W decreases continulously with increasing magnitude of g. g = -0.0527 and κ = 0.0 give the value of R = 0.9 at W = 0.0 where L = 1.0056. The integrated reflection is given by $(1/2)\int_{-1}^{1}R(W)dW$ and shown in Fig. 2.6. For a given value of κ, the integrated reflection is monotonically decreasing function of $|g|$.

ψ_r's and ψ_i's are real and imaginary parts of the susceptibility for the particular reflection, in which the temperature factor is included.

$$\psi_{h(r,i)}=-\frac{r_e\lambda^2}{\pi V}F_{h(r,i)}e^{-M}, \tag{7}$$

where the structure factor takes the forms

$$F_{hr}=\sum_j (f^0+\Delta f')_j e^{2\pi i h r_j}, \tag{8}$$

$$F_{hi}=\sum_j (\Delta f'')_j e^{2\pi i h r_j}. \tag{9}$$

The atomic scattering factor of the j-th atom in the unit cell is written as

$$f_j = (f^0+\Delta f'+i\Delta f'')_j, \tag{10}$$

where $\Delta f'$ and $\Delta f''$ are the real and imaginary parts of the anomalous dispersion correction, which are virtually independent of $\sin\theta_B/\lambda$. The anomalous scattering factor accounts for the absorption of x-rays by electrons of finite binding energy in an atom. The anomalous scattering effect is strongest at absorption edges. nevertheless, the effect is not entirely negligible to calculate the scattering amplitude even for wavelengths away from the absorption edge. r_e is the classical electron radius given by h/mc = 2.63 x 10^{-13} cm. V is the volume of unit cell of crystal. r_j stands for positions of atom within the unit cell. f^0 is the atomic scattering factor of the j-th atom in the unit cell, taking account of the spacial distribution of electrons in the atom. ψ_{0i} is related to absorption coefficient as follows:

$$\psi_{0i}=-\mu\lambda/2\pi. \tag{11}$$

Table 2.1 lists the absorption coefficients of Si and Ge over the energy range from 1.0 keV to 123.93 keV (Fig. 2.7)[6]. C is the polarization factor, and C = 1 for the normal component (σ component) of polarization and C = $|\cos 2\theta_B|$ for the parallel component (π component). Subscripts 0 and h refer to the forward

and Bragg-reflected directions. e^{-M} is the Debye-Waller factor which will be discussed in chapter 5. W is a parameter representing the deviation of the angle of the incidence θ_0 from the Bragg angle θ_B , which is given by the Bragg equation (1). Typically, for silicon crystals, the bandwidth will be of order 1 eV about the Bragg energy

$$E = hc/2d\sin\theta_B. \tag{12}$$

A common monochromator configuration consists of two parallel perfect crystals. From geometry, any light ray that satisfies the Bragg condition for one crystal automatically satisfies it for the second. An advantage of having two crystals is that the beam leaving the second crystal is parallel to the incident beam which makes the design of experimental apparatus simpler. A second crystal serves to reject fluorescence radiation that is emitted from the first crystal due to incoherent absorption.

The intrinsic width of the Bragg reflection, w_s, is given by[7]

$$w_s = \frac{2}{\sin 2\theta_B}\frac{r_e\lambda^2}{\pi V}C|F_{hr}|e^{-M}. \tag{13}$$

In the zero-absorption approximation, the reflectivity is unity in this angular range and total reflection occurs. The center of $R(\theta_0)$, where W = 0, is deviated from the Bragg angle due to refraction by an amount[7]

$$\Delta\theta_s = \frac{1}{\sin 2\theta_B}\frac{r_e\lambda^2}{\pi V}F_{0r}e^{-M}. \tag{14}$$

The values for F_h's can be calculated from the known atomic scattering factors. Except in the close vicinity of absorption edges, $\Delta f'$ and $\Delta f''$ are only small parts of f_h for a given Bragg

reflection. From the equations (1) and (5), we find[7]

$$\frac{\Delta\lambda}{\lambda}=\frac{\Delta E}{E}=\frac{4r_e}{\pi V}d^2C\,|F_{hr}|\,e^{-M}. \tag{15}$$

Thus, the intrinsic energy resolution of a Bragg reflection is independent of photon energy E, if F_{hr} is constant.

The integral reflecting power for a particular state of polarization is given by

$$I=\int_{-\infty}^{\infty}R(\theta_0)\,d\theta_0. \tag{16}$$

This can be well approximated by[7]

$$I=\frac{8}{3\sin 2\theta_B}\frac{r_e\lambda^2}{\pi V}C\,|F_{hr}|\,e^{-M}. \tag{17}$$

for weakly absorbing crystals.

Table 2.1 Absorption coefficients of Si and Ge (cited from Ref.(6))

Energy (keV)	Wavelength (Å)	Absorption coefficient (cm^2/g)	
		Si(Z=14)	Ge(Z=32)
123.93	0.10	0.16	0.35
82.62	0.15	0.22	0.89
61.96	0.20	0.31	1.90
49.57	0.25	0.45	3.50
41.31	0.30	0.67	5.85
35.41	0.35	0.96	9.00
30.98	0.40	1.35	13.0
27.54	0.45	1.80	19.0
24.79	0.50	2.40	24.5
22.53	0.55	3.15	31.5
20.65	0.60	4.05	40.5
19.07	0.65	5.20	48.5
17.70	0.70	6.40	60.0
16.52	0.75	7.75	72.0
15.49	0.80	9.20	87.0
14.58	0.85	10.0	107.0
13.77	0.90	13.5	126.0
13.04	0.95	15.5	133.0
12.39	1.00	17.5	152.0
11.80	1.05	20.5	173.0
11.27	1.10	23.5	210.0
10.78	1.15	26.5	30.0
10.33	1.20	29.5	34.0
9.91	1.25	33.5	38.0
9.53	1.30	37.5	43.0
9.18	1.35	42.0	47.0
8.85	1.40	47.0	53.0
8.26	1.50	57.0	63.0
7.75	1.60	69.0	76.0
7.47	1.66	76.0	84.0
6.92	1.79	94.0	104.0
6.42	1.93	116.0	128.0
5.90	2.10	146.0	158.0
5.63	2.20	172.0	178.0
5.44	2.28	193.0	198.0

Table 2.1 Absorption coefficients of Si and Ge (continued)
(cited from Ref.(6))

Energy (keV)	Wavelength (Å)	Absorption coefficient (cm^2/g)	
		Si(Z=14)	Ge(Z=32)
5.23	2.37	217.0	218.0
5.04	2.46	241.0	240.0
4.88	2.54	260.0	260.0
4.62	2.68	302.0	300.0
4.49	2.76	328.0	325.0
4.29	2.89	369.0	370.0
4.06	3.05	426.0	415.0
3.93	3.15	464.0	440.0
3.77	3.29	520.0	490.0
3.59	3.45	591.0	595.0
3.44	3.60	665.0	730.0
3.31	3.74	735.0	760.0
3.14	3.95	950.0	840.0
2.99	4.15	965.0	920.0
2.82	4.40	1125.0	1095.0
2.70	4.59	1265.0	1210.0
2.62	4.73	1375.0	1320.0
2.39	5.18	1730.0	1500.0
2.29	5.40	1960.0	1670.0
2.15	5.77	2260.0	1895.0
2.04	6.07	2565.0	2110.0
2.00	6.21	2725.0	2180.0
1.92	6.45	3000.0	2300.0
1.81	6.86	290.0	2575.0
1.75	7.08	315.0	2750.0
1.49	8.34	480.0	3995.0
1.25	9.89	740.0	
1.04	11.90	1230.0	

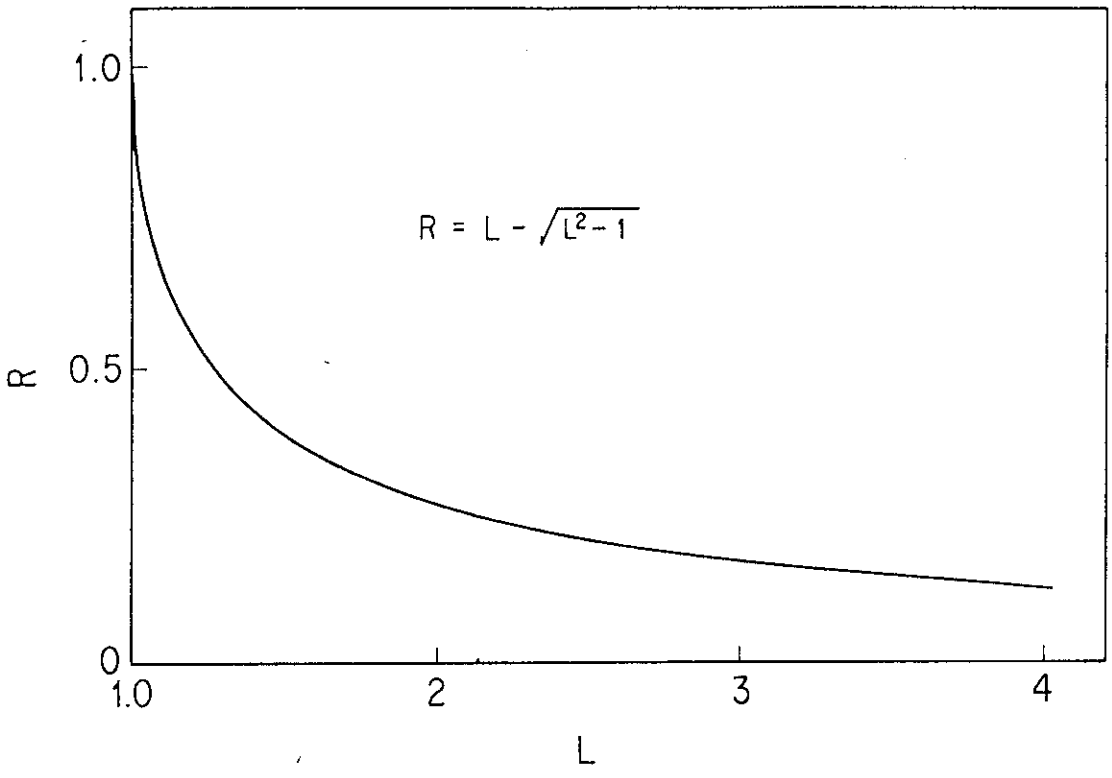

Fig.2.1 Dependency of reflectivity R on L defined by Eq. (3)

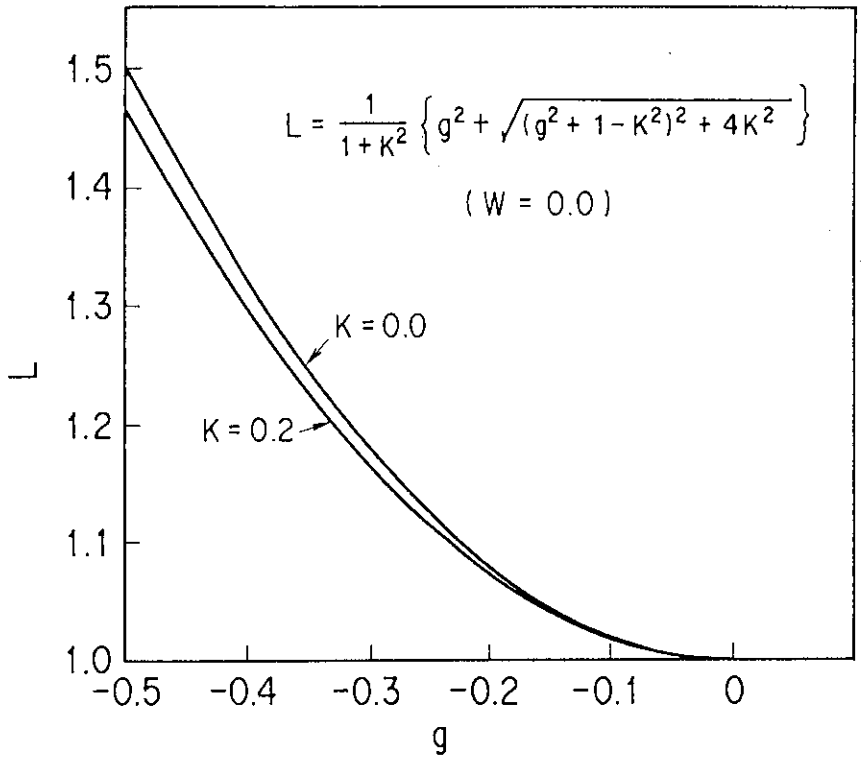

Fig.2.2 Dependency of L on g and κ at W = 0.0

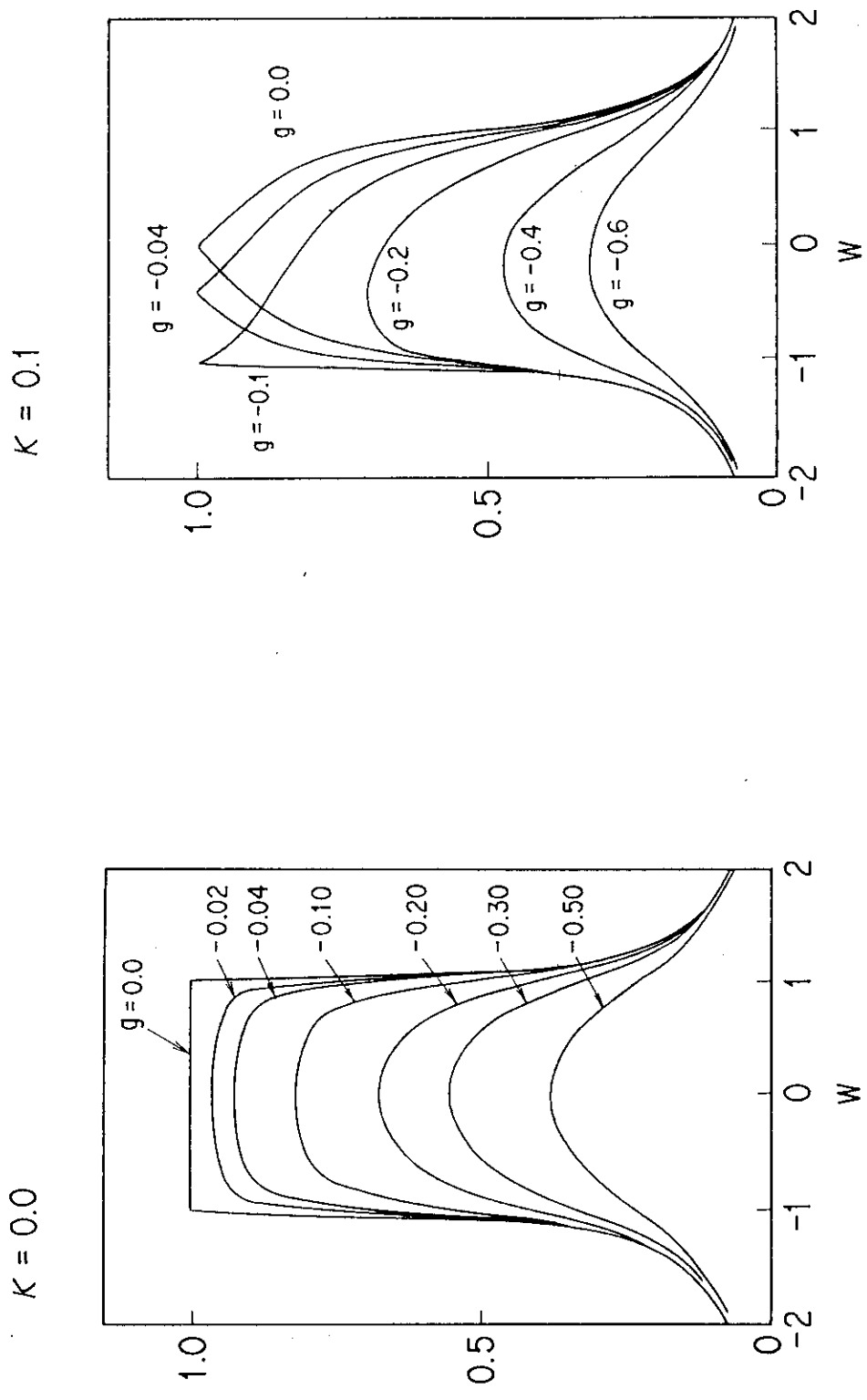

Fig.2.4 Rocking curves for a perfect crystal for various values of g at $\kappa = 0.1$

Fig.2.3 Rocking curves for a perfect crystal for various values of g at $\kappa = 0.0$

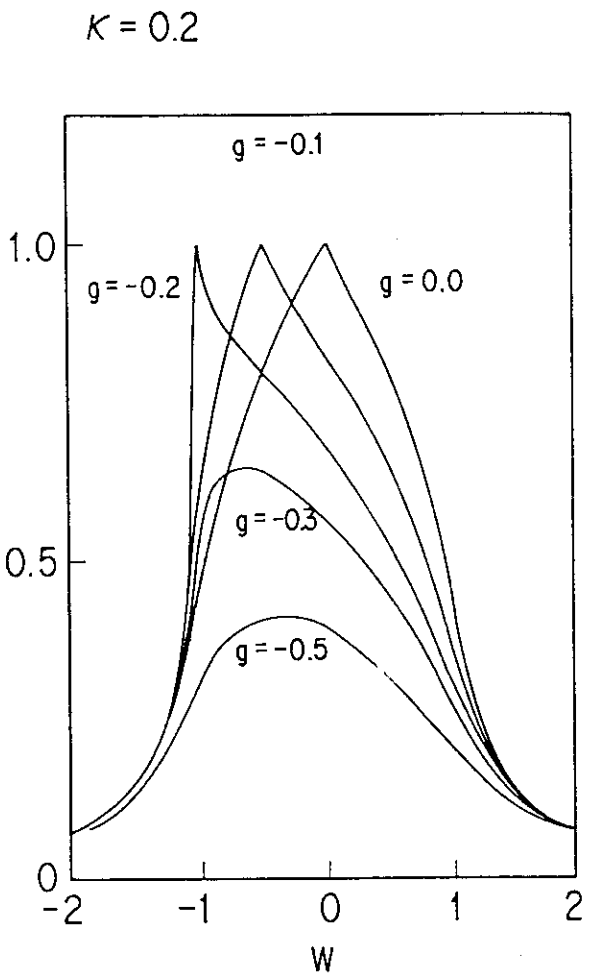

Fig.2.5 Rocking curves for a perfect crystal for various values of g at κ = 0.2

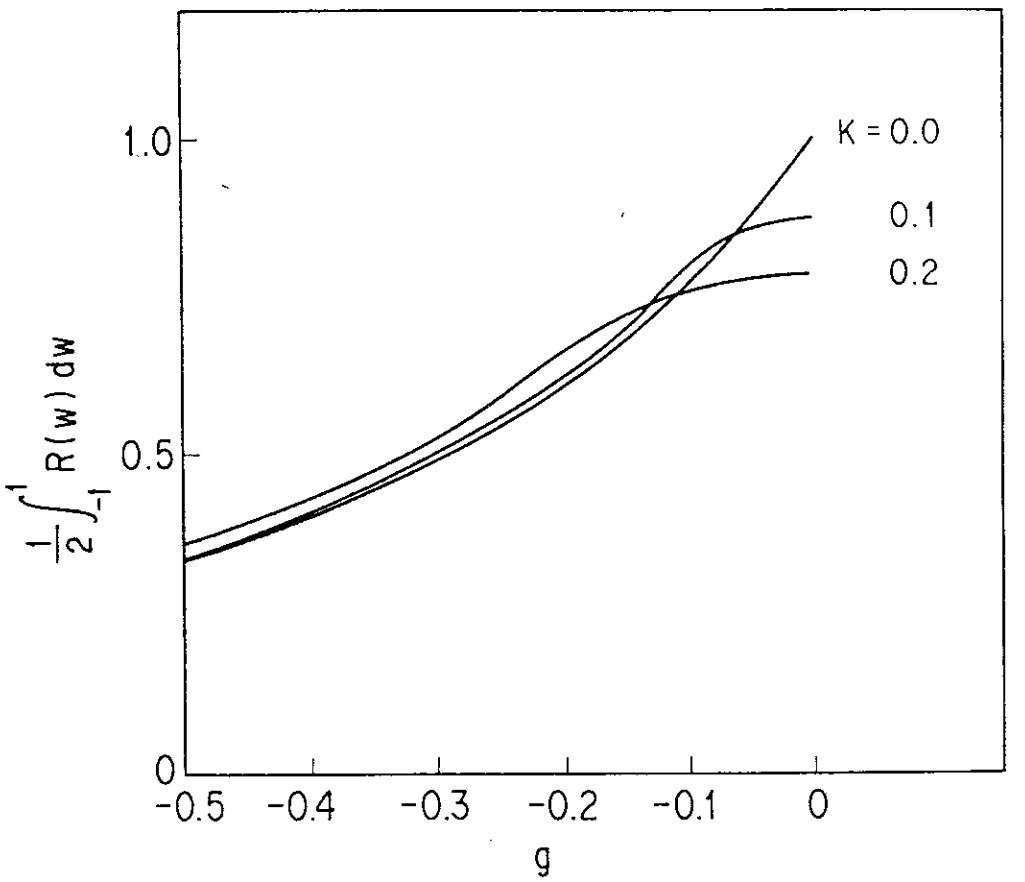

Fig.2.6 Dependency of integrated rocking curve $(1/2)\int_{-1}^{1} R(W)dW$ on g and κ

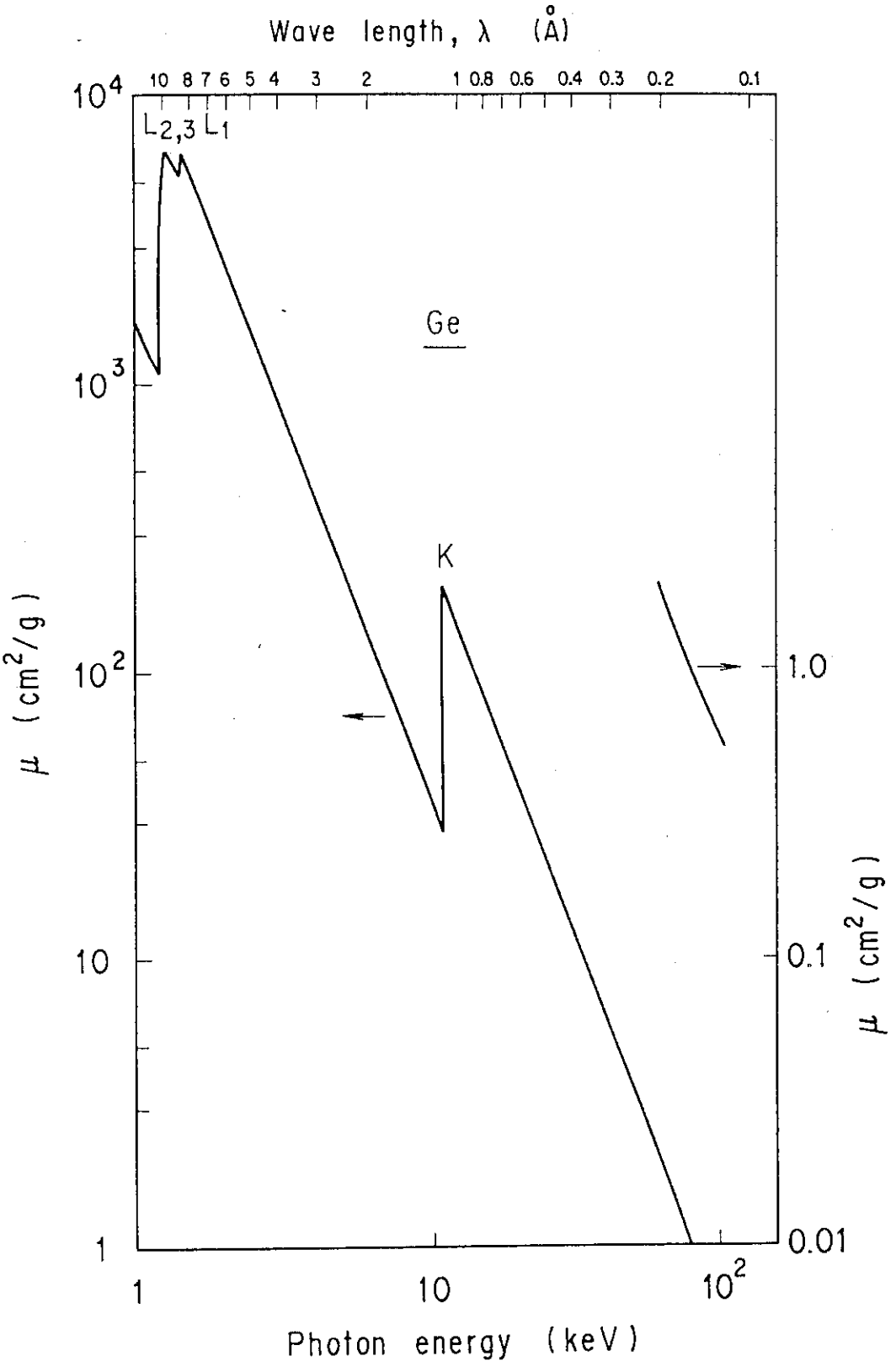

Fig.2.7 Absorption coefficients of Si and Ge as a function of photon energy

3. STRUCTURE OF Si AND Ge CRYSTALS

Si and Ge are the materials most commonly used for monochromator crystals since large perfect crystals are readily available. For a Bragg reflection with Miller indices (hkl), the structure factor takes the form, as shown in equations (8) and (9),

$$F_{h(r,i)}=\sum_j f_{(r,i)}e^{2\pi i(hx_j+ky_j+lz_j)}, \tag{18}$$

where f_r stands for $f^0 + \Delta f'$ and f_i for $\Delta f''$ which are real and imaginary part of the scattering factor, respectively. If $\vec{a}$, $\vec{b}$ and $\vec{c}$ are the cell vectors along the principal axes of the unit cell, the j-th atom is located at position $\vec{r_j} = x_j \vec{a} + y_j \vec{b} + z_j \vec{c}$ within the unit cell where x_j, y_j and z_j are fractional coordinates between zero and one.

The unit cell for Si and Ge contains 8 atoms in a diamond lattice located at the positions shown in Table 3.1[8]. Each atom is surrounded by four equidistant neighbors at the corners of a regular tetrahedron. The structure factor takes one of three forms depending on the value of (hkl):

(1) for h,k,l mixed $\quad F_{h(r,i)} = 0$,

(2) for h,k,l all odd or all even

$h + k + l = 4n \quad F_{h(r,i)} = 8\, f_{(r,i)}$,

$h + k + l = 4n\pm1 \quad F_{h(r,i)} = 4\, f_{(r,i)}(1\pm i)$,

$h + k + l = 4n\pm2 \quad F_{h(r,i)} = 0$.

The physical properties of Si and Ge crystals are shown in Table 3.2.

To use the Bragg law of Eq.(1), we need the value of the planar

spacing d_{hkl}:

$$d_{hkl}=\frac{a}{\sqrt{h^2+k^2+l^2}}. \tag{19}$$

a is the lattice constant of Si or Ge crystals. Table 3.3 shows the spacings of lattice planes in Si and Ge crystals.

Table 3.1 Coordinates of the atoms in the silicon unit cell

x_n	y_n	z_n
0	0	0
1/2	1/2	0
1/2	0	1/2
0	1/2	1/2
1/4	1/4	1/4
3/4	3/4	1/4
3/4	1/4	3/4
1/4	3/4	3/4

Table 3.3 Spacing, atomic scattering factor and Debye-Waller factor of lattice planes in Si and Ge crystals

hkl	$d_{hkl} = a/(h^2 + k^2 + l^2)^{1/2}$		$1/2d_{hkl} = \sin\theta_B/\lambda$		f^0		$\exp\{-B(\sin\theta/\lambda)^2\}$ (30°C)	
	Si	Ge	Si	Ge	Si	Ge	Si	Ge
111	3.136	3.267	0.159	0.153	10.537	27.335	0.988	0.986
220	1.921	2.001	0.260	0.250	8.710	23.770	0.969	0.964
311	1.637	1.706	0.305	0.293	8.163	22.341	0.958	0.951
331	1.246	1.298	0.401	0.385	7.185	19.456	0.929	0.916
333	1.045	1.089	0.478	0.459	6.440	17.305	0.900	0.883
400	1.358	1.414	0.368	0.354	7.509	20.425	0.940	0.929
422	1.109	1.155	0.451	0.433	6.704	18.050	0.911	0.895
440	0.960	1.000	0.521	0.500	6.035	16.194	0.883	0.863
444	0.784	0.817	0.638	0.612	4.972	13.448	0.829	0.802
511	1.045	1.089	0.478	0.459	6.440	17.305	0.900	0.883
531	0.918	0.956	0.545	0.523	5.810	15.594	0.872	0.851
551	0.761	0.792	0.657	0.631	4.806	13.039	0.820	0.791
553	0.707	0.737	0.707	0.678	4.406	12.075	0.795	0.762
555	0.627	0.653	0.797	0.766	3.759	10.584	0.747	0.707

Table 3.2 Physical properties of Si and Ge crystals

Items	Si	Ge
Atomic number	14	32
Atomic weight	28.09	72.59
Crystal structure	diamond type	diamond type
Lattice constant (Å)	5.43070 (25°C) 5.445 (1300°C)	5.65735 (20°C) 5.65695 (18°C)
Melting point (°C)	1410	937.4
Density(25°C) (g/cm^3)	2.33	5.32
Thermal capacity (J/K·mol)	20.0	23.4
Thermal conductivity (W/m·K)	148	59.9
Linear expansion rate (x 10-4/K)	0.0415	0.077
Characteristic temperature Θ_M (K)	543	290

4. SCATTERING FACTORS OF Si and Ge ATOMS

X-ray scattering factor for Si and Ge are computed from numerical Hartree-Fock wave functions. The results are given in the form of coefficients for an analytical function[9].

$$f^0(\sin\theta_B/\lambda) = \sum_{i=1}^{4} a_i \exp(-b_i \sin^2\theta_B/\lambda^2) + c. \qquad (20)$$

The coefficients for Si and Ge are listed in Table 4.1. Table 3.3 lists the atomic scattering factor for the various Bragg reflections of Si and Ge crystals. Figure 4.1 shows the atomic scattering factors of Si and Ge as a function of $\sin\theta_B/\lambda$.

Anomalous scattering factors $\Delta f'$ and $\Delta f''$ are calculated for the atoms Li through Bi plus U, using the relativistic treatment described by Cromer and Liberman and tabulated at 0.01 Å intervals in the wavelength range from 0.1 and 2.89 Å and at 0.0001 Å intervals in the neighborhood of the K, L1, L2 and L3 absorption edges[10]. Table 4.2 and 4.3 list the anomalous scattering factors, $\Delta f'$ and $\Delta f''$ of Si and Ge ,respectively. Figure 4.2 and 4.3 show $\Delta f'$ and $\Delta f''$, respectively, of Si as a function of photon wavelength. Figure 4.4 and 4.5 show $\Delta f'$ and $\Delta f''$, respectively, of Ge as a function of photon wavelength.

Table 4.1 Coefficients for analytic approximations of Hartree-Fock scattering factors

	Si	Ge
a1	5.79411	15.4378
a2	3.22390	6.00432
a3	2.42795	3.05158
a4	1.32149	2.93572
b1	2.57104	3.39715
b2	34.1775	0.73097
b3	0.86937	18.9533
b4	85.3410	63.7969
c	1.23139	4.56068

Table 4.2 Anomalous scattering factors for Si atom (cited from Ref.(10).)

Energy (Å)	Δf'	Δf''
0.26	-0.007	0.008
0.27	-0.006	0.009
0.28	-0.004	0.010
0.29	-0.003	0.011
0.51	0.033	0.036
0.52	0.034	0.037
0.53	0.036	0.039
0.85	0.101	0.102
0.86	0.103	0.104
0.87	0.105	0.107
1.46	0.228	0.298
1.47	0.230	0.302
1.48	0.232	0.306
1.98	0.317	0.530
1.99	0.318	0.535
2.00	0.320	0.540

Table 4.3 Anomalous scattering factors for Ge atom (cited from Ref.(10).)

Energy (Å)	Δf'	Δf''
0.26	0.064	0.286
0.27	0.075	0.308
0.28	0.086	0.330
0.29	0.097	0.353
0.51	0.235	1.009
0.52	0.235	1.045
0.53	0.234	1.081
0.85	-0.309	2.443
0.86	-0.355	2.491
0.87	-0.399	2.539
1.46	-1.304	0.804
1.47	-1.285	0.814
1.48	-1.266	0.824
1.98	-0.679	1.383
1.99	-0.671	1.395
2.00	-0.662	1.408

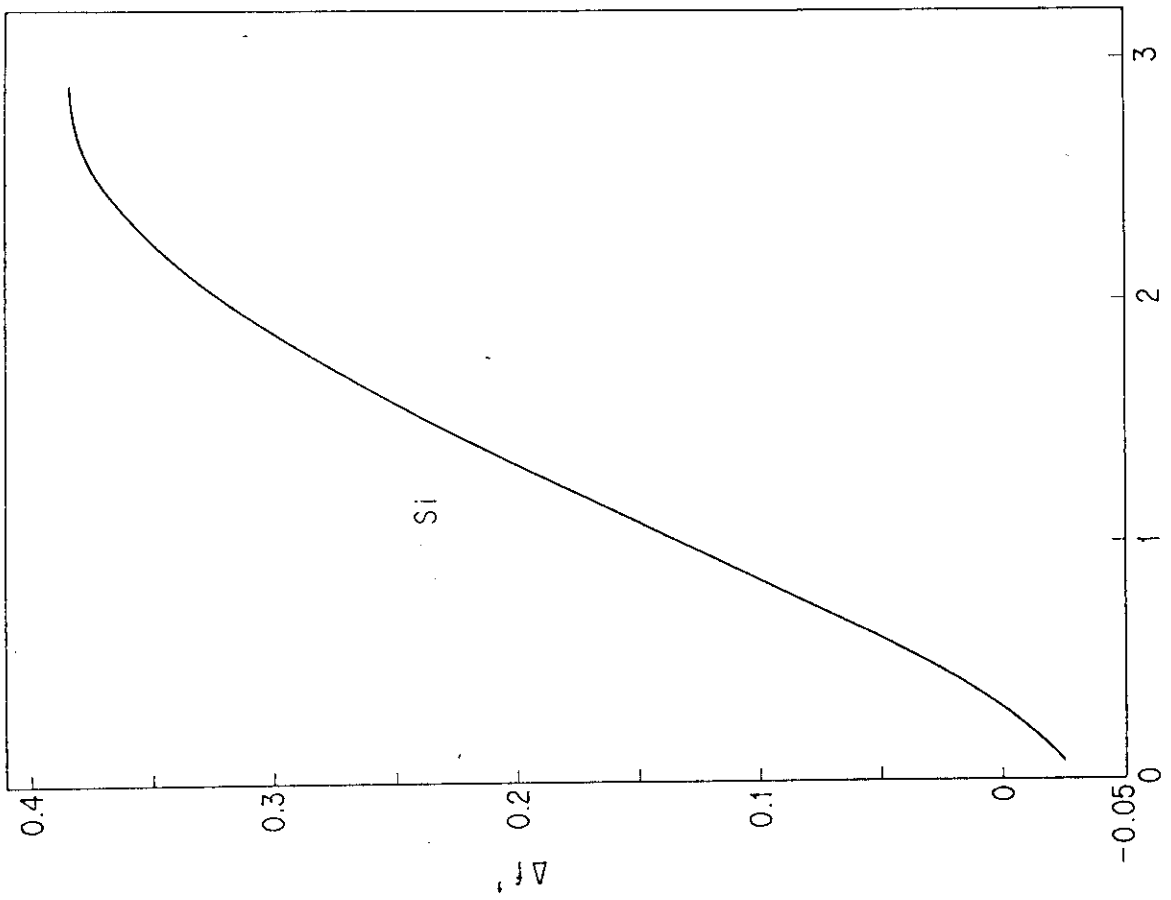

Fig.4.2 Real part of anomalous scattering factors of Si as a function of photon wavelength

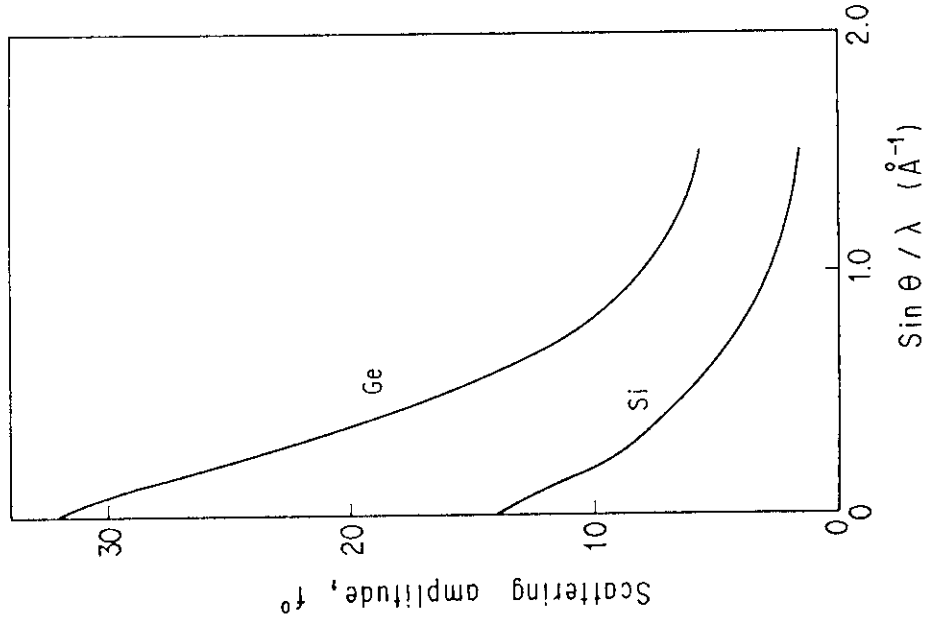

Fig.4.1 Atomic scattering factors of Si and Ge as a function of $\sin\theta_B/\lambda$

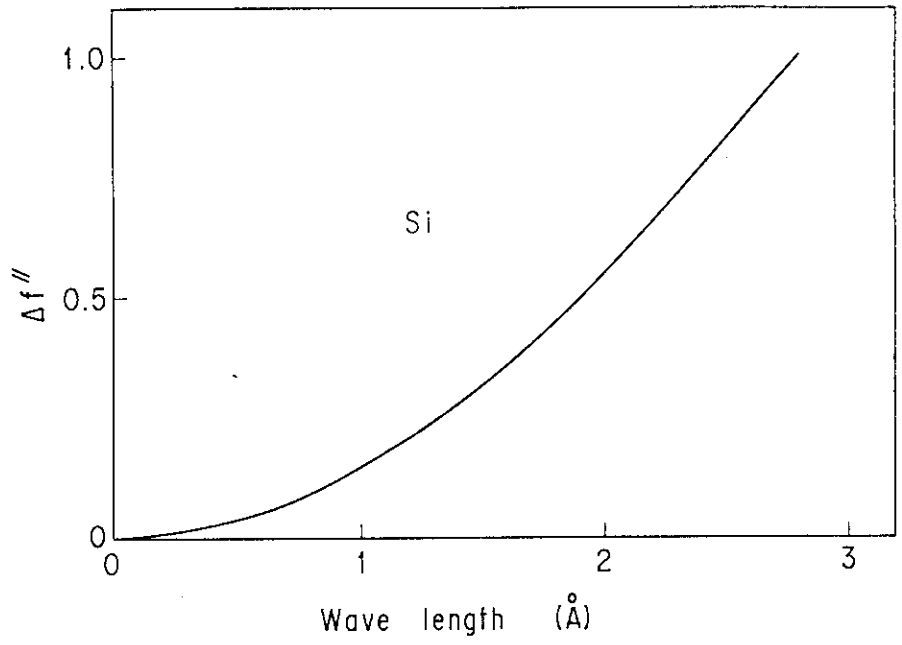

Fig.4.3 Imaginary part of anomalous scattering factors of Si as a function of photon wavelength

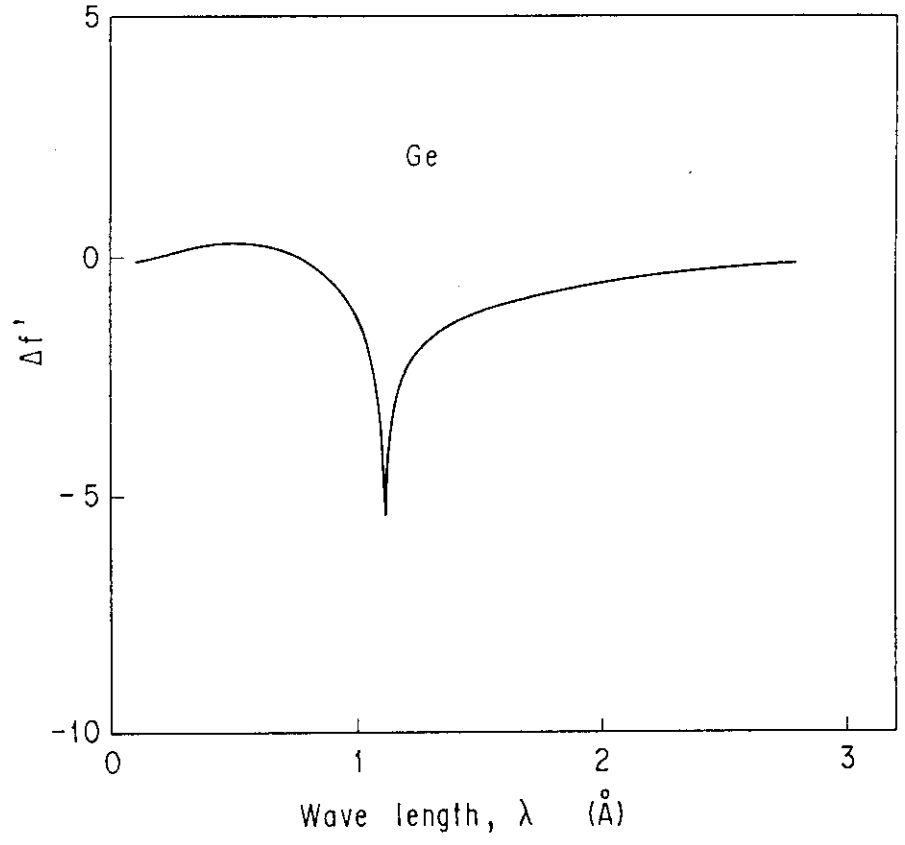

Fig.4.4 Real part of anomalous scattering factors of Ge as a function of photon wavelength

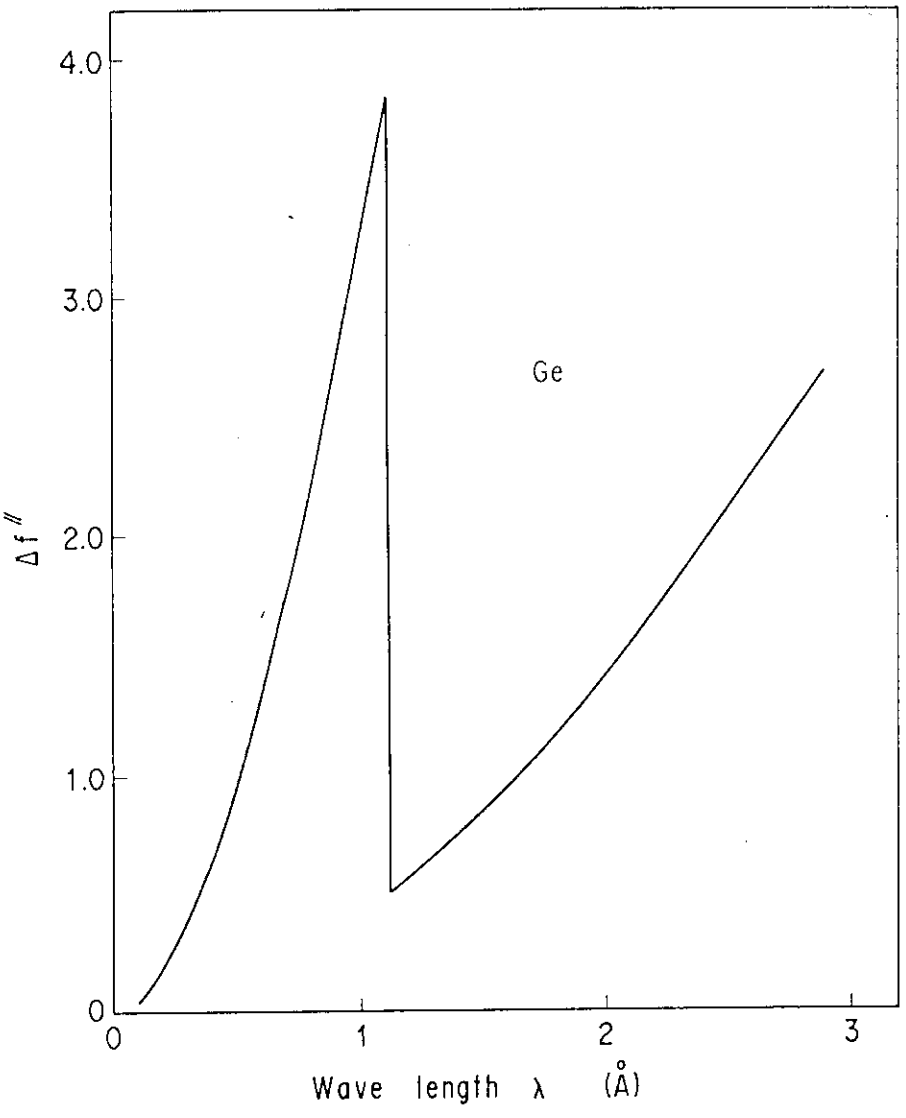

Fig.4.5 Imaginary part of anomalous scattering factors of Ge as a function of photon wavelength

5. DEBYE WALLER FACTORS

The familiar effect of temperature vibration is the reduction of the intensities of the crystalline reflections by the well-known Debye temperature factor e^{-2M}[11].

$$M=B\left(\frac{\sin\theta_B}{\lambda}\right)^2, \tag{21}$$

$$B=\frac{6h^2T}{mk\Theta_M^2}\left(\Phi(x)+\frac{x}{4}\right), \tag{22}$$

$$\Phi(x)=\frac{1}{x}\int_0^x \frac{\varepsilon d\varepsilon}{e^{\varepsilon}-1}, \tag{23}$$

$$x=\Theta_M/T. \tag{24}$$

h is Planck constant, k is Boltzmann constant, m is mass of atom, Θ_M is the average characteristic Debye temperature. Values $\exp(-B\sin^2\theta_B/\lambda^2)$ are shown in Fig. 5.1 as functions of constant B and $\sin\theta_B/\lambda$. Figure 5.2 shows the functions of $\Phi(x)$ and $\Phi(x)+x/4$. For $x < 2.0$, $\Phi(x) + x/4$ can be approximated by $1 + x^2/36 - x^4/3600$. Using the average Debye temperatures listed in Table 3.2, B is calculated and shown in Fig. 5.3 for Si and Ge crystals as a function of temperature. Values of $\exp(-B\sin^2\theta_B/\lambda^2)$ at 30 ℃ are shown in Table 3.3 for the various reflections of Si and Ge crystals.

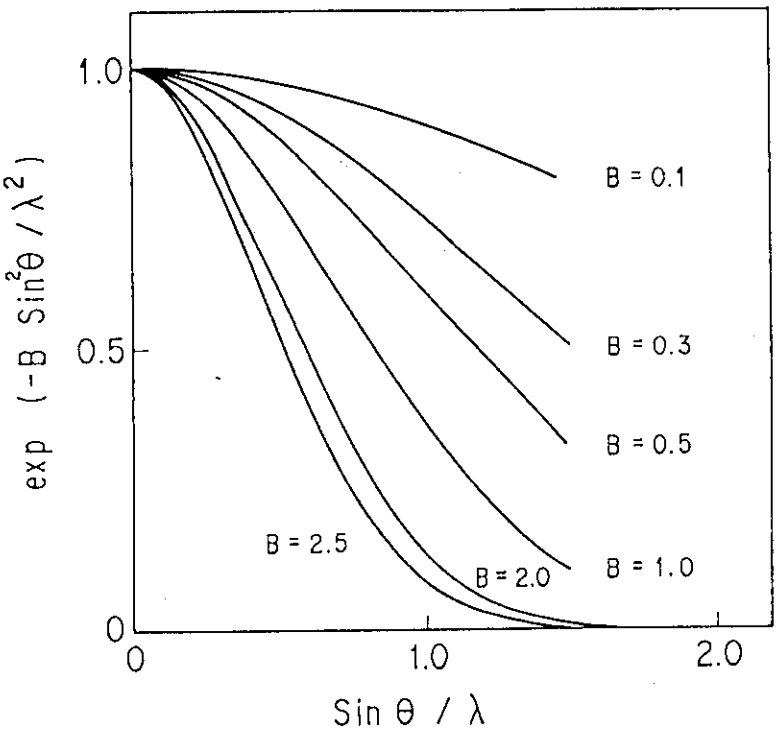

Fig.5.1 Values of $\exp(-B\sin^2\theta_B/\lambda^2)$ function of photon wavelength

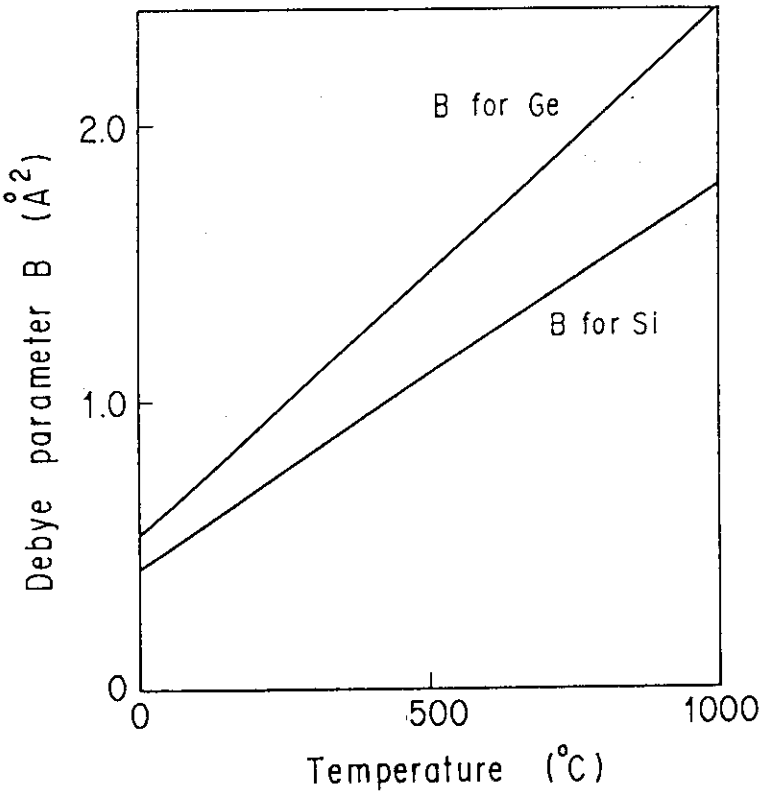

Fig.5.3 Debye parameter B of Si and Ge crystals as a function of temperature

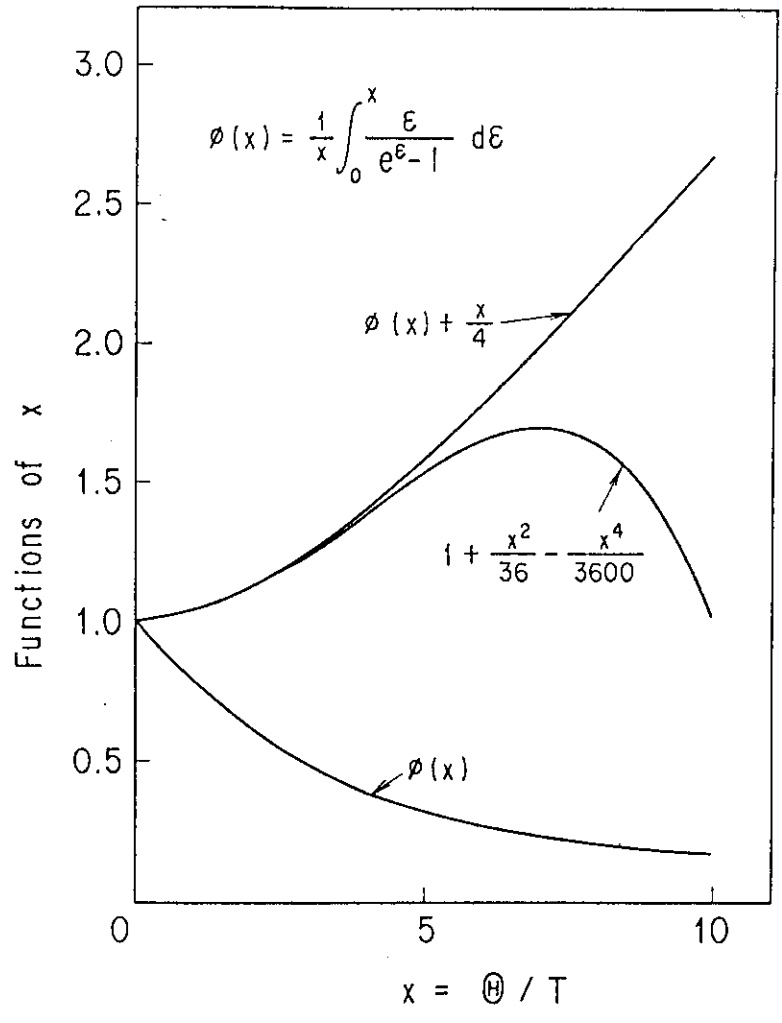

Fig.5.2 Functions of Φ(x) and Φ(x)+ x/4 function of photon wavelength

6. PREMONOCHROMATOR CHARACTERISTICS FOR NUCLEAR BRAGG SCATTERING

In this chapter, we will discuss the premonochromator characteristics of Si and Ge crystals for the nuclear Bragg scattering photon, using the formulae and data described in the previous chapters. We will focus our attention to nuclear Bragg scattering for the photon energy below 50 keV, using the Mössbauer nuclei of ^{181}Ta(1.996 Å), ^{169}Tm(1.472 Å), ^{57}Fe(0.860 Å), ^{119}Sn(0.519 Å) and ^{238}U(0.277 Å).

The energy width of the most common nuclear Mössbauer transitions is typically less than 10^{-7} eV. It is necessary to separate the corresponding band of resonant photons from the white photon of the synchrotron radiation. The source of synchrotron radiation is generated by an undulator. The premonochromator of Si or Ge crystal is used to reduce the band width photon from the undulator to 0.1 ~ 5 eV depending on the geometry chosen.

Figures 6.1 and 6.2 show the Bragg relations of Si and Ge crystals, respectively, for the Mössbauer photons of 1.996, 1.472, 0.860, 0.519 and 0.277 Å. Tables 6.1 through 6.10 present the parameters g and κ defined in Eqs.(5) and (6), intrinsic Bragg reflection width ω_s, angle deviation $\Delta\theta_s$ of W = 0 point from the Bragg angle, intrinsic energy resolution $\Delta\lambda/\lambda$, integral reflecting power I of Si and Ge crystals at 1.996, 1.472, 0.860, 0.519 and 0.277 Å with θ and π polarizations. Bragg reflection angles, atomic scattering factors and susceptibilities of Si and Ge crystals are shown in appendices 1 and 2 for θ and π polarizations, respectively. Figures of rocking curves of the various reflection of Si crystal

are presented in appendices 3 and 4 for θ and π polarizations, respectively. Figures of rocking curves of the various reflection of Ge crystal are presented in appendices 5 and 6 for θ and π polarizations , respectively.

Table 6.1 Intrinsic Bragg reflection width ω_s, angle deviation $\Delta\theta$ of W=0 point from the Bragg angle, intrinsic energy resolution $\Delta\lambda/\lambda$, integral reflecting power I, and parameters g and κ defined in Eqs. (5) and (6) of Si and Ge crystals at 1.996 Å with σ polarization and 30°C temperature.

For Si crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.0698	0.0493	4.508E-5	3.187E-5	1.343E-4	6.010E-5
220	-0.0593	0.0593	3.534E-5	1.767E-5	5.808E-5	4.712E-5
311	-0.0893	0.0631	2.133E-5	1.508E-5	2.774E-5	2.843E-5
331	-0.1009	0.0714	1.843E-5	1.303E-5	1.378E-5	2.458E-5
333	-0.1121	0.0792	2.722E-5	1.925E-5	8.465E-6	3.630E-5
400	-0.0684	0.0684	2.647E-5	1.323E-5	2.441E-5	3.529E-5
422	-0.0763	0.0763	2.928E-5	1.464E-5	1.416E-5	3.904E-5
440	- - -	- - -	- - -	- - -	- - -	- - -
444	- - -	- - -	- - -	- - -	- - -	- - -
511	-0.1121	0.0792	2.722E-5	1.925E-5	8.465E-6	3.630E-5
531	- - -	- - -	- - -	- - -	- - -	- - -
551	- - -	- - -	- - -	- - -	- - -	- - -
553	- - -	- - -	- - -	- - -	- - -	- - -
555	- - -	- - -	- - -	- - -	- - -	- - -

For Ge crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.0744	0.0526	1.014E-4	7.169E-5	3.159E-4	1.352E-4
220	-0.0607	0.0607	8.169E-5	4.085E-5	1.419E-4	1.089E-4
311	-0.0915	0.0647	4.871E-5	3.445E-5	6.752E-5	6.495E-5
331	-0.1056	0.0747	3.930E-5	2.779E-5	3.268E-5	5.240E-5
333	-0.1192	0.0843	4.502E-5	3.183E-5	1.963E-5	6.003E-5
400	-0.0710	0.0710	5.825E-5	2.913E-5	5.850E-5	7.767E-5
422	-0.0807	0.0807	5.683E-5	2.841E-5	3.308E-5	7.577E-5
440	-0.0903	0.0903	3.303E-4	1.651E-4	2.137E-5	4.404E-4
444	- - -	- - -	- - -	- - -	- - -	- - -
511	-0.1192	0.0843	4.502E-5	3.183E-5	1.963E-5	6.003E-5
531	- - -	- - -	- - -	- - -	- - -	- - -
551	- - -	- - -	- - -	- - -	- - -	- - -
553	- - -	- - -	- - -	- - -	- - -	- - -
555	- - -	- - -	- - -	- - -	- - -	- - -

Table 6.2 Intrinsic Bragg reflection width ω_s, angle deviation $\Delta\theta$ of W=0 point from the Bragg angle, intrinsic energy resolution $\Delta\lambda/\lambda$, integral reflecting power I, and parameters g and κ defined in Eqs. (5) and (6) of Si and Ge crystals at 1.472 Å with σ polarization and 30°C temperature.

For Si crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.0398	0.0281	3.215E-5	2.274E-5	1.332E-4	4.287E-5
220	-0.0339	0.0339	2.387E-5	1.193E-5	5.751E-5	3.182E-5
311	-0.0510	0.0361	1.381E-5	9.766E-6	2.745E-5	1.842E-5
331	-0.0577	0.0408	9.966E-6	7.047E-6	1.361E-5	1.329E-5
333	-0.0642	0.0454	8.286E-6	5.859E-6	8.354E-6	1.105E-5
400	-0.0391	0.0391	1.557E-5	7.786E-6	2.414E-5	2.076E-5
422	-0.0437	0.0437	1.241E-5	6.205E-6	1.398E-5	1.655E-5
440	-0.0483	0.0483	1.097E-5	5.483E-6	9.184E-6	1.462E-5
444	-0.0582	0.0582	1.304E-5	6.522E-6	4.779E-6	1.739E-5
511	-0.0642	0.0454	8.286E-6	5.859E-6	8.354E-6	1.105E-5
531	-0.0501	0.0501	1.074E-5	5.368E-6	8.002E-6	1.432E-5
551	-0.0850	0.0601	1.171E-5	8.281E-6	3.044E-6	1.562E-5
553	- - -	- - -	- - -	- - -	- - -	- - -
555	- - -	- - -	- - -	- - -	- - -	- - -

For Ge crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.0443	0.0313	7.139E-5	5.048E-5	3.087E-4	9.518E-5
220	-0.0363	0.0363	5.465E-5	2.733E-5	1.381E-4	7.287E-5
311	-0.0548	0.0388	3.138E-5	2.219E-5	6.560E-5	4.184E-5
331	-0.0635	0.0449	2.176E-5	1.539E-5	3.160E-5	2.901E-5
333	-0.0720	0.0509	1.734E-5	1.226E-5	1.891E-5	2.312E-5
400	-0.0426	0.0426	3.454E-5	1.727E-5	5.668E-5	4.605E-5
422	-0.0487	0.0487	2.639E-5	1.320E-5	3.191E-5	3.519E-5
440	-0.0547	0.0547	2.231E-5	1.115E-5	2.052E-5	2.974E-5
444	-0.0671	0.0671	2.159E-5	1.080E-5	1.038E-5	2.879E-5
511	-0.0720	0.0509	1.734E-5	1.226E-5	1.891E-5	2.312E-5
531	-0.0570	0.0570	2.141E-5	1.071E-5	1.776E-5	2.855E-5
551	-0.0982	0.0694	1.654E-5	1.169E-5	6.583E-6	2.205E-5
553	-0.1069	0.0756	1.334E-4	9.435E-5	5.037E-6	1.779E-4
555	- - -	- - -	- - -	- - -	- - -	- - -

Table 6.3 Intrinsic Bragg reflection width ω_s, angle deviation $\Delta\theta$ of W=0 point from the Bragg angle, intrinsic energy resolution $\Delta\lambda/\lambda$, integral reflecting power I, and parameters g and κ defined in Eqs. (5) and (6) of Si and Ge crystals at 0.860 Å with σ polarization and 30°C temperature.

For Si crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.0138	0.0098	1.822E-5	1.288E-5	1.316E-4	2.429E-5
220	-0.0118	0.0118	1.303E-5	6.513E-6	5.669E-5	1.737E-5
311	-0.0178	0.0126	7.357E-6	5.202E-6	2.703E-5	9.809E-6
331	-0.0202	0.0143	4.920E-6	3.479E-6	1.338E-5	6.560E-6
333	-0.0225	0.0159	3.699E-6	2.616E-6	8.194E-6	4.932E-6
400	-0.0137	0.0137	7.927E-6	3.964E-6	2.374E-5	1.057E-5
422	-0.0153	0.0153	5.774E-6	2.887E-6	1.372E-5	7.699E-6
440	-0.0169	0.0169	4.507E-6	2.254E-6	8.997E-6	6.010E-6
444	-0.0205	0.0205	3.069E-6	1.530E-6	4.662E-6	4.079E-6
511	-0.0225	0.0159	3.699E-6	2.616E-6	8.194E-6	4.932E-6
531	-0.0176	0.0176	4.153E-6	2.077E-6	7.834E-6	5.538E-6
551	-0.0300	0.0212	2.034E-6	1.438E-6	2.967E-6	2.712E-6
553	-0.0326	0.0231	1.750E-6	1.237E-6	2.284E-6	2.333E-6
555	-0.0381	0.0269	1.363E-6	9.637E-7	1.447E-6	1.817E-6

For Ge crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.1306	0.0923	4.245E-5	3.002E-5	3.196E-4	5.660E-5
220	-0.1064	0.1064	3.165E-5	1.583E-5	1.438E-4	4.220E-5
311	-0.1602	0.1133	1.784E-5	1.262E-5	6.849E-5	2.379E-5
331	-0.1844	0.1304	1.166E-5	8.247E-6	3.322E-5	1.555E-5
333	-0.2078	0.1470	8.597E-6	6.079E-6	2.000E-5	1.146E-5
400	-0.1241	0.1241	1.896E-5	9.481E-6	5.942E-5	2.528E-5
422	-0.1408	0.1408	1.351E-5	6.755E-6	3.367E-5	1.801E-5
440	-0.1573	0.1573	1.038E-5	5.190E-6	2.180E-5	1.384E-5
444	-0.1903	0.1903	6.917E-6	3.459E-6	1.117E-5	9.223E-6
511	-0.2078	0.1470	8.597E-6	6.079E-6	2.000E-5	1.146E-5
531	-0.1635	0.1635	9.521E-6	4.761E-6	1.891E-5	1.270E-5
551	-0.2777	0.1964	4.590E-6	3.246E-6	7.102E-6	6.120E-6
553	-0.3006	0.2126	3.933E-6	2.781E-6	5.469E-6	5.244E-6
555	-0.3444	0.2435	3.052E-6	2.158E-6	3.491E-6	4.070E-6

Table 6.4 Intrinsic Bragg reflection width ω_s, angle deviation $\Delta\theta$ of W=0 point from the Bragg angle, intrinsic energy resolution $\Delta\lambda/\lambda$, integral reflecting power I, and parameters g and κ defined in Eq. (5) and (6) of Si and Ge crystals at 0.519 Å with σ polarization and 30°C temperature.

For Si crystal

h k l	g	κ	ω_s	Δθ	Δλ/λ	I
111	-0.0050	0.0035	1.086E-5	7.677E-6	1.307E-4	1.448E-5
220	-0.0042	0.0042	7.672E-6	3.836E-6	5.625E-5	1.023E-5
311	-0.0064	0.0045	4.303E-6	3.042E-6	2.681E-5	5.737E-6
331	-0.0072	0.0051	2.822E-6	1.996E-6	1.325E-5	3.763E-6
333	-0.0081	0.0057	2.078E-6	1.470E-6	8.108E-6	2.771E-6
400	-0.0049	0.0049	4.581E-6	2.290E-6	2.352E-5	6.108E-6
422	-0.0055	0.0055	3.270E-6	1.635E-6	1.358E-5	4.360E-6
440	-0.0061	0.0061	2.498E-6	1.249E-6	8.896E-6	3.330E-6
444	-0.0074	0.0074	1.614E-6	8.067E-7	4.599E-6	2.151E-6
511	-0.0081	0.0057	2.078E-6	1.470E-6	8.108E-6	2.771E-6
531	-0.0063	0.0063	2.282E-6	1.141E-6	7.742E-6	3.042E-6
551	-0.0108	0.0076	1.062E-6	7.509E-7	2.925E-6	1.416E-6
553	-0.0118	0.0083	8.872E-7	6.274E-7	2.249E-6	1.183E-6
555	-0.0138	0.0098	6.459E-7	4.567E-7	1.421E-6	8.611E-7

For Ge crystal

h k l	g	κ	ω_s	Δθ	Δλ/λ	I
111	-0.0534	0.0378	2.603E-5	1.841E-5	3.266E-4	3.471E-5
220	-0.0434	0.0434	1.929E-5	9.644E-6	1.474E-4	2.572E-5
311	-0.0652	0.0461	1.083E-5	7.654E-6	7.033E-5	1.443E-5
331	-0.0748	0.0529	6.987E-6	4.941E-6	3.424E-5	9.317E-6
333	-0.0840	0.0594	5.079E-6	3.591E-6	2.069E-5	6.772E-6
400	-0.0504	0.0504	1.142E-5	5.708E-6	6.116E-5	1.522E-5
422	-0.0570	0.0570	8.024E-6	4.012E-6	3.480E-5	1.070E-5
440	-0.0634	0.0634	6.074E-6	3.037E-6	2.261E-5	8.099E-6
444	-0.0761	0.0761	3.911E-6	1.956E-6	1.167E-5	5.215E-6
511	-0.0840	0.0594	5.079E-6	3.591E-6	2.069E-5	6.772E-6
531	-0.0658	0.0658	5.539E-6	2.769E-6	1.965E-5	7.385E-6
551	-0.1110	0.0785	2.577E-6	1.822E-6	7.432E-6	3.436E-6
553	-0.1196	0.0846	2.163E-6	1.529E-6	5.744E-6	2.883E-6
555	-0.1361	0.0963	1.598E-6	1.130E-6	3.692E-6	2.131E-6

Table 6.5 Intrinsic Bragg reflection width ω_s, angle deviation $\Delta\theta$ of W=0 point from the Bragg angle, intrinsic energy resolution $\Delta\lambda/\lambda$, integral reflecting power I, and parameters g and κ defined in Eqs. (5) and (6) of Si and Ge crystals at 0.277 Å with σ polarization and 30°C temperature.

For Si crystal

h k l	g	κ	ω_s	Δθ	Δλ/λ	I
111	-0.0013	0.00092	5.759E-6	4.072E-6	1.303E-4	7.679E-6
220	-0.0011	0.0011	4.050E-6	2.025E-6	5.600E-5	5.400E-6
311	-0.0017	0.0012	2.265E-6	1.602E-6	2.668E-5	3.020E-6
331	-0.0019	0.0014	1.474E-6	1.043E-6	1.318E-5	1.966E-6
333	-0.0021	0.0015	1.078E-6	7.620E-7	8.060E-6	1.437E-6
400	-0.0013	0.0013	2.400E-6	1.200E-6	2.340E-5	3.200E-6
422	-0.0014	0.0014	1.701E-6	8.502E-7	1.350E-5	2.267E-6
440	-0.0016	0.0016	1.289E-6	6.444E-7	8.839E-6	1.718E-6
444	-0.0020	0.0020	8.192E-7	4.096E-7	4.563E-6	1.092E-6
511	-0.0021	0.0015	1.078E-6	7.620E-7	8.060E-6	1.437E-6
531	-0.0017	0.0017	1.174E-6	5.869E-7	7.691E-6	1.565E-6
551	-0.0029	0.0020	5.375E-7	3.800E-7	2.902E-6	7.166E-7
553	-0.0031	0.0022	4.453E-7	3.149E-7	2.229E-6	5.937E-7
555	-0.0037	0.0026	3.185E-7	2.252E-7	1.406E-6	4.246E-7

For Ge crystal

h k l	g	κ	ω_s	Δθ	Δλ/λ	I
111	-0.0167	0.0118	1.379E-5	9.748E-6	3.248E-4	1.838E-5
220	-0.0136	0.0136	1.017E-5	5.084E-6	1.465E-4	1.356E-5
311	-0.0204	0.0144	5.691E-6	4.024E-6	6.985E-5	7.587E-6
331	-0.0234	0.0166	3.647E-6	2.579E-6	3.398E-5	4.862E-6
333	-0.0263	0.0186	2.631E-6	1.860E-6	2.052E-5	3.508E-6
400	-0.0158	0.0158	5.974E-6	2.987E-6	6.071E-5	7.966E-6
422	-0.0178	0.0178	4.169E-6	2.084E-6	3.451E-5	5.558E-6
440	-0.0199	0.0199	3.132E-6	1.566E-6	2.240E-5	4.176E-6
444	-0.0239	0.0239	1.986E-6	9.931E-7	1.154E-5	2.648E-6
511	-0.0263	0.0186	2.631E-6	1.860E-6	2.052E-5	3.508E-6
531	-0.0206	0.0206	2.848E-6	1.424E-6	1.946E-5	3.797E-6
551	-0.0349	0.0247	1.305E-5	9.225E-7	7.347E-6	1.739E-6
553	-0.0376	0.0266	1.086E-6	7.680E-7	5.673E-6	1.448E-6
555	-0.0429	0.0303	7.897E-7	5.584E-7	3.640E-6	1.053E-6

Table 6.6 Intrinsic Bragg reflection width ω_s,angle deviation $\Delta\theta$ of W=0 point from the Bragg angle, intrinsic energy resolution $\Delta\lambda/\lambda$, integral reflecting power I, and parameters g and κ defined in Eqs.(5) and (6) of Si and Ge crystals at 1.996 Å with π polarization and 30°C temperature.

For Si crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.0736	0.0493	4.273E-5	3.187E-5	1.273E-4	5.698E-5
220	-0.0694	0.0593	3.019E-5	1.767E-5	4.962E-5	4.025E-5
311	-0.1126	0.0631	1.691E-5	1.508E-5	2.199E-5	2.254E-5
331	-0.1686	0.0714	1.103E-5	1.303E-5	8.246E-6	1.471E-5
333	-0.3774	0.0792	8.083E-6	1.925E-5	2.514E-6	1.078E-5
400	-0.1009	0.0684	1.795E-5	1.324E-5	1.655E-5	2.393E-5
422	-0.1752	0.0763	1.275E-5	1.464E-5	6.162E-6	1.699E-5
440	- - -	- - -	- - -	- - -	- - -	- - -
444	- - -	- - -	- - -	- - -	- - -	- - -
511	-0.3774	0.0792	8.083E-6	1.925E-5	2.514E-6	1.078E-5
531	- - -	- - -	- - -	- - -	- - -	- - -
551	- - -	- - -	- - -	- - -	- - -	- - -
553	- - -	- - -	- - -	- - -	- - -	- - -
555	- - -	- - -	- - -	- - -	- - -	- - -

For Ge crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.0781	0.0526	9.654E-5	7.169E-5	3.008E-4	1.287E-4
220	-0.0701	0.0607	7.080E-5	4.085E-5	1.230E-4	9.439E-5
311	-0.1129	0.0647	3.951E-5	3.445E-5	5.476E-5	5.267E-5
331	-0.1651	0.0747	2.513E-5	2.779E-5	2.089E-5	3.350E-5
333	-0.2983	0.0843	1.800E-5	3.183E-5	7.847E-6	2.399E-5
400	-0.1002	0.0710	4.128E-5	2.913E-5	4.145E-5	5.504E-5
422	-0.1604	0.0807	2.859E-5	2.841E-5	1.664E-5	3.812E-5
440	-1.3993	0.0903	2.132E-5	1.651E-4	1.380E-6	2.843E-5
444	- - -	- - -	- - -	- - -	- - -	- - -
511	-0.2983	0.0843	1.800E-5	3.183E-5	7.847E-6	2.399E-5
531	- - -	- - -	- - -	- - -	- - -	- - -
551	- - -	- - -	- - -	- - -	- - -	- - -
553	- - -	- - -	- - -	- - -	- - -	- - -
555	- - -	- - -	- - -	- - -	- - -	- - -

Table 6.7 Intrinsic Bragg reflection width ω_s, angle deviation $\Delta\theta$ of W=0 point from the Bragg angle, intrinsic energy resolution $\Delta\lambda/\lambda$, integral reflecting power I, and parameters g and κ defined in Eqs.(5) and (6) of Si and Ge crystals at 1.472 Å with π polarization and 30°C temperature.

For Si crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.0409	0.0281	3.126E-5	2.274E-5	1.294E-4	4.167E-5
220	-0.0367	0.0339	2.205E-5	1.193E-5	5.312E-5	2.939E-5
311	-0.0571	0.0361	1.234E-5	9.766E-6	2.452E-5	1.645E-5
331	-0.0716	0.0408	8.041E-6	7.047E-6	1.098E-5	1.072E-5
333	-0.0904	0.0454	5.883E-6	5.859E-6	5.931E-6	7.844E-6
400	-0.0466	0.0391	1.309E-5	7.786E-6	2.028E-5	1.745E-5
422	-0.0584	0.0437	9.280E-6	6.205E-6	1.045E-5	1.237E-5
440	-0.0753	0.0483	7.041E-6	5.483E-6	5.897E-6	9.388E-6
444	-0.1692	0.0582	4.488E-6	6.522E-6	1.644E-6	5.983E-6
511	-0.0904	0.0454	5.883E-6	5.859E-6	5.931E-6	7.844E-6
531	-0.0839	0.0501	6.416E-6	5.368E-6	4.782E-6	8.555E-6
551	-0.3381	0.0601	2.946E-6	8.281E-6	7.656E-7	3.928E-6
553	- - -	- - -	- - -	- - -	- - -	- - -
555	- - -	- - -	- - -	- - -	- - -	- - -

For Ge crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.0455	0.0313	6.955E-5	5.048E-5	3.007E-4	9.273E-5
220	-0.0390	0.0363	5.082E-5	2.733E-5	1.284E-4	6.776E-5
311	-0.0607	0.0388	2.831E-5	2.219E-5	5.918E-5	3.774E-5
331	-0.0771	0.0449	1.792E-5	1.539E-5	2.603E-5	2.390E-5
333	-0.0977	0.0509	1.278E-5	1.226E-5	1.393E-5	1.704E-5
400	-0.0499	0.0426	2.949E-5	1.727E-5	4.840E-5	3.932E-5
422	-0.0632	0.0487	2.034E-5	1.320E-5	2.459E-5	2.712E-5
440	-0.0808	0.0547	1.510E-5	1.115E-5	1.389E-5	2.014E-5
444	-0.1549	0.0671	9.353E-6	1.080E-5	4.494E-6	1.247E-5
511	-0.0977	0.0509	1.278E-5	1.226E-5	1.393E-5	1.704E-5
531	-0.0893	0.0570	1.367E-5	1.071E-5	1.134E-5	1.823E-5
551	-0.2653	0.0694	6.116E-6	1.169E-5	2.435E-6	8.155E-6
553	-2.8346	0.0756	5.033E-6	9.435E-5	1.900E-7	6.711E-6
555	- - -	- - -	- - -	- - -	- - -	- - -

Table 6.8 Intrinsic Bragg reflection width ω_s,angle deviation $\Delta\theta$ of W=0 point from the Bragg angle, intrinsic energy resolution $\Delta\lambda/\lambda$, integral reflecting power I, and parameters g and κ defined in Eqs.(5) and (6) of Si and Ge crystals at 0.860 Å with π polarization and 30°C temperature.

For Si crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.0140	0.0098	1.805E-5	1.288E-5	1.303E-4	2.406E-5
220	-0.0121	0.0118	1.270E-5	6.513E-6	5.525E-5	1.693E-5
311	-0.0184	0.0126	7.099E-6	5.202E-6	2.608E-5	9.465E-6
331	-0.0215	0.0143	4.617E-6	3.479E-6	1.256E-5	6.157E-6
333	-0.0247	0.0159	3.371E-6	2.616E-6	7.469E-6	4.495E-6
400	-0.0144	0.0137	7.519E-6	3.964E-6	2.252E-5	1.003E-5
422	-0.0166	0.0153	5.322E-6	2.887E-6	1.265E-5	7.096E-6
440	-0.0190	0.0170	4.030E-6	2.254E-6	8.044E-6	5.373E-6
444	-0.0245	0.0205	2.558E-6	1.530E-6	3.898E-6	3.410E-6
511	-0.0247	0.0159	3.371E-6	2.616E-6	7.469E-6	4.495E-6
531	-0.0199	0.0176	3.670E-6	2.077E-6	6.921E-6	4.893E-6
551	-0.0363	0.0212	1.678E-6	1.438E-6	2.447E-6	2.237E-6
553	-0.0411	0.0231	1.389E-6	1.237E-6	1.813E-6	1.852E-6
555	-0.0523	0.0269	9.920E-7	9.637E-7	1.053E-6	1.323E-6

For Ge crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.1317	0.0923	4.208E-5	3.002E-5	3.168E-4	5.610E-5
220	-0.1089	0.1064	3.091E-5	1.583E-5	1.404E-4	4.122E-5
311	-0.1656	0.1133	1.727E-5	1.262E-5	6.628E-5	2.302E-5
331	-0.1955	0.1304	1.100E-5	8.247E-6	3.134E-5	1.467E-5
333	-0.2262	0.1470	7.898E-6	6.079E-6	1.837E-5	1.053E-5
400	-0.1303	0.1241	1.807E-5	9.481E-6	5.661E-5	2.409E-5
422	-0.1517	0.1408	1.254E-5	6.755E-6	3.125E-5	1.672E-5
440	-0.1742	0.1573	9.371E-6	5.190E-6	1.968E-5	1.250E-5
444	-0.2238	0.1903	5.880E-6	3.459E-6	9.493E-6	7.840E-6
511	-0.2262	0.1470	7.898E-6	6.079E-6	1.837E-5	1.053E-5
531	-0.1830	0.1635	8.504E-6	4.761E-6	1.689E-5	1.134E-5
551	-0.3307	0.1964	3.855E-6	3.246E-6	5.964E-6	5.140E-6
553	-0.3703	0.2126	3.193E-6	2.781E-6	4.440E-6	4.257E-6
555	-0.4575	0.2435	2.298E-6	2.158E-6	2.628E-6	3.064E-6

Table 6.9 Intrinsic Bragg reflection width ω_s,angle deviation $\Delta\theta$ of W=0 point from the Bragg angle, intrinsic energy resolution $\Delta\lambda/\lambda$, integral reflecting power I, and parameters g and κ defined in Eqs.(5) and (6) of Si and Ge crystals at 0.519 Å with π polarization and 30°C temperature.

For Si crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.0050	0.0035	1.082E-5	7.677E-6	1.303E-4	1.443E-5
220	-0.0043	0.0042	7.602E-6	3.836E-6	5.573E-5	1.014E-5
311	-0.0065	0.0045	4.248E-6	3.043E-6	2.647E-5	5.664E-6
331	-0.0074	0.0051	2.760E-6	1.996E-6	1.296E-5	3.680E-6
333	-0.0083	0.0057	2.013E-6	1.470E-6	7.854E-6	2.684E-6
400	-0.0050	0.0049	4.496E-6	2.290E-6	2.309E-5	5.995E-6
422	-0.0056	0.0055	3.179E-6	1.635E-6	1.320E-5	4.239E-6
440	-0.0063	0.0061	2.405E-6	1.249E-6	8.565E-6	3.206E-6
444	-0.0078	0.0074	1.523E-6	8.067E-7	4.340E-6	2.030E-6
511	-0.0083	0.0057	2.013E-6	1.470E-6	7.854E-6	2.684E-6
531	-0.0066	0.0063	2.189E-6	1.141E-6	7.426E-6	2.918E-6
551	-0.0115	0.0076	9.981E-7	7.509E-7	2.749E-6	1.331E-6
553	-0.0127	0.0083	8.253E-7	6.274E-7	2.092E-6	1.100E-6
555	-0.0152	0.0098	5.880E-7	4.567E-7	1.293E-6	7.839E-7

For Ge crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.0536	0.0378	2.595E-5	1.841E-5	3.256E-4	3.460E-5
220	-0.0438	0.0434	1.913E-5	9.644E-6	1.462E-4	2.550E-5
311	-0.0660	0.0461	1.070E-5	7.654E-6	6.951E-5	1.427E-5
331	-0.0763	0.0529	6.846E-6	4.941E-6	3.355E-5	9.128E-6
333	-0.0865	0.0594	4.932E-6	3.591E-6	2.010E-5	6.577E-6
400	-0.0513	0.0504	1.122E-5	5.708E-6	6.013E-5	1.496E-5
422	-0.0585	0.0570	7.819E-6	4.012E-6	3.391E-5	1.043E-5
440	-0.0656	0.0634	5.866E-6	3.037E-6	2.183E-5	7.822E-6
444	-0.0803	0.0761	3.709E-6	1.956E-6	1.107E-5	4.945E-6
511	-0.0865	0.0594	4.932E-6	3.591E-6	2.010E-5	6.577E-6
531	-0.0684	0.0658	5.331E-6	2.769E-6	1.891E-5	7.108E-6
551	-0.1174	0.0785	2.435E-6	1.822E-6	7.022E-6	3.246E-6
553	-0.1278	0.0846	2.024E-6	1.529E-6	5.376E-6	2.699E-6
555	-0.1483	0.0963	1.467E-6	1.130E-6	3.388E-6	1.956E-6

Table 6.10 Intrinsic Bragg reflection width ω_s,angle deviation $\Delta\theta$ of W=0 point from the Bragg angle, intrinsic energy resolution $\Delta\lambda/\lambda$, integral reflecting power I, and parameters g and κ defined in Eqs.(5) and (6) of Si and Ge crystals at 0.277 Å with π polarization and 30°C temperature.

For Si crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.0013	0.0009	5.753E-6	4.072E-6	1.301E-4	7.671E-6
220	-0.0011	0.0011	4.039E-6	2.025E-6	5.585E-5	5.386E-6
311	-0.0017	0.0012	2.257E-6	1.602E-6	2.658E-5	3.009E-6
331	-0.0019	0.0014	1.465E-6	1.043E-6	1.310E-5	1.954E-6
333	-0.0022	0.0015	1.068E-6	7.620E-7	7.989E-6	1.424E-6
400	-0.0013	0.0013	2.388E-6	1.200E-6	2.328E-5	3.183E-6
422	-0.0015	0.0014	1.687E-6	8.502E-7	1.340E-5	2.250E-6
440	-0.0016	0.0016	1.275E-6	6.444E-7	8.747E-6	1.700E-6
444	-0.0020	0.0020	8.063E-7	4.096E-7	4.492E-6	1.075E-6
511	-0.0022	0.0015	1.068E-6	7.620E-7	7.989E-6	1.424E-6
531	-0.0017	0.0017	1.160E-6	5.869E-7	7.603E-6	1.547E-6
551	-0.0029	0.0020	5.285E-7	3.800E-7	2.853E-6	7.046E-7
553	-0.0032	0.0022	4.367E-7	3.149E-7	2.186E-6	5.822E-7
555	-0.0037	0.0026	3.106E-7	2.252E-7	1.372E-6	4.141E-7

For Ge crystal

h k l	g	κ	ω_s	$\Delta\theta$	$\Delta\lambda/\lambda$	I
111	-0.0167	0.0118	1.377E-5	9.748E-6	3.245E-4	1.836E-5
220	-0.0136	0.0136	1.014E-5	5.084E-6	1.461E-4	1.352E-5
311	-0.0205	0.0144	5.672E-6	4.024E-6	6.962E-5	7.562E-6
331	-0.0235	0.0166	3.626E-6	2.579E-6	3.378E-5	4.834E-6
333	-0.0265	0.0186	2.610E-6	1.860E-6	2.035E-5	3.480E-6
400	-0.0158	0.0158	5.945E-6	2.987E-6	6.042E-5	7.927E-6
422	-0.0180	0.0178	4.138E-6	2.084E-6	3.426E-5	5.518E-6
440	-0.0201	0.0199	3.102E-6	1.566E-6	2.218E-5	4.136E-6
444	-0.0243	0.0239	1.957E-6	9.931E-7	1.137E-5	2.610E-6
511	-0.0265	0.0186	2.610E-6	1.860E-6	2.035E-5	3.480E-6
531	-0.0209	0.0206	2.818E-6	1.424E-6	1.925E-5	3.757E-6
551	-0.0354	0.0247	1.284E-6	9.225E-7	7.234E-6	1.713E-6
553	-0.0383	0.0266	1.067E-6	7.680E-7	5.572E-6	1.422E-6
555	-0.0439	0.0303	7.718E-7	5.584E-7	3.557E-6	1.029E-6

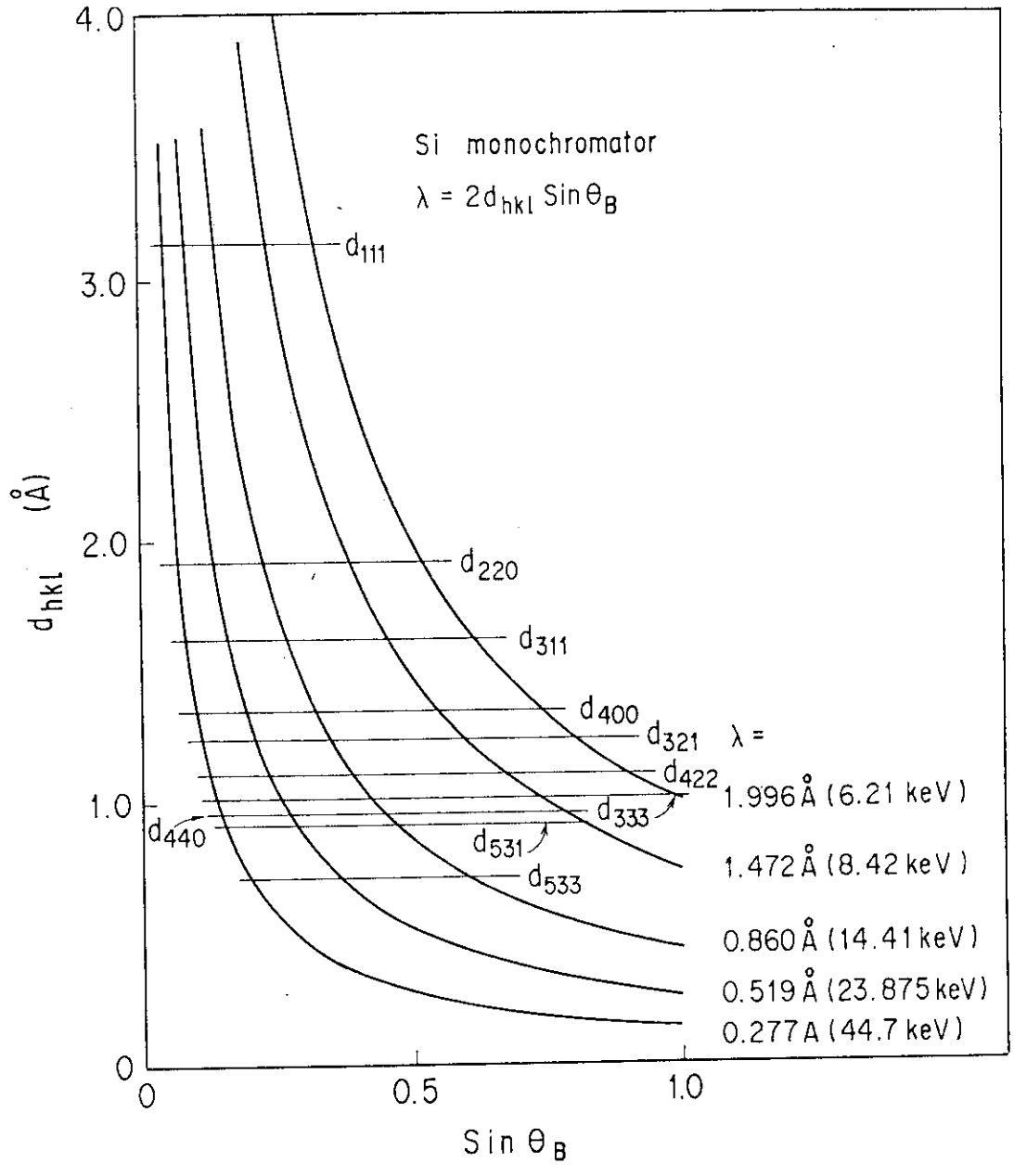

Fig.6.1 Bragg condition of Si crystal for some Mössbauer photons

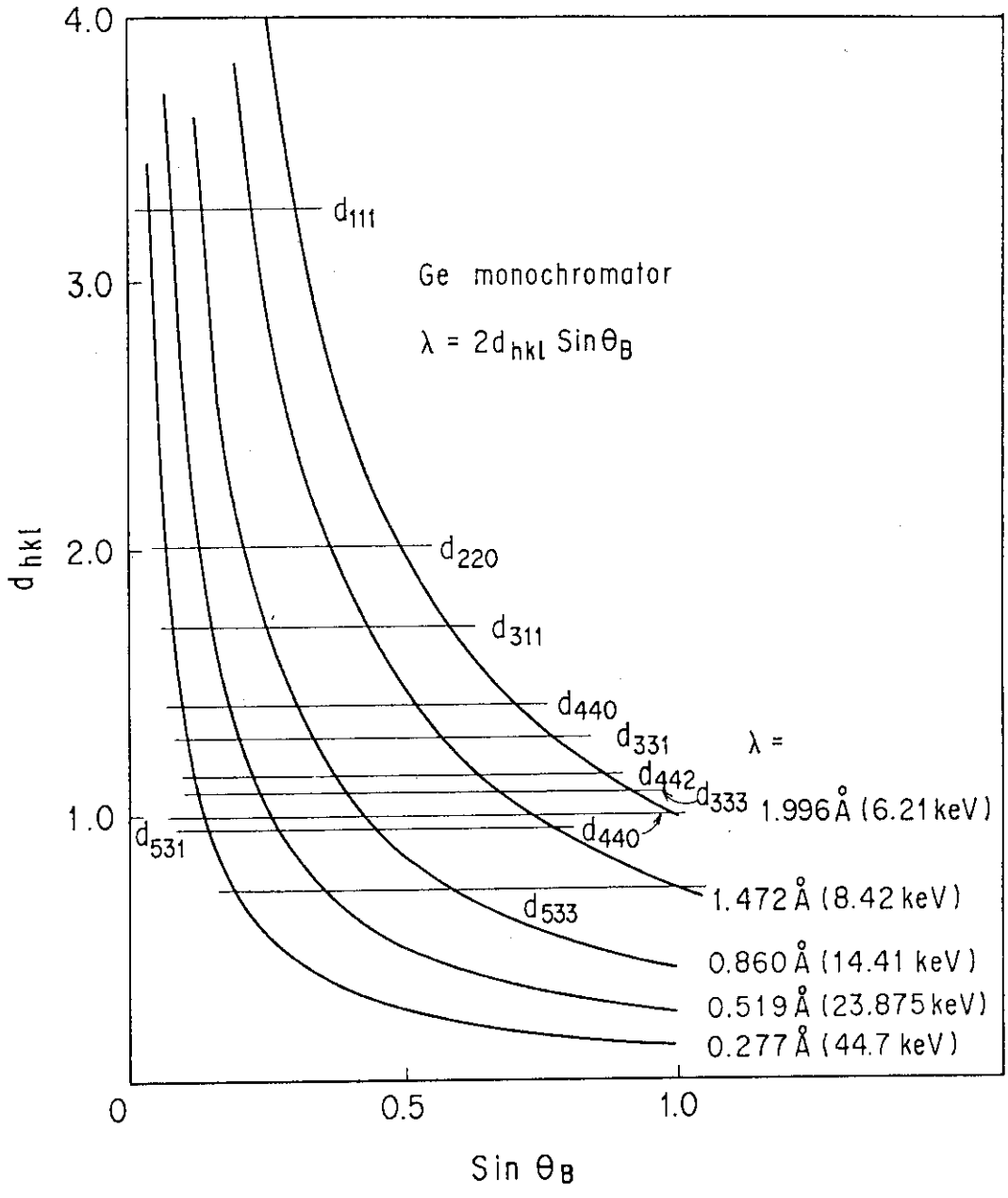

Fig.6.2 Bragg condition of Ge crystal for some Mössbauer photons

7. CONCLUDING REMARKS

This paper has described the dynamical diffraction formulae and collected the characteristics data of premonochromators of Si and Ge crystals for nuclear Bragg scattering; reflectivity, Bragg reflection width, energy resolution and integral reflecting power for the various reflections of Si and Ge crystals at the excitation photon wavelength of some Mössbauer nuclei, Bragg reflection angle, spacing between Bragg reflecting planes, scattering factor and anomalous scattering factor of Si and Ge atoms, Debye Waller factor, susceptibilities, rocking curves for the various reflections of Si and Ge crystals.

These data are useful to design and construct the X-ray beam line devices for nuclear Bragg scattering. The monochromator of nuclear Bragg scattering will be studied in the following paper.

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Appendix 1 Tables of Bragg reflection angles, atomic scattering factors and susceptibilities of Si and Ge crystals at λ = 1.996 , 1.472, 0.860 , 0.519 and 0.277 Å with σ polarization.

Table A 1.1 Bragg reflection angles θ_B, atomic scattering factors f, and susceptibilities Ψ of Si and Ge crystals at 1.996 Å (σ polarization,30°C)

For Si crystal ($\Delta f' = 0.536$)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.318	10.856	-1.360E-5	-6.710E-7	-1.924E-5	-9.489E-7
220	0.520	9.028	-1.569E-5	-9.307E-7	-1.569E-5	-9.307E-7
311	0.610	8.482	-1.030E-5	-6.506E-7	-1.457E-5	-9.200E-7
331	0.801	7.504	-8.839E-6	-6.308E-7	-1.250E-5	-8.920E-7
333	0.955	6.759	-7.719E-6	-6.116E-7	-1.092E-5	-8.649E-7
400	0.735	7.828	-1.319E-5	-9.024E-7	-1.319E-5	-9.024E-7
422	0.900	7.022	-1.147E-5	-8.750E-7	-1.147E-5	-8.750E-7
440	> 1.0					
444	> 1.0					
511	0.955	6.759	-7.719E-6	-6.116E-7	-1.092E-5	-8.649E-7
531	> 1.0					
551	> 1.0					
553	> 1.0					
555	> 1.0					

For Ge crystal ($\Delta f' = 1.403$)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.306	26.669	-2.950E-5	-1.552E-6	-4.171E-5	-2.194E-6
220	0.499	23.104	-3.532E-5	-2.145E-6	-3.532E-5	-2.145E-6
311	0.585	21.675	-2.311E-5	-1.496E-6	-3.269E-5	-2.116E-6
331	0.769	18.790	-1.932E-5	-1.442E-6	-2.732E-5	-2.040E-6
333	0.917	16.639	-1.650E-5	-1.391E-6	-2.333E-5	-1.967E-6
400	0.706	19.759	-2.913E-5	-2.068E-6	-2.913E-5	-2.068E-6
422	0.864	17.384	-2.471E-5	-1.994E-6	-2.471E-5	-1.994E-6
440	0.998	15.527	-2.128E-5	-1.922E-6	-2.128E-5	-1.922E-6
444	> 1.0					
511	0.917	16.639	-1.650E-5	-1.391E-6	-2.333E-5	-1.967E-6
531	> 1.0					
551	> 1.0					
553	> 1.0					
555	> 1.0					

Table A 1.2 Bragg reflection angles θ_B, atomic scattering factors f, and susceptibilities Ψ of Si and Ge crystals at 1.472 Å (σ polarization,30°C)

For Si crystal ($\Delta f'$ = 0.303)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.235	10.767	-7.337E-6	-2.063E-7	-1.038E-5	-2.918E-7
220	0.383	8.939	-8.450E-6	-2.862E-7	-8.450E-6	-2.862E-7
311	0.449	8.393	-5.546E-6	-2.001E-7	-7.843E-6	-2.829E-7
331	0.591	7.415	-4.750E-6	-1.940E-7	-6.718E-6	-2.743E-7
333	0.704	6.670	-4.143E-6	-1.881E-7	-5.859E-6	-2.660E-7
400	0.542	7.739	-7.093E-6	-2.775E-7	-7.093E-6	-2.775E-7
422	0.664	6.934	-6.162E-6	-2.691E-7	-6.162E-6	-2.691E-7
440	0.767	6.265	-5.398E-6	-2.609E-7	-5.398E-6	-2.609E-7
444	0.939	5.202	-4.214E-6	-2.453E-7	-4.214E-6	-2.453E-7
511	0.704	6.670	-4.143E-6	-1.881E-7	-5.859E-6	-2.660E-7
531	0.802	6.040	-5.144E-6	-2.579E-7	-5.144E-6	-2.579E-7
551	0.968	5.036	-2.851E-6	-1.714E-7	-4.032E-6	-2.425E-7
553	> 1.0					
555	> 1.0					

For Ge crystal ($\Delta f'$ = 0.816)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.225	26.054	-1.567E-5	-4.908E-7	-2.216E-5	-6.941E-7
220	0.368	22.489	-1.870E-5	-6.785E-7	-1.870E-5	-6.785E-7
311	0.431	21.059	-1.221E-5	-4.733E-7	-1.727E-5	-6.693E-7
331	0.567	18.174	-1.016E-5	-4.563E-7	-1.437E-5	-6.453E-7
333	0.676	16.023	-8.639E-6	-4.400E-7	-1.222E-5	-6.222E-7
400	0.520	19.143	-1.535E-5	-6.542E-7	-1.535E-5	-6.542E-7
422	0.637	16.768	-1.296E-5	-6.308E-7	-1.296E-5	-6.308E-7
440	0.736	14.912	-1.111E-5	-6.082E-7	-1.111E-5	-6.082E-7
444	0.901	12.166	-8.430E-6	-5.654E-7	-8.430E-6	-5.654E-7
511	0.676	16.023	-8.639E-6	-4.400E-7	-1.222E-5	-6.222E-7
531	0.770	14.312	-1.052E-5	-5.999E-7	-1.052E-5	-5.999E-7
551	0.929	11.757	-5.682E-6	-3.944E-7	-8.036E-6	-5.577E-7
553	0.999	10.793	-5.029E-6	-3.803E-7	-7.113E-6	-5.378E-7
555	> 1.0					

Table A 1.3 Bragg reflection angles θ_B, atomic scattering factors f, and susceptibilities Ψ of Si and Ge crystals at 0.860 Å (σ polarization,30°C)

For Si crystal ($\Delta f'' = 0.104$)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.137	10.639	-2.475E-6	-2.419E-8	-3.500E-6	-3.421E-8
220	0.224	8.812	-2.843E-6	-3.356E-8	-2.843E-6	-3.356E-8
311	0.263	8.266	-1.864E-6	-2.346E-8	-2.636E-6	-3.317E-8
331	0.345	7.288	-1.594E-6	-2.274E-8	-2.254E-6	-3.216E-8
333	0.411	6.542	-1.387E-6	-2.205E-8	-1.962E-6	-3.118E-8
400	0.317	7.612	-2.381E-6	-3.254E-8	-2.381E-6	-3.254E-8
422	0.388	6.806	-2.065E-6	-3.155E-8	-2.065E-6	-3.155E-8
440	0.448	6.137	-1.805E-6	-3.059E-8	-1.805E-6	-3.059E-8
444	0.549	5.074	-1.403E-6	-2.876E-8	-1.403E-6	-2.876E-8
511	0.411	6.542	-1.387E-6	-2.205E-8	-1.962E-6	-3.119E-8
531	0.468	5.913	-1.719E-6	-3.024E-8	-1.719E-6	-3.024E-8
551	0.565	4.908	-9.486E-7	-2.010E-8	-1.342E-6	-2.842E-8
553	0.608	4.508	-8.447E-7	-1.949E-8	-1.195E-6	-2.756E-8
555	0.686	3.861	-6.802E-7	-1.832E-8	-9.620E-7	-2.591E-8

For Ge crystal ($\Delta f'' = 2.491$)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.132	26.980	-5.540E-6	-5.115E-7	-7.834E-6	-7.233E-7
220	0.215	23.415	-6.646E-6	-7.070E-7	-6.646E-6	-7.070E-7
311	0.252	21.985	-4.352E-6	-4.931E-7	-6.155E-6	-6.974E-7
331	0.331	19.101	-3.646E-6	-4.755E-7	-5.156E-6	-6.724E-7
333	0.395	16.949	-3.119E-6	-4.585E-7	-4.411E-6	-6.483E-7
400	0.304	20.070	-5.492E-6	-6.817E-7	-5.492E-6	-6.817E-7
422	0.372	17.694	-4.669E-6	-6.573E-7	-4.669E-6	-6.573E-7
440	0.430	15.838	-4.029E-6	-6.337E-7	-4.029E-6	-6.337E-7
444	0.527	13.093	-3.097E-6	-5.892E-7	-3.097E-6	-5.892E-7
511	0.395	16.949	-3.119E-6	-4.585E-7	-4.411E-6	-6.483E-7
531	0.450	15.238	-3.824E-6	-6.251E-7	-3.824E-6	-6.251E-7
551	0.543	12.684	-2.092E-6	-4.109E-7	-2.959E-6	-5.812E-7
553	0.584	11.719	-1.864E-6	-3.962E-7	-2.636E-6	-5.603E-7
555	0.658	10.228	-1.513E-6	-3.684E-7	-2.139E-6	-5.209E-7

Table A 1.4 Bragg reflection angles θ_B, atomic scattering factors f, and susceptibilities Ψ of Si and Ge crystals at 0.519 Å (σ polarization,30°C)

For Si crystal ($\Delta f'$ = 0.037)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.083	10.570	-8.954E-7	-3.134E-9	-1.266E-6	-4.433E-9
220	0.135	8.743	-1.027E-6	-4.348E-9	-1.027E-6	-4.348E-9
311	0.158	8.197	-6.733E-7	-3.039E-9	-9.521E-7	-4.298E-9
331	0.208	7.219	-5.749E-7	-2.947E-9	-8.130E-7	-4.167E-9
333	0.248	6.473	-4.999E-7	-2.857E-9	-7.069E-7	-4.040E-9
400	0.191	7.543	-8.594E-7	-4.216E-9	-8.594E-7	-4.216E-9
422	0.234	6.737	-7.443E-7	-4.088E-9	-7.443E-7	-4.088E-9
440	0.270	6.068	-6.500E-7	-3.963E-9	-6.500E-7	-3.963E-9
444	0.331	5.005	-5.040E-7	-3.726E-9	-5.040E-7	-3.726E-9
511	0.248	6.473	-4.999E-7	-2.857E-9	-7.069E-7	-4.040E-9
531	0.283	5.844	-6.187E-7	-3.918E-9	-6.187E-7	-3.918E-9
551	0.341	4.840	-3.406E-7	-2.604E-9	-4.817E-7	-3.683E-9
553	0.367	4.439	-3.029E-7	-2.525E-9	-4.284E-7	-3.571E-9
555	0.414	3.792	-2.433E-7	-2.374E-9	-3.441E-7	-3.357E-9

For Ge crystal ($\Delta f'$ = 1.041)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.079	27.570	-2.062E-6	-7.787E-8	-2.916E-6	-1.101E-7
220	0.130	24.005	-2.481E-6	-1.077E-7	-2.481E-6	-1.077E-7
311	0.152	22.575	-1.628E-6	-7.508E-8	-2.302E-6	-1.062E-7
331	0.200	19.691	-1.369E-6	-7.240E-8	-1.936E-6	-1.024E-7
333	0.238	17.539	-1.176E-6	-6.980E-8	-1.663E-6	-9.872E-8
400	0.183	20.660	-2.059E-6	-1.038E-7	-2.059E-6	-1.038E-7
422	0.225	18.284	-1.757E-6	-1.001E-7	-1.757E-6	-1.001E-7
440	0.259	16.428	-1.522E-6	-9.649E-8	-1.522E-6	-9.649E-8
444	0.318	13.683	-1.179E-6	-8.970E-8	-1.179E-6	-8.970E-8
511	0.238	17.539	-1.176E-6	-6.980E-8	-1.663E-6	-9.872E-8
531	0.271	15.828	-1.447E-6	-9.518E-8	-1.447E-6	-9.518E-8
551	0.328	13.274	-7.975E-7	-6.257E-8	-8.849E-8	-1.128E-6
553	0.352	12.309	-7.131E-7	-6.033E-8	-1.008E-6	-8.532E-8
555	0.397	10.818	-5.826E-7	-5.608E-8	-8.240E-7	-7.932E-8

Table A 1.5 Bragg reflection angles θ_B, atomic scattering factors f, and susceptibilities Ψ of Si and Ge crystals at 0.277 Å (σ polarization,30°C)

For Si crystal ($\Delta f'$ = 0.010)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.044	10.532	-2.541E-7	-2.341E-10	-3.594E-7	-3.310E-10
220	0.072	8.704	-2.914E-7	-3.247E-10	-2.914E-7	-3.247E-10
311	0.085	8.158	-1.909E-7	-2.270E-10	-2.700E-7	-3.210E-10
331	0.111	7.180	-1.629E-7	-2.201E-10	-2.304E-7	-3.112E-10
333	0.133	6.434	-1.415E-7	-2.134E-10	-2.002E-7	-3.017E-10
400	0.102	7.504	-2.436E-7	-3.148E-10	-2.436E-7	-3.148E-10
422	0.125	6.698	-2.108E-7	-3.053E-10	-2.108E-7	-3.053E-10
440	0.144	6.030	-1.840E-7	-2.960E-10	-1.840E-7	-2.960E-10
444	0.177	4.967	-1.425E-7	-2.782E-10	-1.425E-7	-2.782E-10
511	0.133	6.435	-1.415E-7	-2.134E-10	-2.002E-7	-3.017E-10
531	0.151	5.805	-1.751E-7	-2.926E-10	-1.751E-7	-2.926E-10
551	0.182	4.801	-9.625E-8	-1.945E-10	-1.361E-7	-2.750E-10
553	0.196	4.400	-8.554E-8	-1.886E-10	-1.210E-7	-2.667E-10
555	0.221	3.754	-6.860E-8	-1.773E-10	-9.702E-8	-2.507E-10

For Ge crystal ($\Delta f'$ = 0.323)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.042	27.418	-5.840E-7	-6.889E-9	-8.259E-7	-9.742E-9
220	0.069	23.853	-7.023E-7	-9.522E-9	-7.023E-7	-9.522E-9
311	0.081	22.423	-4.605E-7	-6.642E-9	-6.513E-7	-9.393E-9
331	0.107	19.538	-3.869E-7	-6.404E-9	-5.472E-7	-9.057E-9
333	0.127	17.387	-3.320E-7	-6.175E-9	-4.695E-7	-8.732E-9
400	0.098	20.507	-5.822E-7	-9.181E-9	-5.822E-7	-9.181E-9
422	0.120	18.132	-4.963E-7	-8.853E-9	-4.963E-7	-8.853E-9
440	0.138	16.276	-4.296E-7	-8.536E-9	-4.296E-7	-8.536E-9
444	0.170	13.530	-3.320E-7	-7.935E-9	-3.320E-7	-7.935E-9
511	0.127	17.387	-3.320E-7	-6.175E-9	-4.695E-7	-8.732E-9
531	0.145	15.676	-4.081E-7	-8.420E-9	-4.081E-7	-8.420E-9
551	0.175	13.121	-2.246E-7	-5.535E-9	-3.176E-7	-7.827E-9
553	0.188	12.157	-2.006E-7	-5.337E-9	-2.837E-7	-7.547E-9
555	0.212	10.666	-1.636E-7	-4.961E-9	-2.314E-7	-7.016E-9

Appendix 2 Tables of Bragg reflection angles, atomic scattering factors and susceptibilities of Si and Ge crystals at λ = 1.996 , 1.472 , 0.860 , 0.519 and 0.277 Å with π polarization.

Table A 2.1 Bragg reflection angles θ_B, atomic scattering factors f, and susceptibilities Ψ of Si and Ge crystals at 1.996 Å (π polarization, 30°C)

For Si crystal ($\Delta f' = 0.536$)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.318	10.856	-1.360E-5	-6.710E-7	-1.924E-5	-9.489E-7
220	0.520	9.028	-1.569E-5	-9.307E-7	-1.569E-5	-9.307E-7
311	0.610	8.482	-1.030E-5	-6.506E-7	-1.457E-5	-9.200E-7
331	0.801	7.504	-8.839E-6	-6.308E-7	-1.250E-5	-8.920E-7
333	0.955	6.759	-7.719E-6	-6.116E-7	-1.092E-5	-8.649E-7
400	0.735	7.828	-1.319E-5	-9.024E-7	-1.319E-5	-9.024E-7
422	0.900	7.022	-1.147E-5	-8.750E-7	-1.147E-5	-8.750E-7
440	> 1.0					
444	> 1.0					
511	0.955	6.759	-7.719E-6	-6.116E-7	-1.092E-5	-8.649E-7
531	> 1.0					
551	> 1.0					
553	> 1.0					
555	> 1.0					

For Ge crystal ($\Delta f' = 1.403$)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.306	26.669	-2.950E-5	-1.552E-6	-4.171E-5	-2.194E-6
220	0.499	23.104	-3.532E-5	-2.145E-6	-3.532E-5	-2.145E-6
311	0.585	21.675	-2.311E-5	-1.496E-6	-3.269E-5	-2.116E-6
331	0.769	18.790	-1.932E-5	-1.442E-6	-2.732E-5	-2.040E-6
333	0.917	16.639	-1.650E-5	-1.391E-6	-2.333E-5	-1.967E-6
400	0.706	19.759	-2.913E-5	-2.068E-6	-2.913E-5	-2.068E-6
422	0.864	17.384	-2.471E-5	-1.994E-6	-2.471E-5	-1.994E-6
440	0.998	15.527	-2.128E-5	-1.922E-6	-2.128E-5	-1.922E-6
444	> 1.0					
511	0.917	16.639	-1.650E-5	-1.391E-6	-2.333E-5	-1.967E-6
531	> 1.0					
551	> 1.0					
553	> 1.0					
555	> 1.0					

Table A 2.2 Bragg reflection angles θ_B, atomic scattering factors f, and susceptibilities Ψ of Si and Ge crystals at 1.472 Å (π polarization, 30°C)

For Si crystal ($\Delta f'' = 0.303$)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.235	10.767	-7.337E-6	-2.063E-7	-1.038E-5	-2.918E-7
220	0.383	8.939	-8.450E-6	-2.862E-7	-8.450E-6	-2.862E-7
311	0.449	8.393	-5.546E-6	-2.001E-7	-7.843E-6	-2.829E-7
331	0.591	7.415	-4.750E-6	-1.940E-7	-6.718E-6	-2.743E-7
333	0.704	6.670	-4.143E-6	-1.881E-7	-5.859E-6	-2.660E-7
400	0.542	7.739	-7.093E-6	-2.775E-7	-7.093E-6	-2.775E-7
422	0.664	6.933	-6.162E-6	-2.691E-7	-6.162E-6	-2.691E-7
440	0.767	6.265	-5.398E-6	-2.609E-7	-5.398E-6	-2.609E-7
444	0.939	5.202	-4.214E-6	-2.453E-7	-4.214E-6	-2.453E-7
511	0.704	6.670	-4.143E-6	-1.881E-7	-5.859E-6	-2.660E-7
531	0.802	6.040	-5.144E-6	-2.579E-7	-5.144E-6	-2.579E-7
551	0.968	5.036	-2.851E-6	-1.714E-7	-4.032E-6	-2.424E-7
553	> 1.0					
555	> 1.0					

For Ge crystal ($\Delta f'' = 0.816$)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.225	26.054	-1.567E-5	-4.908E-7	-2.216E-5	-6.942E-7
220	0.368	22.489	-1.870E-5	-6.785E-7	-1.870E-5	-6.785E-7
311	0.431	21.059	-1.221E-5	-4.733E-7	-1.727E-5	-6.693E-7
331	0.567	18.174	-1.016E-5	-4.563E-7	-1.437E-5	-6.453E-7
333	0.676	16.023	-8.639E-6	-4.400E-7	-1.222E-5	-6.222E-7
400	0.520	19.143	-1.535E-5	-6.542E-7	-1.535E-5	-6.542E-7
422	0.637	16.768	-1.296E-5	-6.308E-7	-1.296E-5	-6.308E-7
440	0.736	14.912	-1.111E-5	-6.082E-7	-1.111E-5	-6.082E-7
444	0.901	12.166	-8.430E-6	-5.654E-7	-8.430E-6	-5.654E-7
511	0.676	16.023	-8.639E-6	-4.400E-7	-1.222E-5	-6.222E-7
531	0.770	14.312	-1.052E-5	-5.999E-7	-1.052E-5	-5.999E-7
551	0.929	11.757	-5.682E-6	-3.944E-7	-8.036E-6	-5.577E-7
553	0.999	10.793	-5.029E-6	-3.803E-7	-7.113E-6	-5.378E-7
555	> 1.0					

Table A 2.3 Bragg reflection angles θ_B, atomic scattering factors f, and susceptibilities Ψ of Si and Ge crystals at 0.860 Å (π polarization, 30°C)

For Si crystal ($\Delta f'' = 0.104$)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.137	10.639	-2.475E-6	-2.419E-8	-3.500E-6	-3.421E-8
220	0.224	8.812	-2.843E-6	-3.356E-8	-2.843E-6	-3.356E-8
311	0.263	8.266	-1.864E-6	-2.346E-8	-2.636E-6	-3.317E-8
331	0.345	7.288	-1.594E-6	-2.274E-8	-2.254E-6	-3.216E-8
333	0.411	6.542	-1.387E-6	-2.205E-8	-1.962E-6	-3.118E-8
400	0.317	7.612	-2.381E-6	-3.254E-8	-2.381E-6	-3.254E-8
422	0.388	6.806	-2.065E-6	-3.155E-8	-2.065E-6	-3.155E-8
440	0.448	6.137	-1.805E-6	-3.059E-8	-1.805E-6	-3.059E-8
444	0.549	5.074	-1.403E-6	-2.876E-8	-1.403E-6	-2.876E-8
511	0.411	6.542	-1.387E-6	-2.205E-8	-1.962E-6	-3.118E-8
531	0.468	5.913	-1.719E-6	-3.024E-8	-1.719E-6	-3.024E-8
551	0.565	4.908	-9.486E-7	-2.010E-8	-1.342E-6	-2.842E-8
553	0.608	4.508	-8.447E-7	-1.949E-8	-1.195E-6	-2.756E-8
555	0.686	3.861	-6.802E-7	-1.832E-8	-9.620E-7	-2.591E-8

For Ge crystal ($\Delta f'' = 2.491$)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.132	26.980	-5.540E-6	-5.115E-7	-7.834E-6	-7.233E-7
220	0.215	23.415	-6.646E-6	-7.070E-7	-6.646E-7	-7.070E-7
311	0.252	21.985	-4.352E-6	-4.931E-7	-6.155E-6	-6.974E-7
331	0.331	19.101	-3.646E-6	-4.755E-7	-5.156E-6	-6.724E-7
333	0.395	16.949	-3.119E-6	-4.585E-7	-4.411E-6	-6.483E-7
400	0.304	20.070	-5.492E-6	-6.817E-7	-5.492E-6	-6.817E-7
422	0.372	17.694	-4.669E-6	-6.573E-7	-4.669E-6	-6.573E-7
440	0.430	15.838	-4.029E-6	-6.337E-7	-4.029E-6	-6.337E-7
444	0.527	13.093	-3.097E-6	-5.892E-7	-3.097E-6	-5.892E-7
511	0.395	16.949	-3.119E-6	-4.585E-7	-4.411E-6	-6.483E-7
531	0.450	15.238	-3.824E-6	-6.251E-7	-3.824E-6	-6.251E-7
551	0.543	12.684	-2.092E-6	-4.109E-7	-2.959E-6	-5.812E-7
553	0.584	11.719	-1.864E-6	-3.962E-7	-2.636E-6	-5.603E-7
555	0.658	10.228	-1.513E-6	-3.684E-7	-2.139E-6	-5.209E-7

Table A 2.4 Bragg reflection angles θ_B, atomic scattering factors f, and susceptibilities Ψ of Si and Ge crystals at 0.519 Å (π polarization, 30°C)

For Si crystal ($\Delta f' = 0.037$)

h k l	$\sin\theta_B$	$f^0 + \Delta f$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.083	10.570	-8.954E-7	-3.134E-9	-1.266E-6	-4.433E-9
220	0.135	8.743	-1.027E-6	-4.348E-9	-1.027E-6	-4.348E-9
311	0.158	8.197	-6.733E-7	-3.039E-9	-9.521E-7	-4.298E-9
331	0.208	7.219	-5.749E-7	-2.947E-9	-8.130E-7	-4.167E-9
333	0.248	6.473	-4.999E-7	-2.857E-9	-7.069E-7	-4.040E-9
400	0.191	7.543	-8.594E-7	-4.216E-9	-8.594E-7	-4.216E-9
422	0.234	6.737	-7.443E-7	-4.088E-9	-7.443E-7	-4.088E-9
440	0.270	6.068	-6.500E-7	-3.963E-9	-6.500E-7	-3.963E-9
444	0.331	5.005	-5.040E-7	-3.726E-9	-5.040E-7	-3.726E-9
511	0.248	6.473	-4.999E-7	-2.857E-9	-7.069E-7	-4.040E-9
531	0.283	5.844	-6.187E-7	-3.918E-9	-6.187E-7	-3.918E-9
551	0.341	4.839	-3.406E-7	-2.604E-9	-4.817E-7	-3.683E-9
553	0.367	4.439	-3.029E-7	-2.525E-9	-4.284E-7	-3.571E-9
555	0.414	3.792	-2.433E-7	-2.374E-9	-3.441E-7	-3.357E-9

For Ge crystal ($\Delta f' = 1.041$)

h k l	$\sin\theta_B$	$f^0 + \Delta f$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.079	27.570	-2.062E-6	-7.787E-8	-2.916E-6	-1.101E-7
220	0.130	24.005	-2.481E-6	-1.077E-7	-2.481E-6	-1.077E-7
311	0.152	22.575	-1.628E-6	-7.508E-8	-2.302E-6	-1.062E-7
331	0.200	19.691	-1.369E-6	-7.240E-8	-1.936E-6	-1.024E-7
333	0.238	17.539	-1.176E-6	-6.980E-8	-1.663E-6	-9.872E-8
400	0.183	20.660	-2.059E-6	-1.038E-7	-2.059E-6	-1.038E-7
422	0.225	18.284	-1.757E-6	-1.001E-7	-1.757E-6	-1.001E-7
440	0.259	16.428	-1.522E-6	-9.649E-8	-1.522E-6	-9.649E-8
444	0.318	13.683	-1.179E-6	-8.970E-8	-1.179E-6	-8.970E-8
511	0.238	17.539	-1.176E-6	-6.980E-8	-1.663E-6	-9.872E-8
531	0.271	15.828	-1.447E-6	-9.518E-8	-1.447E-6	-9.518E-8
551	0.328	13.274	-7.975E-7	-6.257E-8	-1.128E-6	-8.849E-8
553	0.352	12.309	-7.131E-7	-6.033E-8	-1.008E-6	-8.532E-8
555	0.397	10.818	-5.826E-7	-5.608E-8	-8.240E-7	-7.932E-8

Table A 2.5 Bragg reflection angles θ_B, atomic scattering factors f, and susceptibilities Ψ of Si and Ge crystals at 0.277 Å (π polarization, 30°C)

For Si crystal ($\Delta f'$ = 0.010)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.044	10.532	-2.541E-7	-2.341E-10	-3.594E-7	-3.310E-10
220	0.072	8.704	-2.914E-7	-3.247E-10	-2.914E-7	-3.247E-10
311	0.085	8.158	-1.909E-7	-2.270E-10	-2.700E-7	-3.210E-10
331	0.111	7.180	-1.629E-7	-2.201E-10	-2.304E-7	-3.112E-10
333	0.133	6.435	-1.415E-7	-2.134E-10	-2.002E-7	-3.017E-10
400	0.102	7.504	-2.436E-7	-3.148E-10	-2.436E-7	-3.148E-10
422	0.125	6.698	-2.108E-7	-3.053E-10	-2.108E-7	-3.053E-10
440	0.144	6.030	-1.840E-7	-2.960E-10	-1.840E-7	-2.960E-10
444	0.177	4.967	-1.425E-7	-2.782E-10	-1.425E-7	-2.782E-10
511	0.133	6.435	-1.415E-7	-2.134E-10	-2.002E-7	-3.017E-10
531	0.151	5.805	-1.751E-7	-2.926E-10	-1.751E-7	-2.926E-10
551	0.182	4.801	-9.625E-8	-1.945E-10	-1.361E-7	-2.750E-10
553	0.196	4.400	-8.554E-8	-1.886E-10	-1.210E-7	-2.667E-10
555	0.221	3.754	-6.860E-8	-1.773E-10	-9.702E-8	-2.507E-10

For Ge crystal ($\Delta f'$ = 0.323)

h k l	$\sin\theta_B$	$f^0 + \Delta f'$	$\Psi_{h,r}$	$\Psi_{h,i}$	$\Psi_{o,r}$	$\Psi_{o,i}$
111	0.042	27.418	-5.840E-7	-6.889E-9	-8.259E-7	-9.742E-9
220	0.069	23.853	-7.023E-7	-9.522E-9	-7.023E-7	-9.522E-9
311	0.081	22.423	-4.605E-7	-6.642E-9	-6.513E-7	-9.393E-9
331	0.107	19.538	-3.869E-7	-6.404E-9	-5.472E-7	-9.057E-9
333	0.127	17.387	-3.320E-7	-6.175E-9	-4.695E-7	-8.732E-9
400	0.098	20.507	-5.822E-7	-9.181E-9	-5.822E-7	-9.181E-9
422	0.120	18.132	-4.963E-7	-8.853E-9	-4.963E-7	-8.853E-9
440	0.138	16.276	-4.296E-7	-8.536E-9	-4.296E-7	-8.536E-9
444	0.170	13.530	-3.320E-7	-7.935E-9	-3.320E-7	-7.935E-9
511	0.127	17.387	-3.320E-7	-6.175E-9	-4.695E-7	-8.732E-9
531	0.145	15.676	-4.081E-7	-8.420E-9	-4.081E-7	-8.420E-9
551	0.175	13.121	-2.246E-7	-5.535E-9	-3.176E-7	-7.827E-9
553	0.188	12.157	-2.006E-7	-5.337E-9	-2.837E-7	-7.547E-9
555	0.212	10.666	-1.636E-7	-4.961E-9	-2.314E-7	-7.016E-9

Appendix 3 Figures of rocking curves of the various reflections of Si crystal at λ = 1.996 , 1.472 , 0.860 , 0.519 and 0.277 Å with σ polarization.

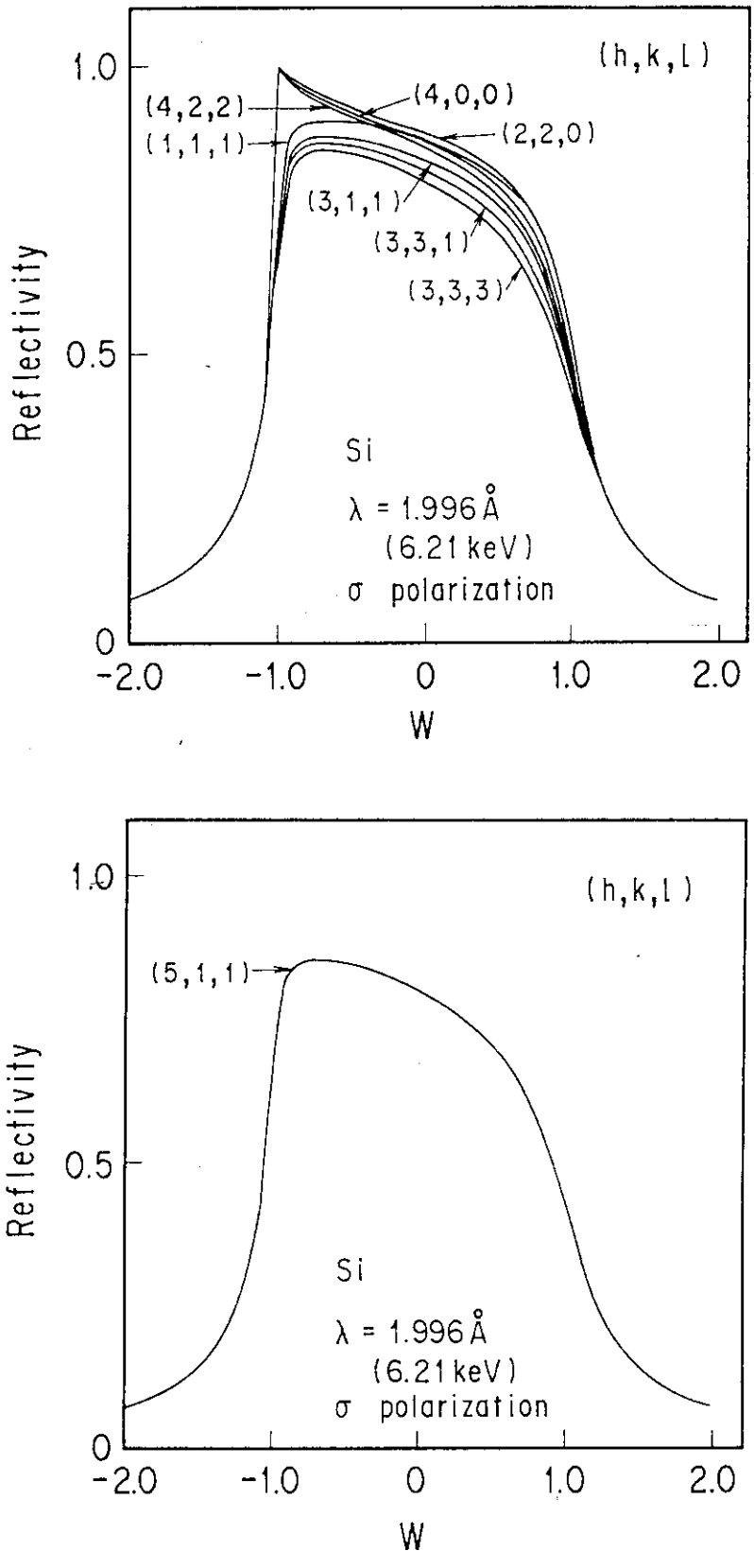

Fig.A3.1 Rocking curves of the various reflections of Si crystal at λ = 1.996 Å with σ polarization

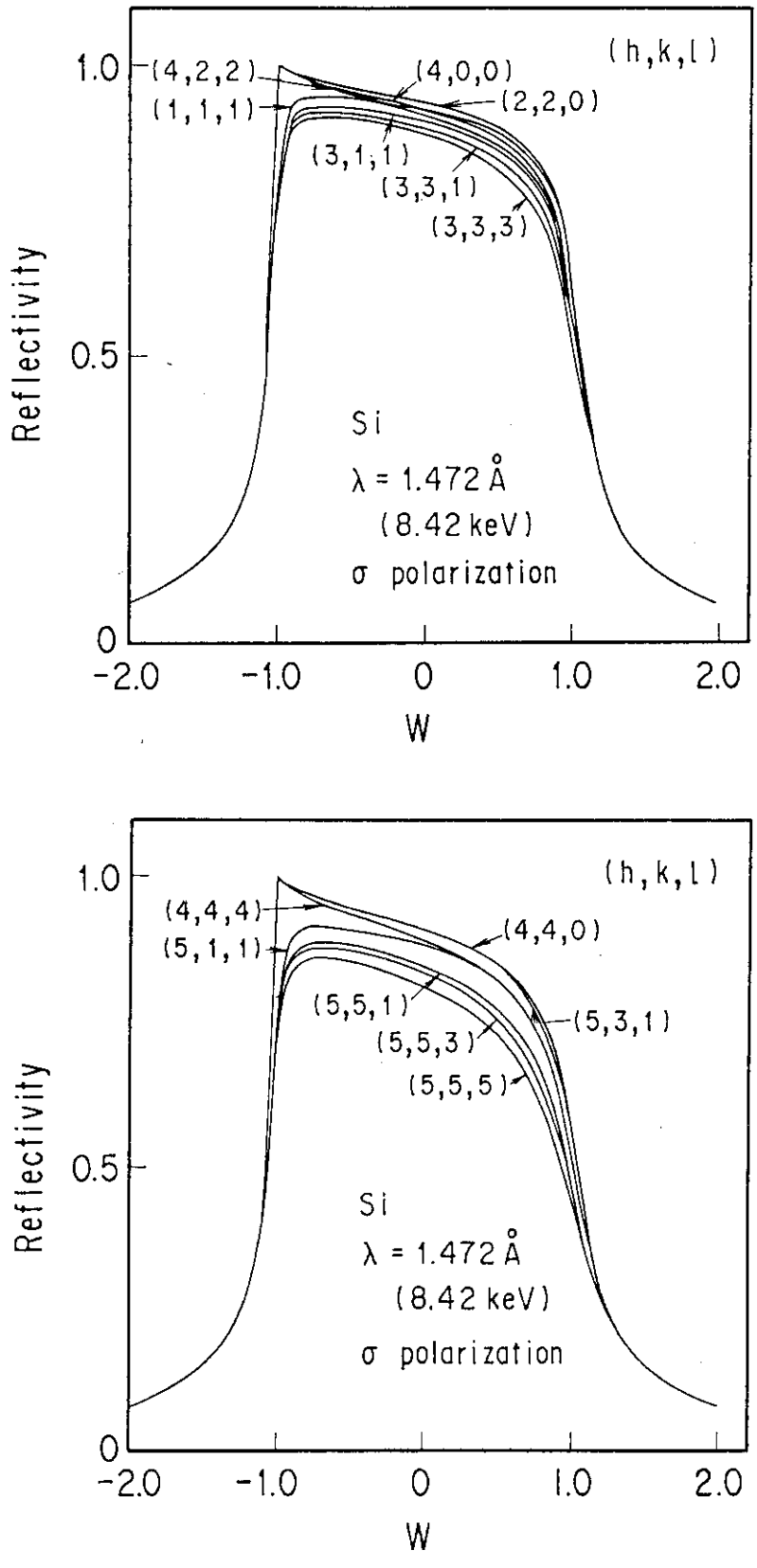

Fig.A3.2 Rocking curves of the various reflections of Si crystal at λ = 1.472 Å with σ polarization

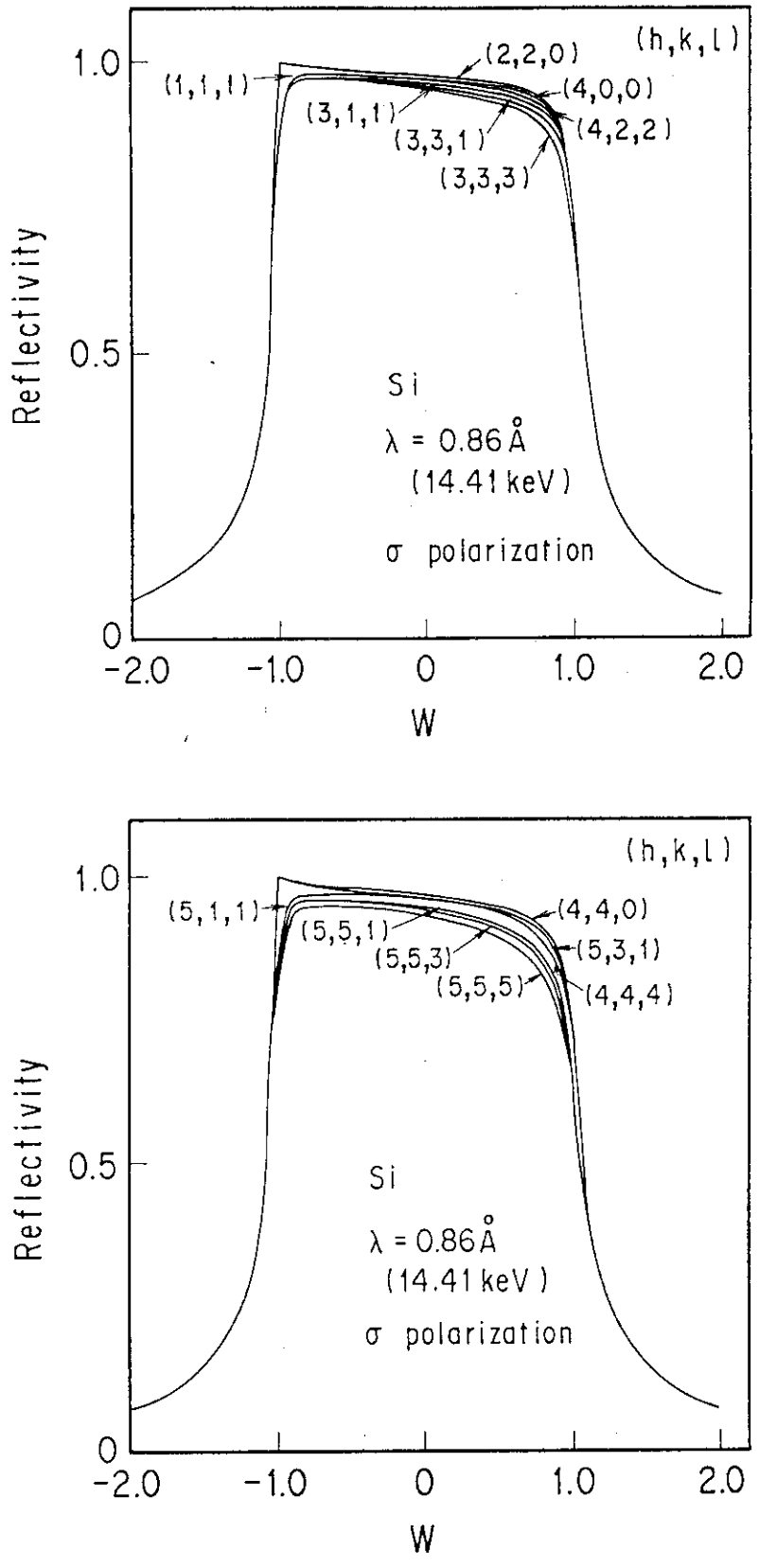

Fig.A3.3 Rocking curves of the various reflections of Si crystal at λ = 0.860 Å with σ polarization

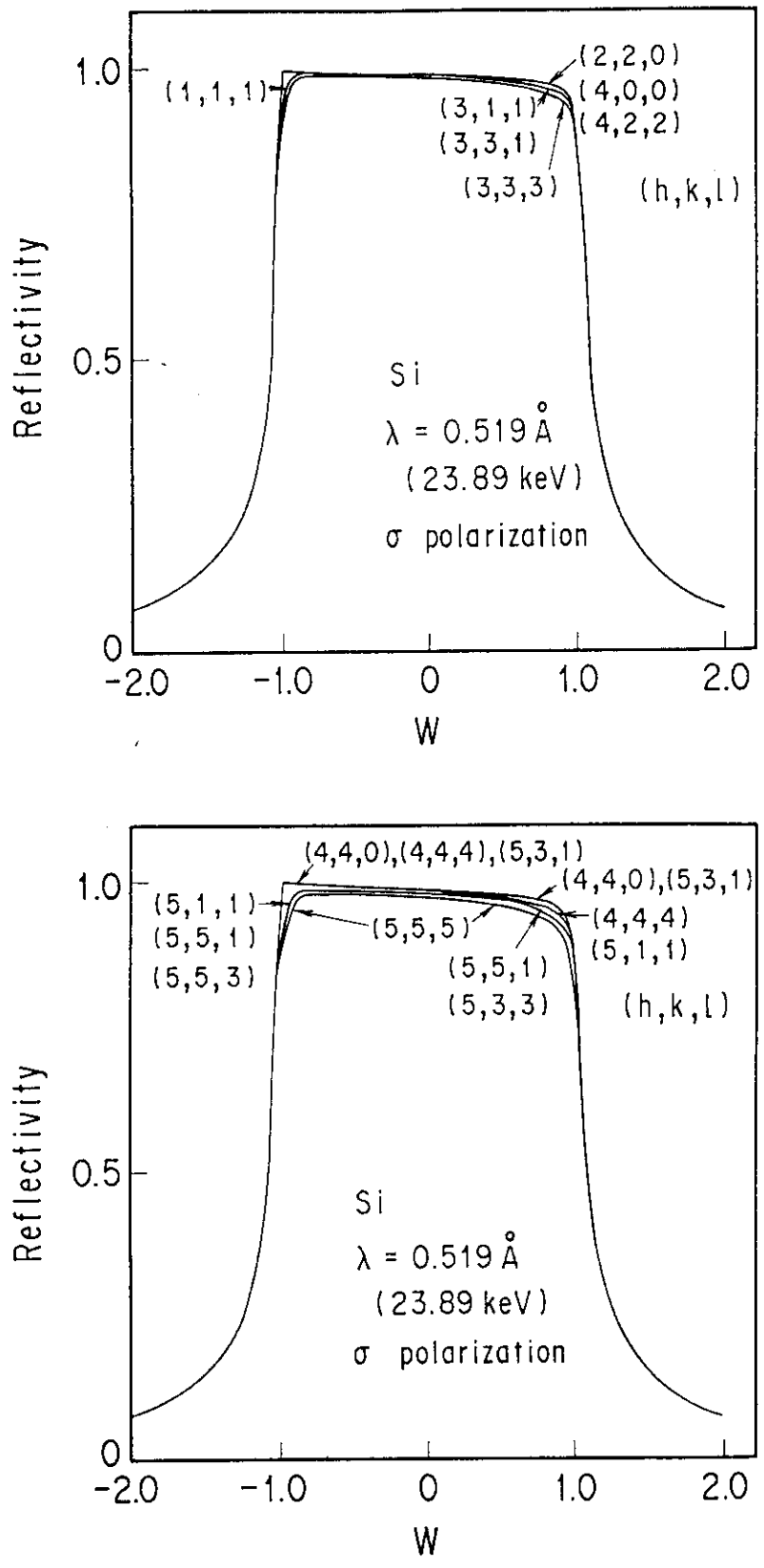

Fig.A3.4 Rocking curves of the various reflections of Si crystal at λ = 0.519 Å with σ polarization

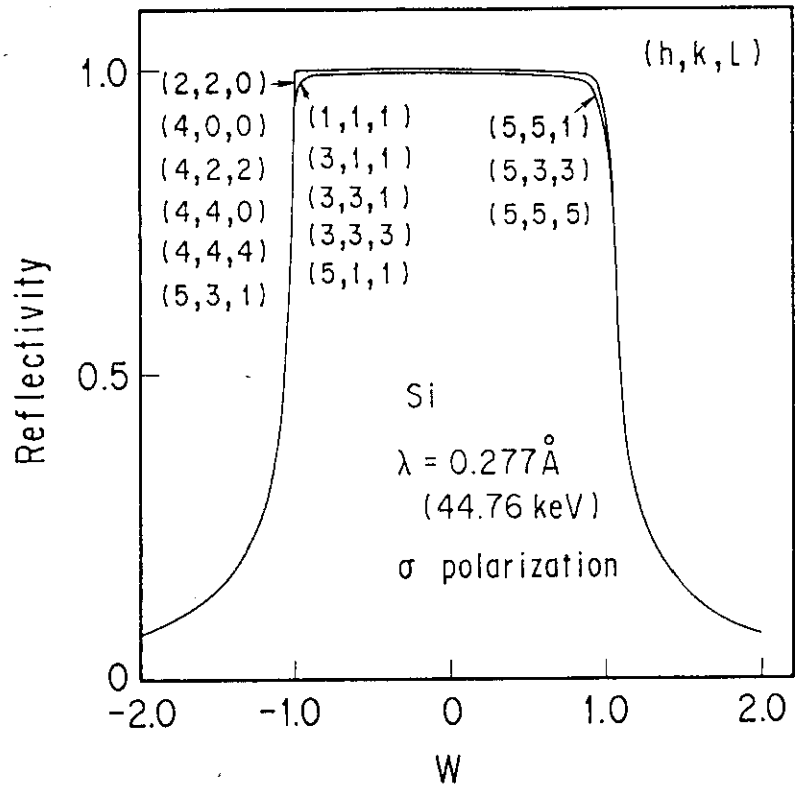

Fig.A3.5 Rocking curves of the various reflections of Si crystal at λ = 0.277 Å with σ polarization

Appendix 4 Figures of rocking curves of the various reflections of Si crystal at λ = 1.996 , 1.472 , 0.860 , 0.519 and 0.277 Å with π polarization

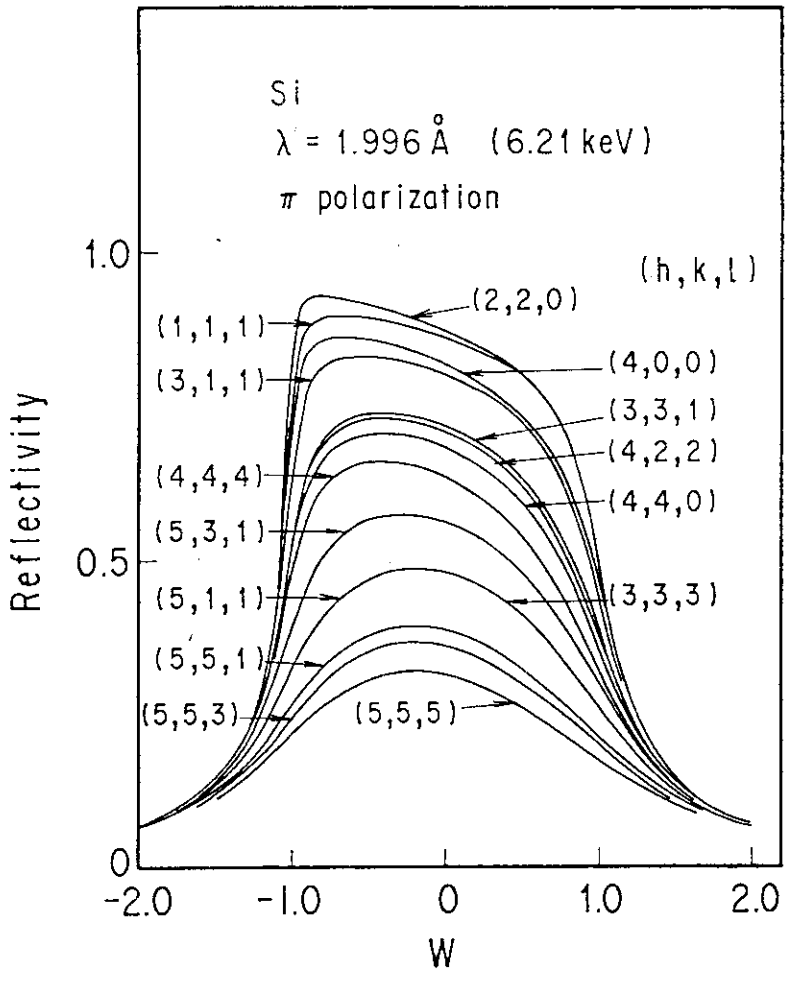

Fig.A4.1 Rocking curves of the various reflections of Si crystal at λ = 1.996 Å with π polarization

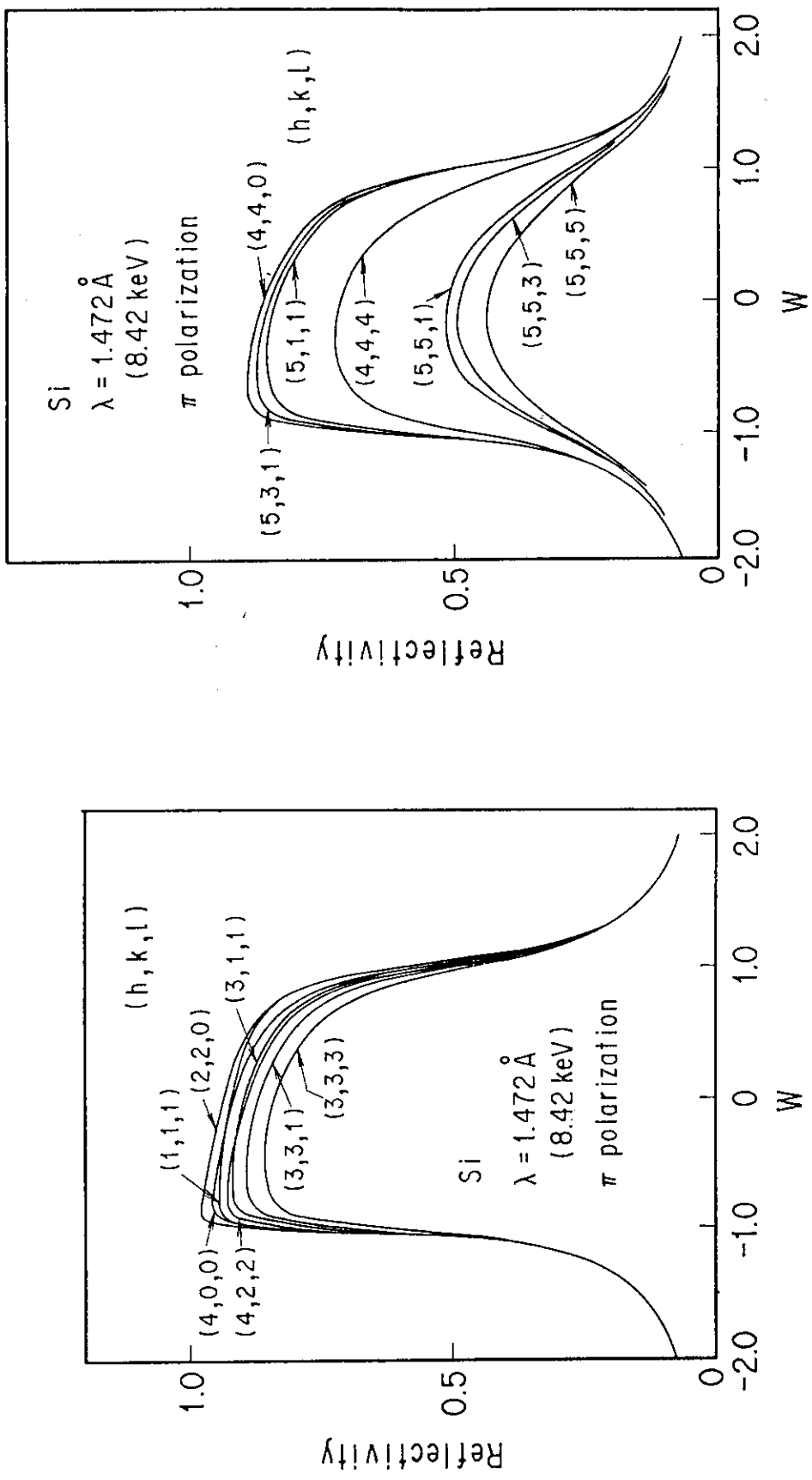

Fig.A4.2 Rocking curves of the various reflections of Si crystal at λ = 1.472 Å with π polarization

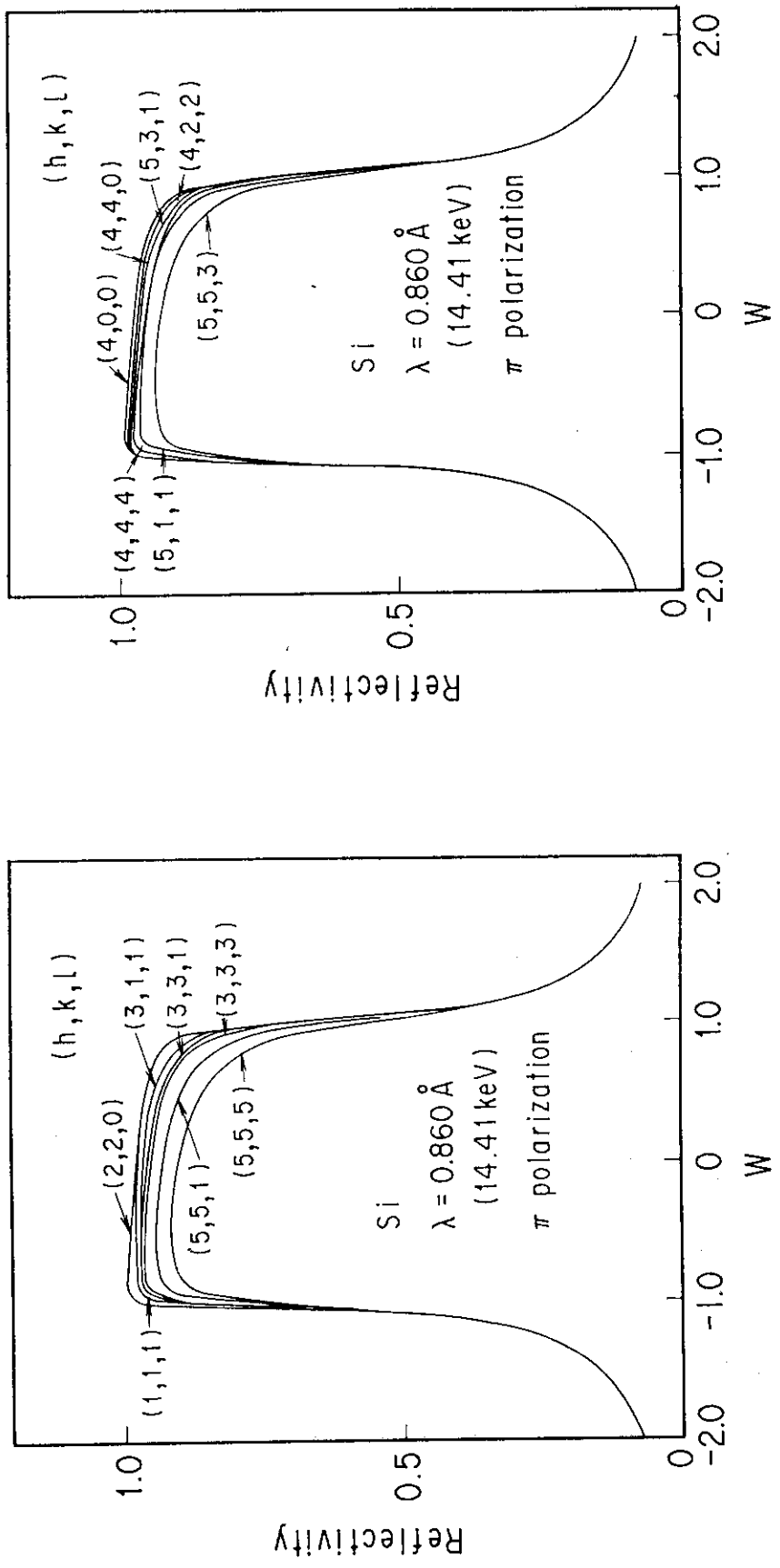

Fig.A4.3 Rocking curves of the various reflections of Si crystal at λ = 0.860 Å with π polarization

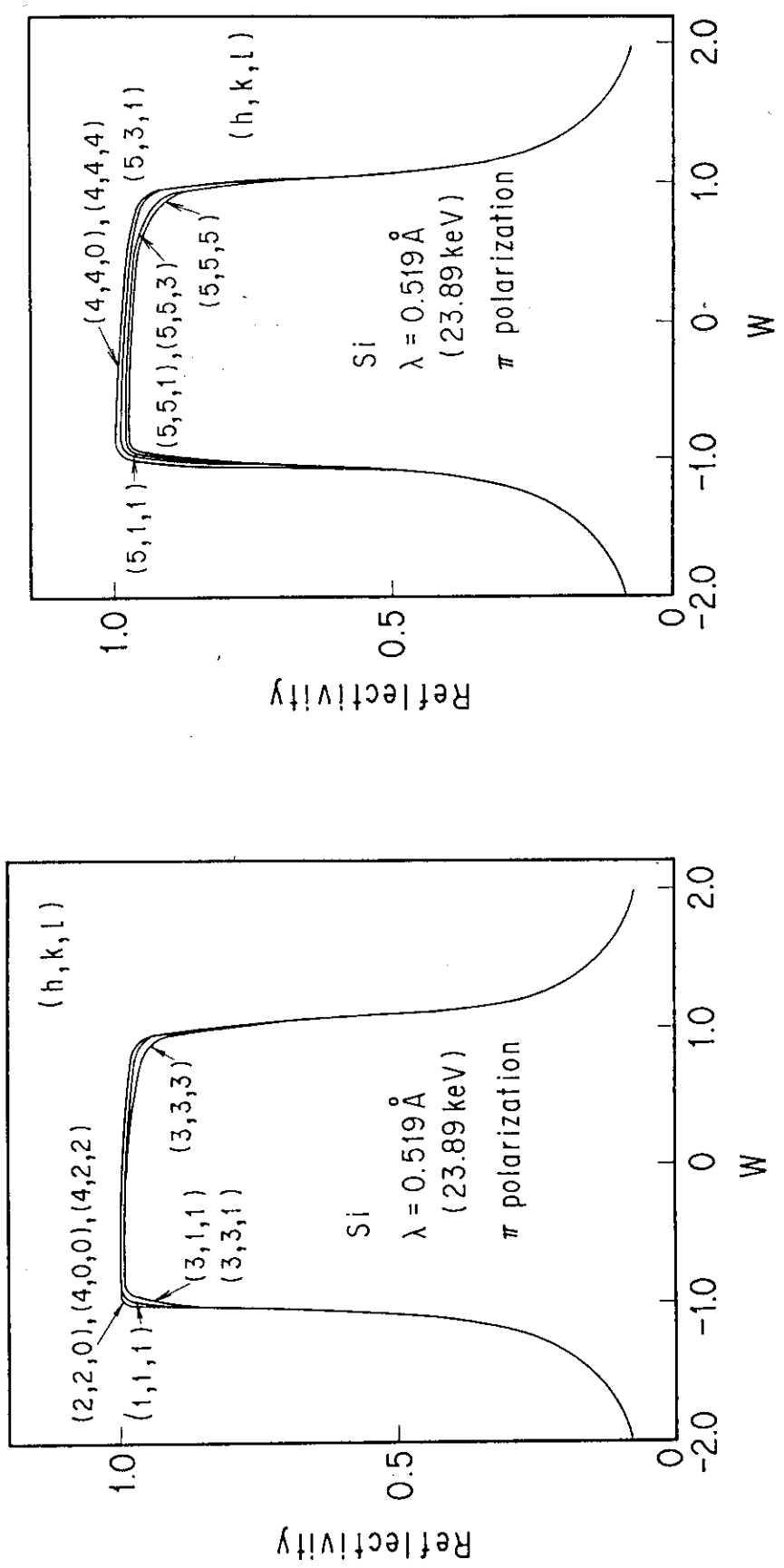

Fig.A4.4 Rocking curves of the various reflections of Si crystal at λ = 0.519 Å with π polarization

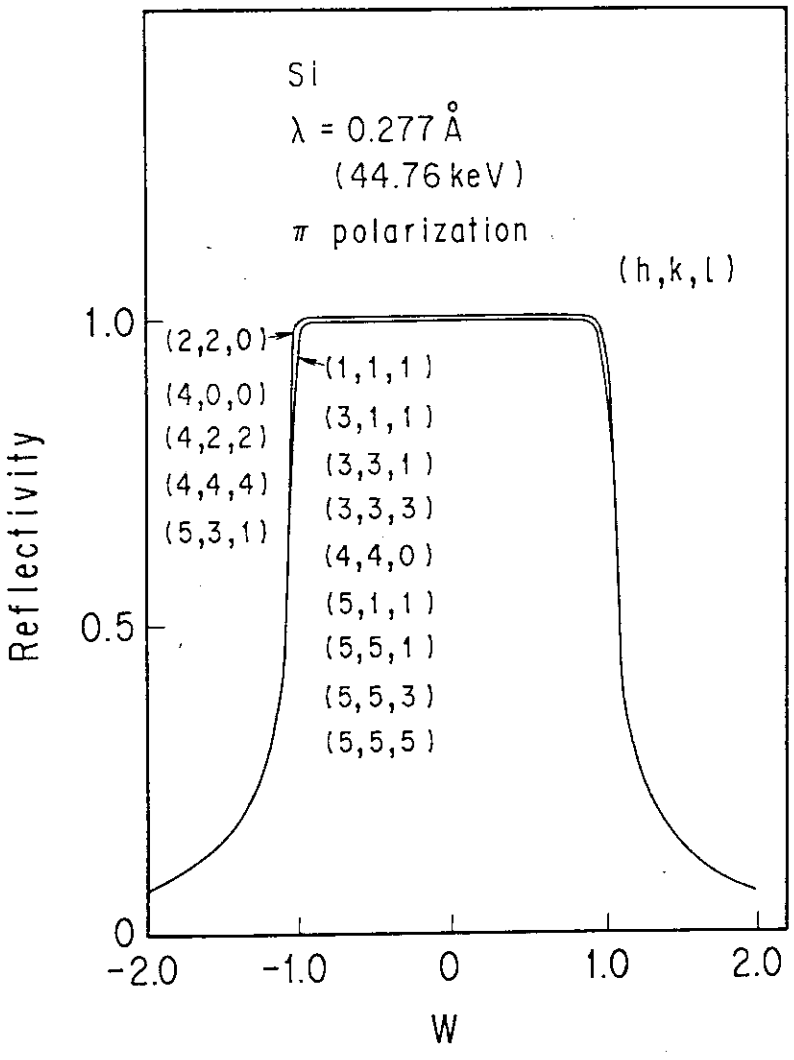

Fig.A4.5 Rocking curves of the various reflections of Si crystal at λ = 0.277 Å with π polarization

Appendix 5 Figures of rocking curves of the various reflections of Ge crystal at λ = 1.996 , 1.472 , 0.860 , 0.519 and 0.277 Å with σ polarization.

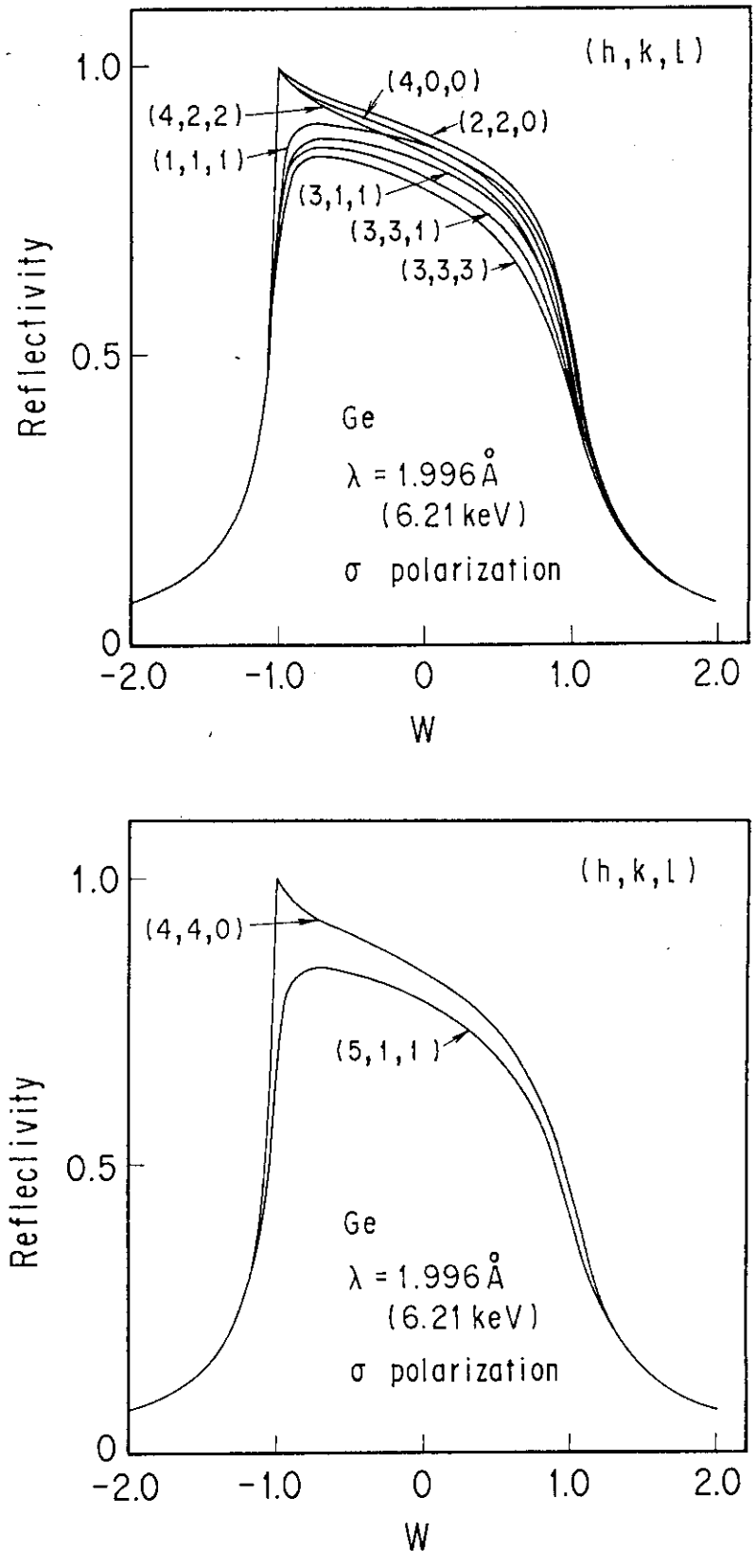

Fig.A5.1 Rocking curves of the various reflections of Ge crystal at λ = 1.996 Å with σ polarization

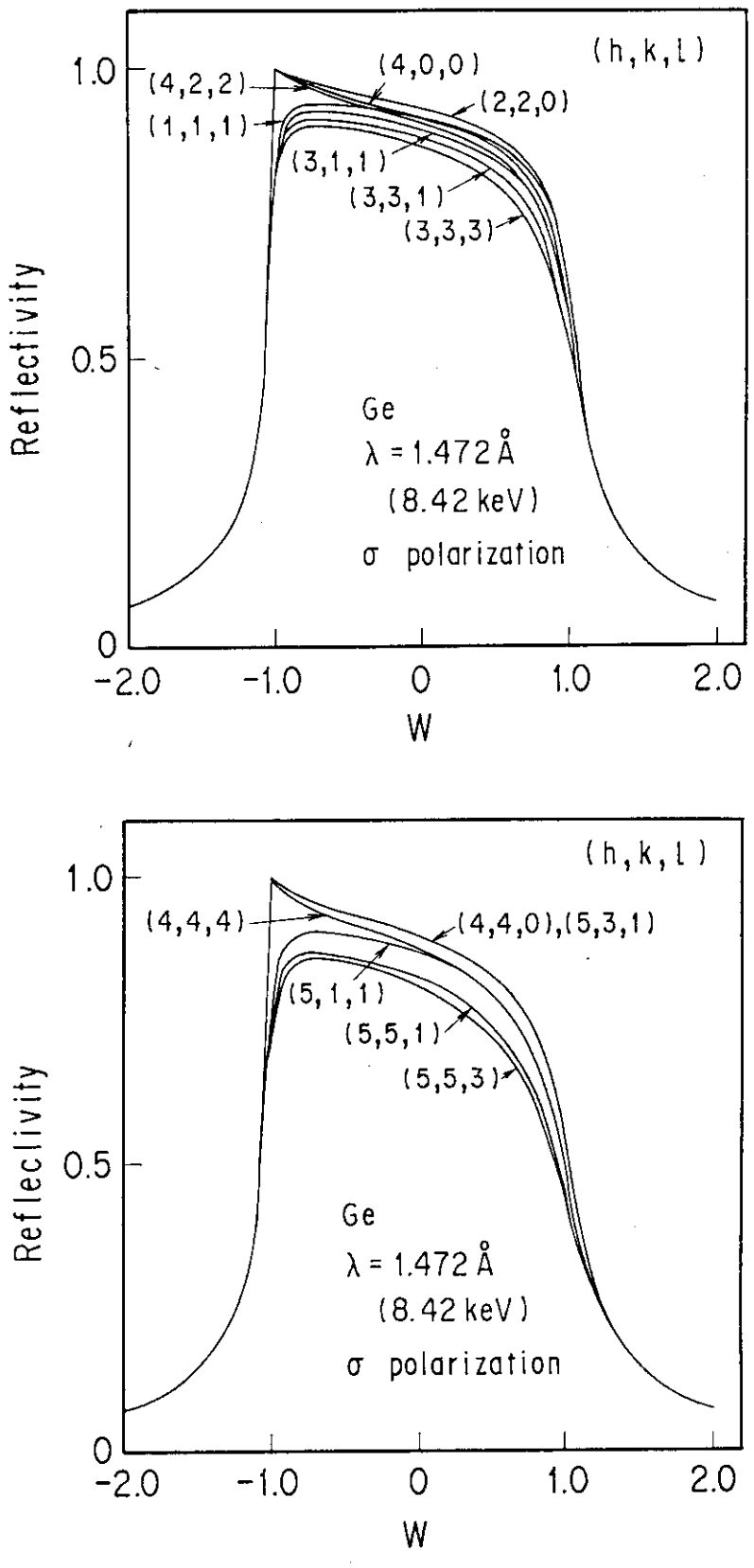

Fig.A5.2 Rocking curves of the various reflections of Ge crystal at λ = 1.472 Å with σ polarization

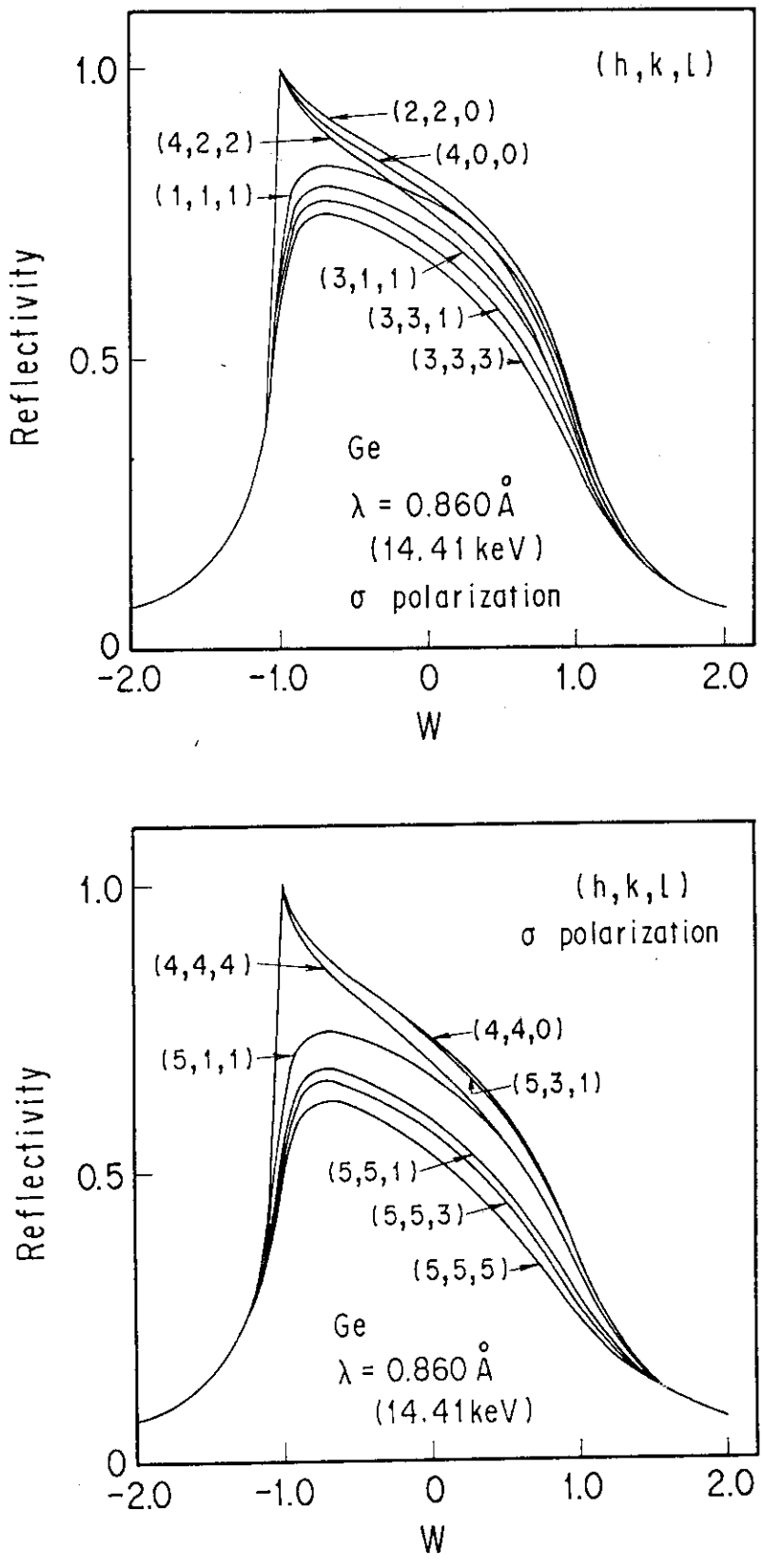

Fig.A5.3 Rocking curves of the various reflections of Ge crystal at λ = 0.860 Å with σ polarization

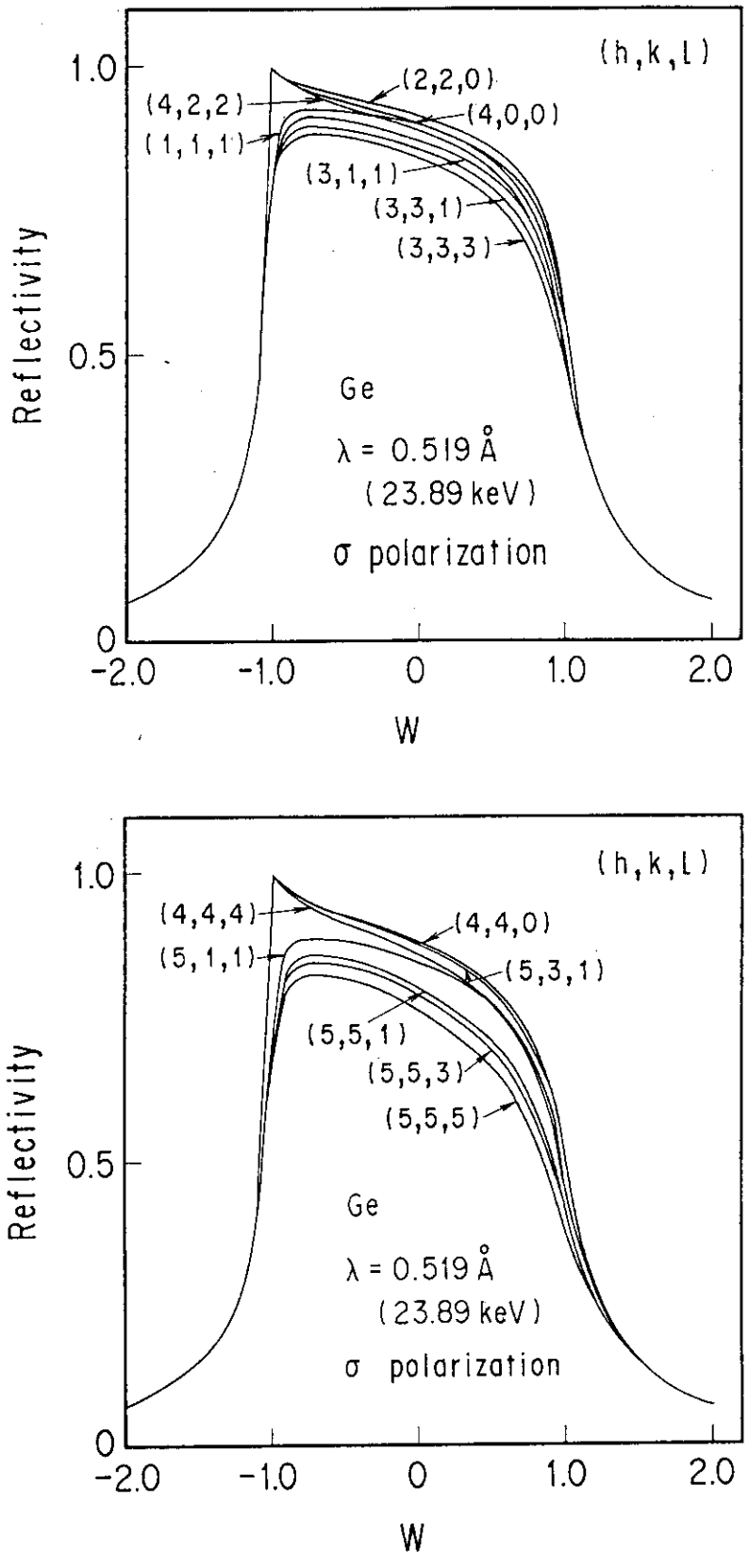

Fig.A5.4 Rocking curves of the various reflections of Ge crystal at λ = 0.519 Å with σ polarization

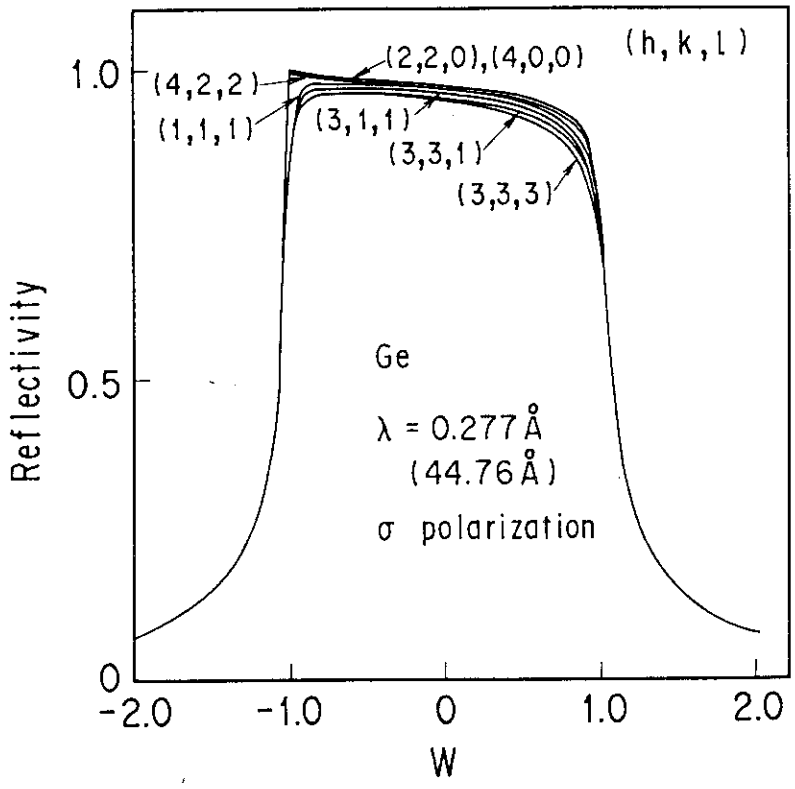

Fig.A5.5 Rocking curves of the various reflections of Ge crystal at λ = 0.277 Å with σ polarization

Appendix 6 Figures of rocking curves of the various reflections of Ge crystal at λ = 1.996 , 1.472 , 0.860 , 0.519 and 0.277 Å with π polarization.

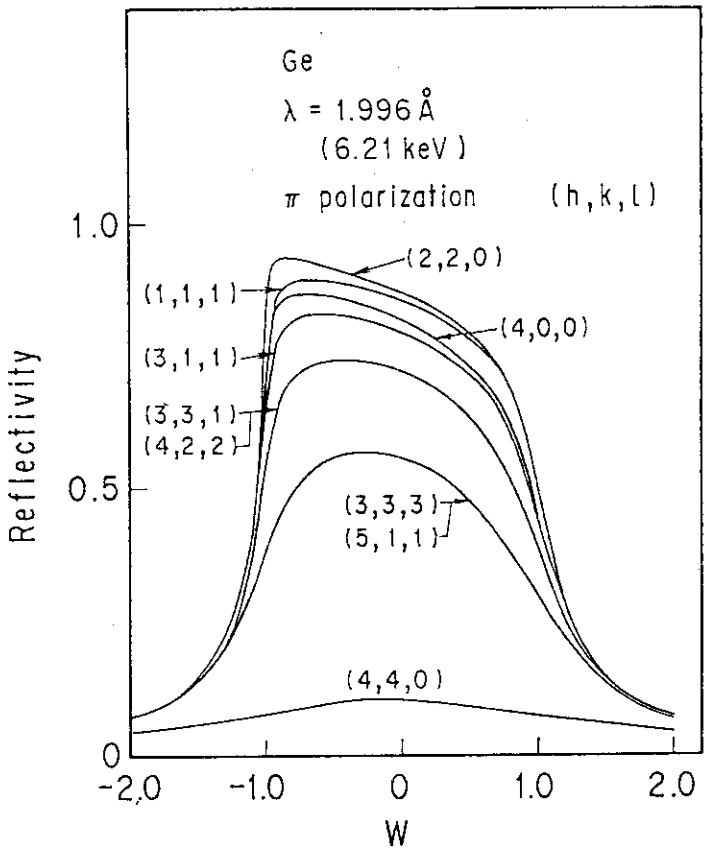

Fig.A6.1 Rocking curves of the various reflections of Ge crystal at λ = 1.996 Å with π polarization

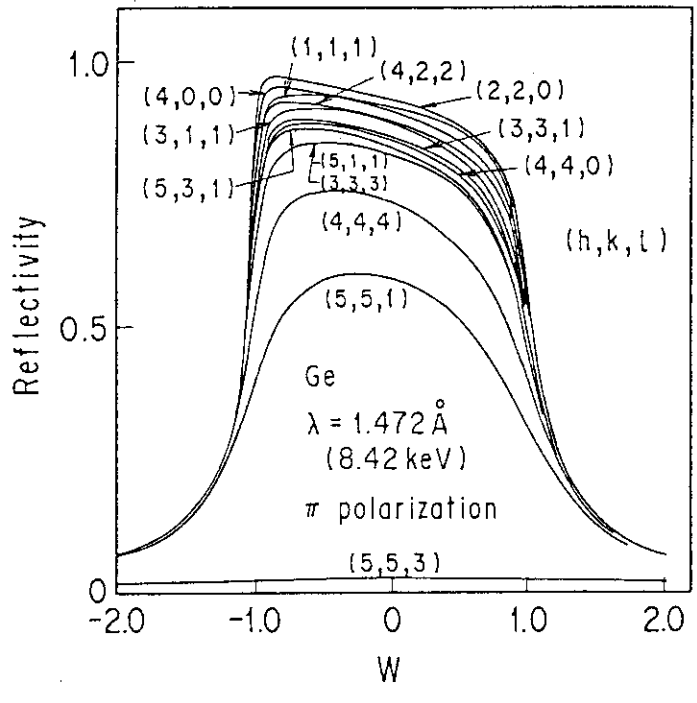

Fig.A6.2 Rocking curves of the various reflections of Ge crystal at λ = 1.472 Å with π polarization

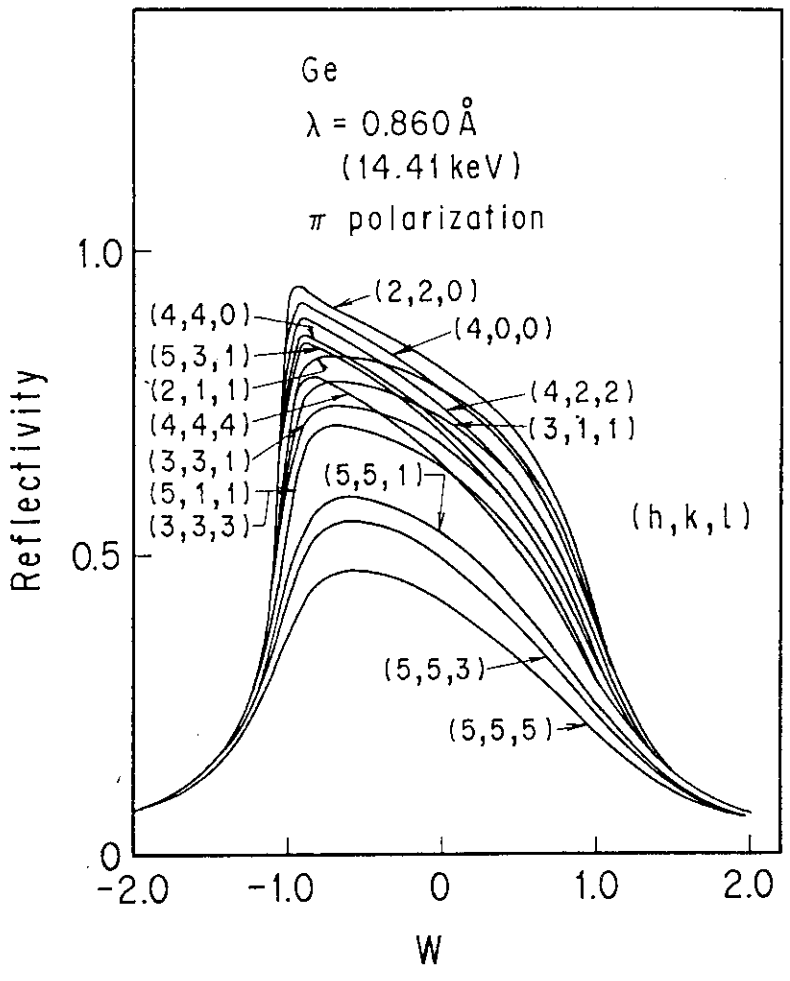

Fig.A6.3 Rocking curves of the various reflections of Ge crystal at λ = 0.860 Å with π polarization

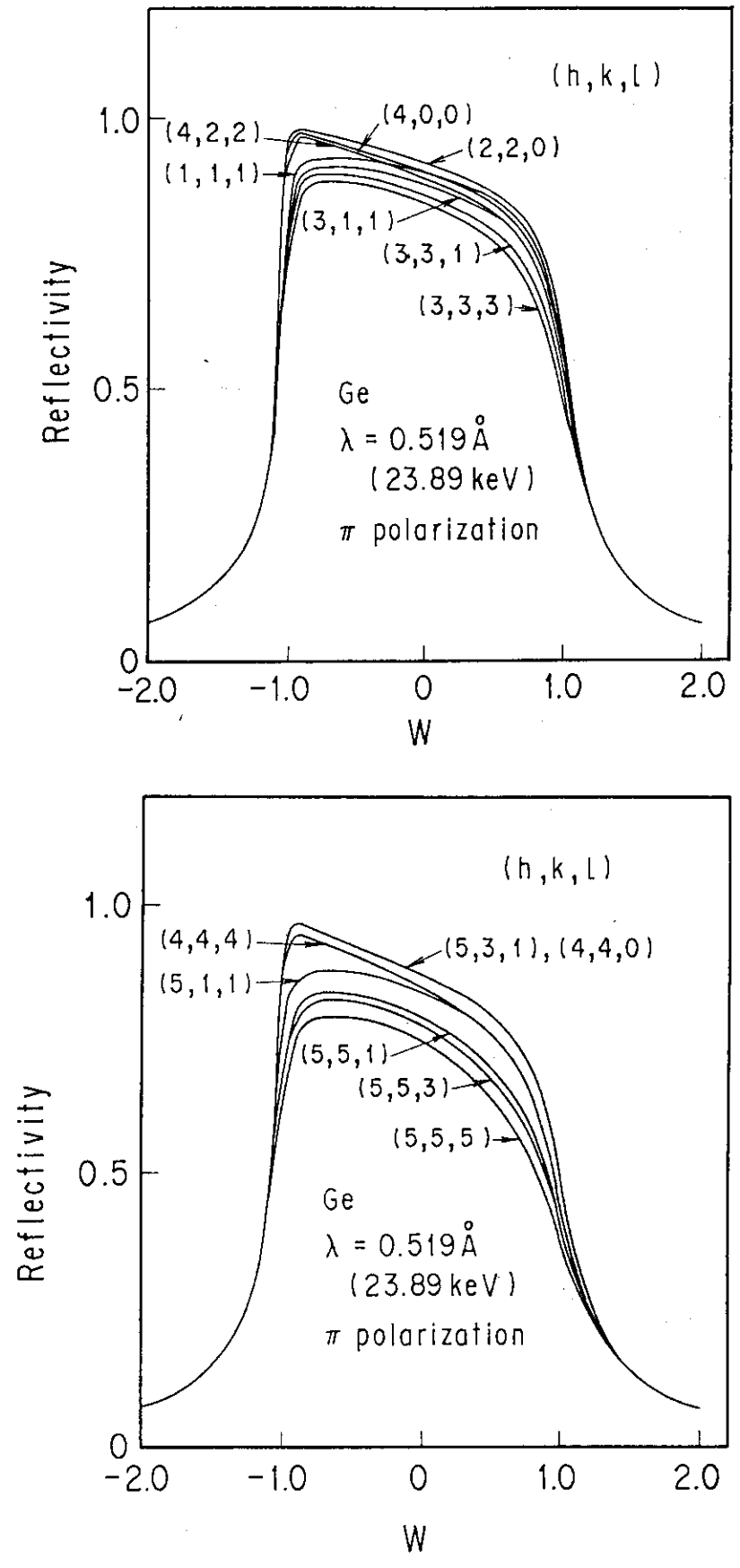

Fig.A6.4 Rocking curves of the various reflections of Ge crystal at λ = 0.519 Å with π polarization

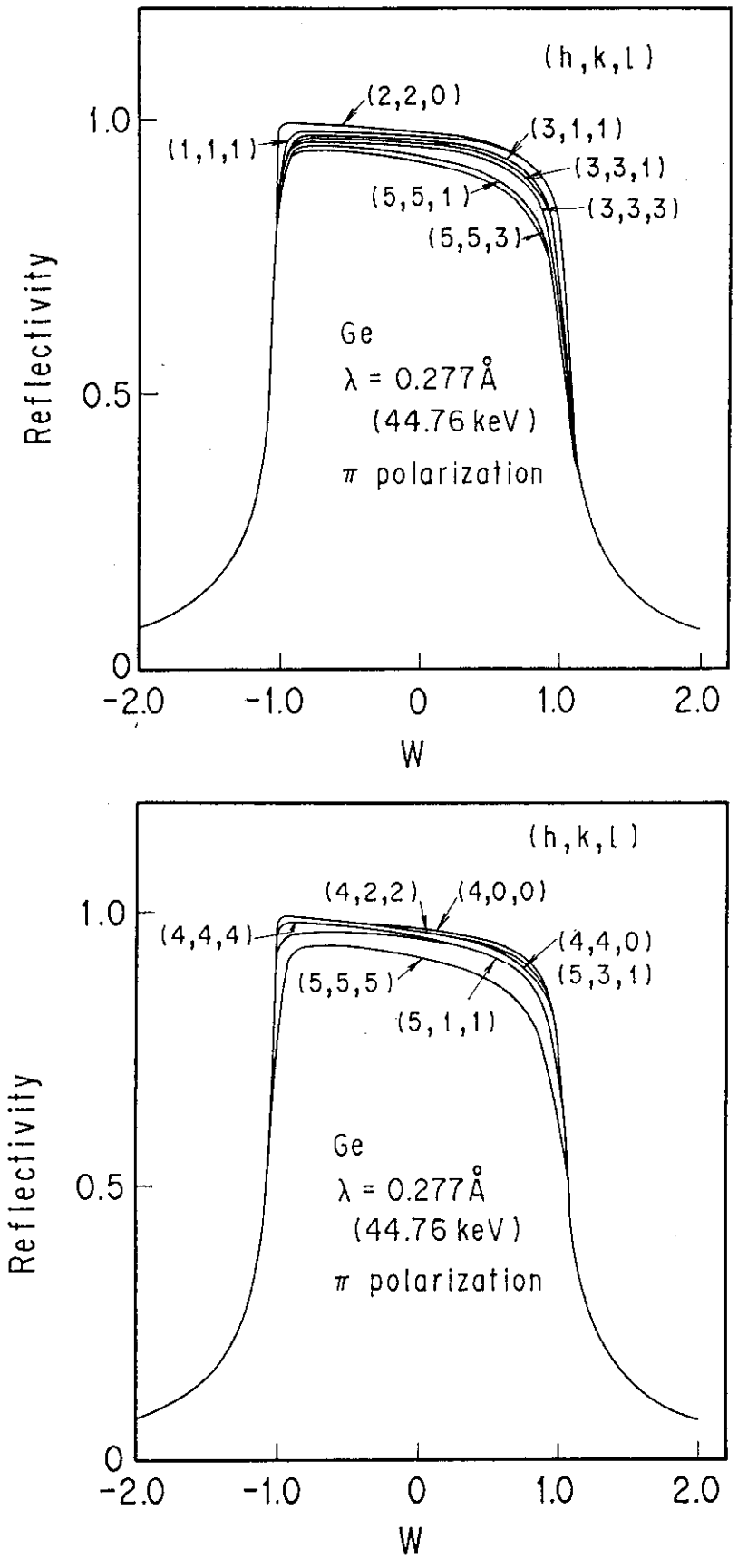

Fig.A6.5 Rocking curves of the various reflections of Ge crystal at λ = 0.277 Å with π polarization

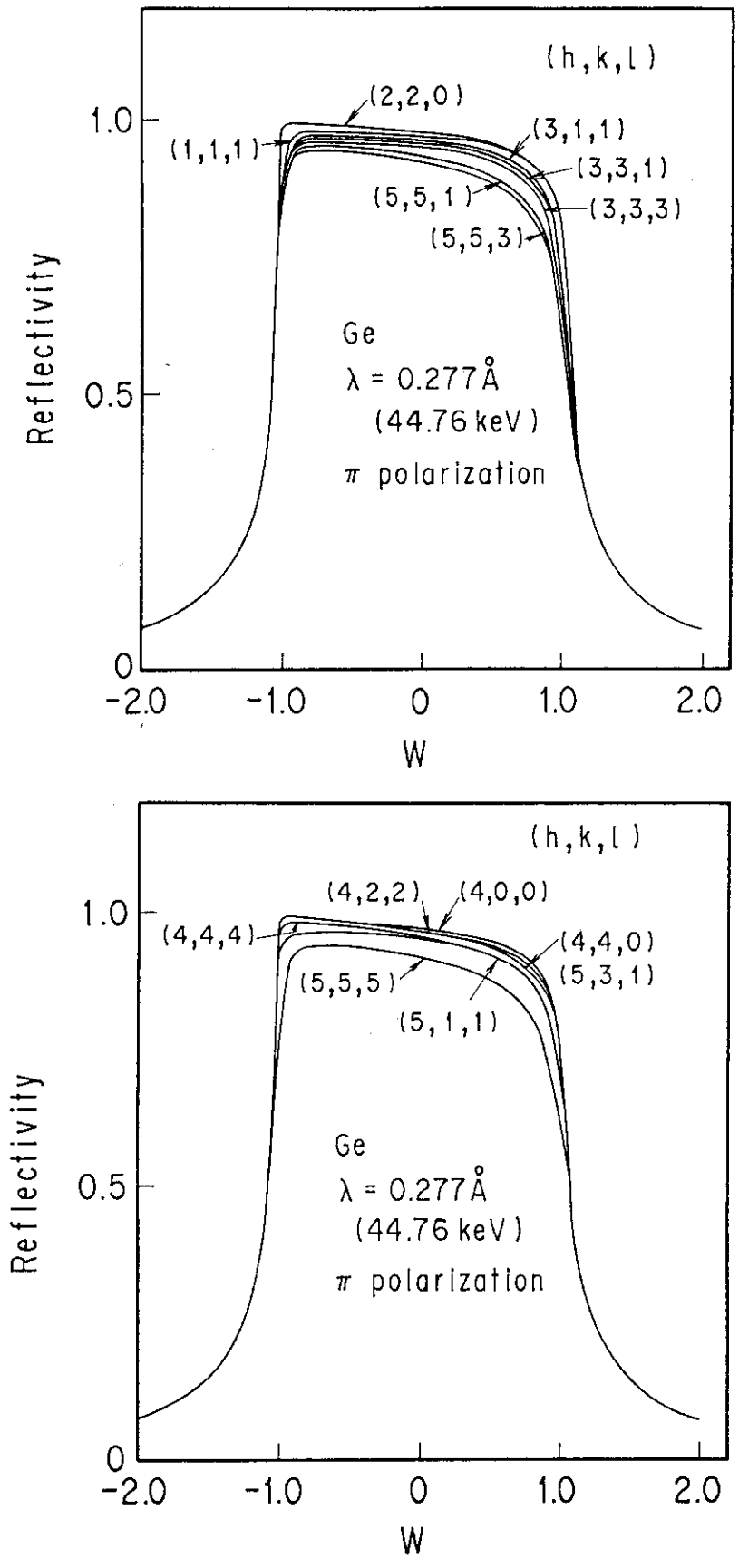

Fig.A6.5 Rocking curves of the various reflections of Ge crystal at λ = 0.277 Å with π polarization