The variation of these indices as a function of y_t for the situation $\langle|\Delta\mathbf{r}|\rangle = 0{\cdot}2$ Å and $\sin\theta/\lambda = 0{\cdot}4$ Å^{-1} is shown in Fig. 1(*a*)–(*f*). A study of these figures shows that, in the *NC* case, as y_t increases, $[R]_t$ decreases. This decrease is much less when y_t is small (say $y_t < 0{\cdot}15$) and becomes more pronounced for larger y_t. This behaviour of $[R]_t$ in the *NC* case may be contrasted with its behaviour in the *C* case (see Fig. 1 of part I). The evaluation of the overall values of the *R* indices for the *NC* case is quite analogous to that described in part I for the *C* case. The values of $[R]_t$ (in percent) as functions of σ_A and y_t required for the evaluation of $[R]_t$ are given in Tables 1–3 for the various *R* indices.

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Absorption Coefficients of Electrons in Crystals

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(*Received* 13 *October* 1980; *accepted* 13 *January* 1981)

Abstract

Absorption coefficients of Si, Ge and InSb are obtained from the analysis of extinction contours in the acceleration voltages ranging from 100 to 750 kV. The cross sections of thermal diffuse scattering, plasmon excitation and electronic excitation are obtained separately. An agreement between theory and experiment is obtained for thermal diffuse scattering and plasmon scattering. The theoretical estimation based on the electron gas statistical model is favourable for the electronic excitation.

1. Introduction

Since the mean and anomalous absorption coefficients are important parameters for electron diffraction and microscopy, many investigations have been carried out experimentally and theoretically. Early attempts to measure absorption coefficients were made on ordinary electron micrographs (Kohra & Watanabe, 1959; Hashimoto, 1964). In these cases some of the inelastic scattering was included in the pattern. It was pointed out, however, that the elastic intensity of the extinction contour of the electron microscopic image did not agree with the theoretical one (Ichimiya, 1969; Takagi & Ishida, 1970). The discrepancy between theory and experiment was shown to be mainly due to technical problems (Kamiya & Gotō, 1980). The aim of the present paper is to extend the experiment to the case of higher accelerating voltages by using electron micrographs. The diffraction pattern was also used for the measurement of absorption coefficients (Molière & Lehmpfuhl, 1961) and later Meyer-Ehmsen (1969) measured them from transmitted and diffracted intensities of elastic scattering at an accelerating voltage of ~50–70 kV. The present results agree quite well with that given by Meyer-Ehmsen. The result also shows that the cross sections due to plasmon excitation and thermal diffuse scattering agree fairly well with theories by Ashley & Ritchie (1970) and Hall & Hirsch (1965), and that the cross section due to electronic excitation agrees with the theory of Ritchie & Howie (1977).

2. Experiments

Experiments were made in the cases of Si, Ge and InSb at several accelerating voltages between 100 and 750 kV and at three different temperatures. The experimental procedure is the same as described previously (Kamiya & Gotō, 1980). The intensities of extinction contours formed by elastic scattering were obtained with a magnetic velocity analyzer (Ichinokawa, 1968; Kamiya, Shimizu & Suzuki, 1974). Most experiments were done at the Bragg position of the 220 reflection. The intensity of the extinction contour is analyzed by a method based on the two-beam approximation (Uyeda

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0567-7394/81/040485-04$01.00

Table 1. *Numerical constants A, A' and extinction distance* t_0 (Å^{-1})

	Si			Ge			InSb		
E(kV)	t_0	A	A'	t_0	A	A'	t_0	A	A'
100	710	0·18	1·15	400	0·275	1·22	390	0·47	1·41
200	890	0·21	1·18	610	0·328	1·26	490	0·54	1·49
400	1050	0·27	1·22	710	0·40	1·32	570	0·66	1·56
600	1110	0·32	1·26	750	0·48	1·37	590	0·78	1·65
800	1140	0·43	1·30	770	0·57	1·61	600	0·88	1·71

& Nonoyama, 1965). The damping of the fringe gives the mean absorption coefficient $\overline{\mu_0}$ and the center of the curve gives the anomalous absorption coefficient $\Delta\mu$. The method can be extended to the N-beam case if the waves with wave points on two main branches of the dispersion surface make a dominant contribution to the extinction contour. The relationship between absorption coefficients $(\overline{\mu_0}, \Delta\mu)$ and the imaginary potential is given by

$$\overline{\mu_0} = 2\pi V^i_{000}/k + 2\pi A V^i_{220}/k$$
$$\Delta\mu = 2\pi A' V^i_{220}/k \qquad (1)$$

and

$$A = a + bV^i_{440}/V^i_{220} + cV^i_{660}/V^i_{220} + \cdots$$
$$A' = a' + b' V^i_{440}/V^i_{220} + c' V^i_{660}/V^i_{220} + \cdots, \qquad (2)$$

where V^i_{000}, V^i_{220} ... are Fourier coefficients of the imaginary potential and k is the wave number of the incident electron. The constants a, b, c, a', *etc.* are determined numerically on the basis of the ten-beam dynamical theory of electron diffraction. The values A and A' are obtained from Radi's (1970) data for ratios V^i_{440}/V^i_{220} and V^i_{660}/V^i_{220} and are listed in Table 1 with the extinction distance t_0.

The results at room temperature are given in Fig. 1 for experiments at 100, 200, 370, 560 and 750 kV. The absorption coefficients at different temperatures (Fig. 2) give the magnitude of the cross section due to thermal diffuse scattering from a comparison with theoretical ones obtained by Hall & Hirsch's (1965) formulae. The cross section of plasmon excitation was evaluated from energy loss spectra obtained from crystals with thicknesses $t_0/2$ and $3t_0/2$. The scattering angle of inelastic scattering is limited by the objective aperture which corresponds to about half of the cut-off angle. The correction for the finite size of the objective aperture was made with the theoretical scattering formula of Ferrel (1956).

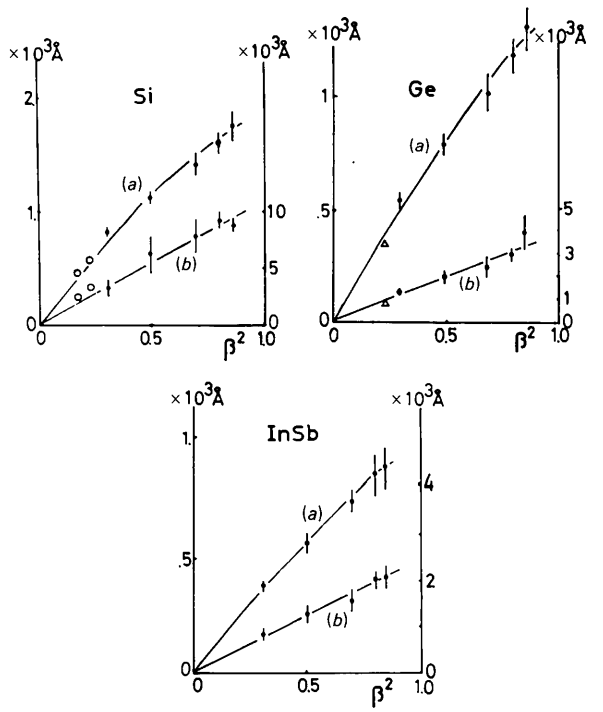

Fig. 1. Mean free path at room temperature. β is the ratio of electron velocity to light velocity. (*a*) $k/(2\pi V^i_{000})$, left ordinate, (*b*) $k/(2\pi V^i_{220})$, right ordinate. ○, △ Meyer-Ehmsen (1969).

3. Discussion

(*a*) *Comparison with theories*

Plasmon excitation. The mean free path obtained experimentally is shown in Fig. 3 in comparison with theoretical values due to Ashley & Ritchie (1970). Agreement is good for light elements but the experimental results are about 15% larger than the theoretical ones for Ge and InSb. Jouffrey, Kihn, Perez, Sevely

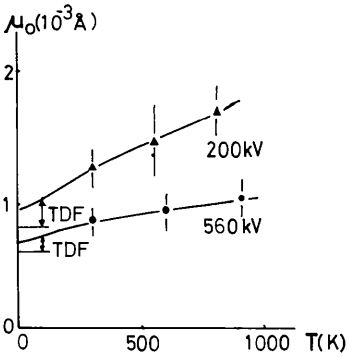

Fig. 2. Variation of absorption coefficient $2\pi V^i_{000}/k$ with specimen temperature for Ge.

& Zanchi (1977) also obtained good agreement between theory and experiment for aluminum and carbon.

Thermal diffuse scattering. The mean free path is nearly proportional to β^2. The mean free paths at 100 kV determined by the least-squares method are given in Table 2. The theoretical values from Radi (1970) are also shown. In the case of Ge, Radi used 0·719 for the Debye–Waller factor at room temperature, but Mair & Barnea (1975) adopted 0·543 in the analysis of X-ray reflection intensities and Batterman & Chipman (1962) obtained experimentally 0·566. Therefore the difference in Table 2 can be attributed to the Debye temperature. Similarly for Si, the Debye–Waller factor used by Radi is 0·355, while the value 0·46 is the recent result (Aldred & Hart, 1973). It must be mentioned that the Debye temperature for Sn is 270 K and it is 200 K for InSb (Keeson & Pearlman, 1963). The mean free path due to thermal diffuse scattering can be obtained by the theory of Hall & Hirsch (1965) with the correct Debye–Waller factor.

Electronic excitation. The theoretical estimations of imaginary potentials made by Yoshioka (1957), Whelan (1965) and Radi (1970) are based on the closure approximation. However, Ritchie & Howie (1977) evaluated them from complex dielectric constants and pointed out that the values obtained previously were overestimated. The imaginary potentials V'_{000}(el) at 100 kV obtained by subtracting that of thermal diffuse scattering from the experimental ones are listed in Table 3. Although Ritchie & Howie did not give the values for Si, Ge and InSb, it is clear that the value given by Radi is larger than the experimental results for heavy elements. The voltage dependence of the absorption coefficient due to electronic excitation (Fig. 4) shows that the mean free path is not proportional to β^2.

Table 2. *Absorption coefficient for thermal diffuse scattering,* μ_{000} (Å^{-1}), 100 kV, *room temperature*

	Experiment	Radi (1970)
Si	$(2{\cdot}2 \pm 0{\cdot}2) \times 10^{-4}$	$1{\cdot}1 \times 10^{-4}$
Ge	$(6{\cdot}0 \pm 1{\cdot}0) \times 10^{-4}$	$9{\cdot}7 \times 10^{-4}$
InSb	$(1{\cdot}3 \pm 0{\cdot}1) \times 10^{-3}$	$1{\cdot}1 \times 10^{-3}$*

* The value for Sn.

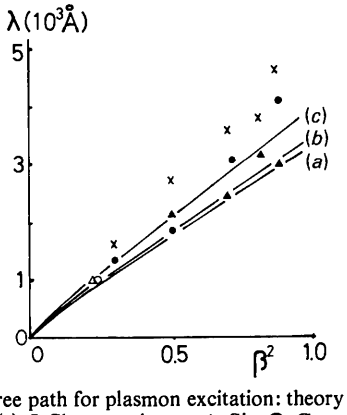

Fig. 3. Mean free path for plasmon excitation: theory solid line, (*a*) Si, (*b*) Ge, (*c*) InSb; experiment ▲ Si, ● Ge, × InSb, △○ Meyer-Ehmsen (1969).

(*b*) *Method of analysis*

In the above analysis, we have assumed that waves associated with wave points on two main branches of the dispersion surface determine the main features of the extinction contour. The effect of Bloch waves on other branches becomes significant for heavy elements and high accelerating voltages. In order to estimate the effect, the intensities of extinction contours were calculated by the ten-beam approximation and also by two-wave interference where the waves on branches except the two main ones are neglected. The mean and anomalous absorption coefficients obtained in the former case are larger than those in the latter case. The differences are 10% for the mean absorption coefficient and 20% for the anomalous one for InSb at 800 kV. Since the difference caused by the assumption is of

Table 3. *Imaginary potential* (eV) *due to electronic excitation,* 100 kV

Z is the atomic number.

	Z	Radi (1970)	Whelan (1965)	Ritchie & Howie (1977)	Experimental
Si	14	0·60			0·50 ± 0·04
Ge	32	1·04			0·70 ± 0·05
InSb	50				0·70 ± 0·03
Sn	50	1·27			
Al	13	0·69	0·57	0·64	
Cu	29	2·74	0·97	0·94	
Ag	47	3·33		0·92	

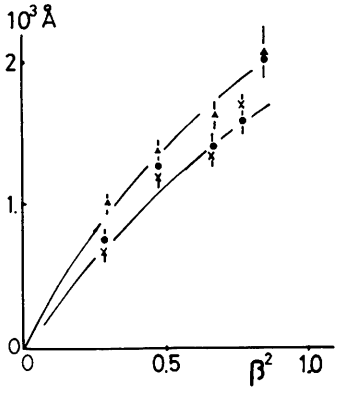

Fig. 4. Mean free path for electronic excitation ▲ Si, ● Ge, × InSb.

the same order as the experimental errors, the effect of many branches is not included in this paper.

The author is grateful to Mr M. Kogiso for critical discussion. Thanks are due to Messrs T. Suzuki and T. Gotō for assistance and the Computation Center of Nagoya University for numerical calculations.

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Eliminating the Small-Angle Component of the Scattering Calculated for Models

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(*Received* 2 *December* 1980; *accepted* 13 *January* 1981)

Abstract

A straightforward procedure (assuming spherical symmetry) is described, which enables the unwanted small-angle component of the scattering for a finite model to be calculated. The method may be applied to models of any shape or size. It is illustrated by means of a single polymer chain.

The use of X-ray scattering to elucidate the local structure of non-crystalline materials is well established. This analysis is facilitated by comparison of the experimental scattering with that calculated from models (Wright, 1974; Adams, Balyuzi & Burge, 1976; Lovell, Mitchell & Windle, 1980). For practical as well as structural reasons the size of these models is limited and consequently the calculated scattering contains an unwanted small-angle component, which is only dependent upon the shape and size of the model. This scattering will be dominant at low angles and may swamp relevant structural detail. To make valid comparisons with experimental data in this region, it is vital to eliminate or at least considerably reduce this scattering.

A method of calculating the small-angle scattering (assuming spherical symmetry) is presented for a model of arbitrary shape and size.

In general, comparisons of experimental and model scattering are made with the s-weighted reduced intensity function $si(s)$

$$i(s) = kI_{\rm corr}(s) - \sum_i^n f_i^2(s)/n, \qquad (1)$$

where $I_{\rm corr}(s)$ is the fully corrected data, k a scaling factor, $\sum_i^n f_i^2(s)$ the independent scattering from one

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