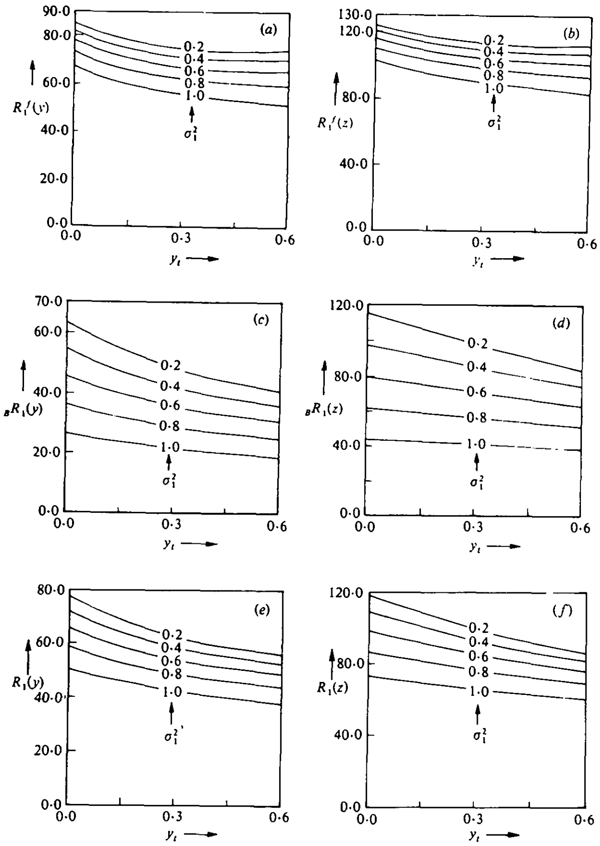

Fig. 1. Variation of the local values of normalized R indices as a function of y_t for different fixed values of σ_1^2. For the definition of $R_1(y)$, $R_1(z)$, *etc.*, see column 6 of Table 1.

P/N. (iii) Divide the range $0 \leq s \leq S_{\max}$ into a number of narrow subintervals. Determine from the data the number (n_s) of observed reflections in each of these sub-intervals. (iv) From the mean value of sin θ/λ corresponding to each sub-interval determine the values of f. (v) Calculate σ_A (by taking $\langle|\Delta\mathbf{r}|\rangle = 0{\cdot}2$ Å) corresponding to each of these sub-intervals. (vi) Make use of the results in Tables 2–4 and determine the values of $[R]_t$ for these sub-intervals by bilinear interpolation. (vii) Make use of the results thus obtained in the appropriate expressions for $[\bar{R}]_t$ and compute the overall values $[\bar{R}]_t$. The values thus obtained represent the theoretical overall values of the normalized R indices corresponding to a model for which $\langle|\Delta\mathbf{r}|\rangle = 0{\cdot}2$ Å and for data in which $y_N \geq y_t$ and $0 \leq s \leq S_{\max}$.

References

PARTHASARATHI, V. & PARTHASARATHY, S. (1977). *Pramana*, **9**, 61–69.

PARTHASARATHY, S. (1975). *J. Indian Inst. Sci.* **57**, 127–159.

PARTHASARATHY, S. & PARTHASARATHI, V. (1975). *Acta Cryst.* A**31**, 178–185.

PONNUSWAMY, M. N. & PARTHASARATHY, S. (1977). *Acta Cryst.* A**33**, 838–844.

SRINIVASAN, R. & PARTHASARATHY, S. (1976). *Some Statistical Applications in X-ray Crystallography*. Oxford: Pergamon Press.

STOUT, G. H. & JENSEN, L. H. (1968). *X-ray Structure Determination*, p. 182. New York: Macmillan.

WILSON, A. J. C. (1949). *Acta Cryst.* **2**, 318–320.

Acta Cryst. (1981). A**37**, 480–485

Theoretical Evaluation of the Overall Values of Discrepancy Indices for Truncated Data. II. Normalized *R* indices for a Non-centrosymmetric Crystal with Similar Atoms

BY D. VELMURUGAN AND S. PARTHASARATHY

Department of Physics (Crystallography and Biophysics), University of Madras, Guindy Campus, Madras-600025, India*

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

Abstract

Theoretical expressions and numerical tables for the local values of six types of normalized R indices are obtained for an imperfectly related incomplete model of a non-centrosymmetric crystal with truncated data. Under similar conditions, the curve of the local value of an R index *versus* the truncation limit y_t is relatively more flat for the non-centrosymmetric case than for the centrosymmetric case particularly in the region where y_t is small.

* Contribution No. 546.

0567-7394/81/040480-06$01.00

1. Introduction

In part I (Parthasarathy & Velmurugan, 1981), we derived the theoretical expressions necessary for calculating the overall values of various normalized R indices for a C crystal with truncated data. In this paper we shall derive the corresponding results applicable to an NC crystal. The notation used here is the same as in part I. Since the method of derivation closely follows that used in part I, we shall give only the essential steps.

2. Derivation of the theoretical expressions for the normalized *R* indices

2.1. *Derivation of the joint p.d.f. of y_N and y_P^c for the truncated data*

The joint p.d.f. of y_N and y_P^c for the NC case is known to be (SP, 1976)

$$P(y_N, y_P^c) = \frac{4y_N y_P^c}{\sigma_B^2}\exp\left[-\frac{(y_N^2 + (y_P^c)^2)}{\sigma_B^2}\right] \times I_0\left(\frac{2\sigma_A y_N y_P^c}{\sigma_B^2}\right),\quad 0 \le y_N < \infty, 0 \le y_p^c < \infty, \tag{1}$$

The joint p.d.f. of y_N and y_P^c applicable to the truncated data will therefore be given by [see (13) and (14) of part I]

$$P_t(y_N, y_P^c) = \frac{4y_N y_P^c}{\sigma_B^2 \beta_{NC}}\exp\left[-\frac{[y_N^2 + (y_P^c)^2]}{\sigma_B^2}\right] \times I_0\left(\frac{2\sigma_A y_N y_P^c}{\sigma_B^2}\right), \tag{2}$$

where β_{NC} can be shown to be [see equation (A-5) of the Appendix*]

$$\beta_{NC} = \exp(-y_t^2). \tag{3}$$

2.2. *Derivation of the theoretical expressions for the normalized R indices*

Index $[R_1(y)]_t$. Equation (21) of part I is valid for this case as well except that β_C is now to be replaced by β_{NC}. Since the first term within the square brackets represents $R_1(y)$ (see §2.3 of part I), and since $\langle y_N \rangle = \sqrt{\pi}/2$ for the NC case (Wilson, 1949), we obtain

$$[R_1(y)]_t = \left[R_1(y) - \frac{2}{\sqrt{\pi}}\int_0^{y_t/(1+y_t)}\int_0^1 \left|\frac{u}{1-u} - \frac{v}{1-v}\right| \times P\left(\frac{u}{1-u}, \frac{v}{1-v}\right)\frac{\mathrm{d}u\mathrm{d}v}{(1-u)^2(1-v)^2}\right] \times [2\pi^{-1/2}\beta_{NC}y_t + \mathrm{erfc}(y_t)]^{-1} \tag{4}$$

where we have used (A-7) of part II and the substitution in (24) of part I. $R_1(y)$ is known to be (Srinivasan & Parthasarathy, 1976; hereafter SP, 1976)

$$R_1(y) = \frac{3\sigma_B^3}{2}\int_0^1 \frac{{}_2F_1(-\frac{1}{4}, -\frac{3}{4}; 1; \sigma_A^2 x^2)x\mathrm{d}x}{(1+x)^{1/2}(1-\sigma_A^2 x^2)^2}. \tag{5}$$

Index $[R_1(z)]_t$. Equation (26) of part I is valid for this case as well. Using (A-11) and following the steps used for the C case, we obtain

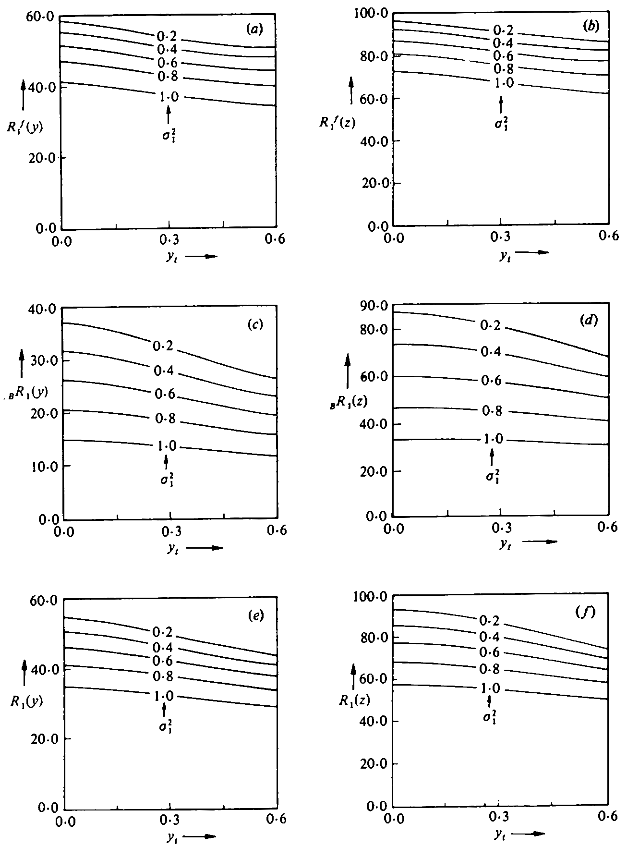

Fig. 1. Variation of the local values of normalized R indices as a function of y_t for different fixed values of σ_1^2. For the definition of $R_1(y)$, $R_1(z)$, *etc.*, see column 6 of Table 1 of part I.

* This appendix has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35849 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

$$[R_1(z)]_t = \left[R_1(z) - \int\limits_0^{y_t/(1+y_t)} \int\limits_0^1 \left| \left(\frac{u}{1-u}\right)^2 - \left(\frac{v}{1-v}\right)^2 \right| \times P\left(\frac{u}{1-u}, \frac{v}{1-v}\right) \frac{\mathrm{d}u\mathrm{d}v}{(1-u)^2(1-v)^2}\right] \times [\beta_{NC}(1+y_t^2)]^{-1}, \quad (6)$$

where $R_1(z)$ has been shown to be (SP, 1976)

$$R_1(z) = \sigma_B. \quad (7)$$

Index $[_BR_1(y)]_t$. Equation (30) of part I is valid for this case as well. Substituting for $\langle y_N^2 \rangle_t$, $\langle (y_P^c)^2 \rangle_t$ and $\langle y_N y_P^c \rangle_t$ from (*A*-11), (*A*-14) and (*A*-16) respectively in equation (30) of part I and simplifying the result, we obtain

$$[_BR_1(y)]_t = \left\{ {}_BR_1(y) + 2(\beta_{NC} - 1) + \beta_{NC} y_t^2 (1 + \sigma_A^2) + \frac{\sqrt{\pi}}{\sigma_B} \int\limits_0^{y_t^2} u^{1/2} \exp[-u(1+\sigma_B^2)/2\sigma_B^2] \times \left[(\sigma_B^2 + \sigma_A^2 u) I_0\left(\frac{\sigma_A^2 u}{2\sigma_B^2}\right) + \sigma_A^2 u I_1\left(\frac{\sigma_A^2 u}{2\sigma_B^2}\right)\right] \mathrm{d}u \right\} \times [\beta_{NC}(1+y_t^2)]^{-1}, \quad (8)$$

where $_BR_1(y)$ is known to be (SP, 1976)

Table 1. *Values of* $[R_1(y)]_t$ *and* $[R_1(z)]_t$ *as functions of* σ_A *and* y_t *for the non-centrosymmetric case*

	$[R_1(y)]_t$					$[R_1(z)]_t$				
σ_A ↓ y_t →	0.00	0.15	0.30	0.45	0.60	y_t → 0.00	0.15	0.30	0.45	0.60
0.000	58.579	56.744	52.846	48.833	45.841	100.000	97.824	92.103	84.755	77.772
0.040	58.536	56.703	52.809	48.801	45.813	99.920	97.747	92.036	84.700	77.728
0.080	58.409	56.581	52.699	48.705	45.729	99.679	97.517	91.834	84.535	77.598
0.120	58.195	56.375	52.514	48.546	45.588	99.277	97.133	91.496	84.258	77.380
0.160	57.895	56.087	52.255	48.320	45.390	98.712	96.592	91.021	83.869	77.071
0.200	57.505	55.712	51.918	48.028	45.132	97.980	95.891	90.404	83.363	76.668
0.240	57.024	55.250	51.502	47.667	44.813	97.077	95.027	89.643	82.736	76.168
0.280	56.449	54.697	51.004	47.234	44.429	96.000	93.995	88.733	81.985	75.566
0.320	55.776	54.050	50.422	46.727	43.978	94.742	92.790	87.668	81.103	74.854
0.360	55.000	53.304	49.749	46.140	43.455	93.295	91.403	86.439	80.082	74.024
0.400	54.116	52.454	48.983	45.470	42.855	91.652	89.825	85.040	78.913	72.401
0.420	53.631	51.988	48.562	45.102	42.524	90.752	88.962	84.272	78.269	71.826
0.440	53.117	51.493	48.115	44.710	42.171	89.800	88.047	83.457	77.565	72.674
0.460	52.571	50.968	47.641	44.294	41.796	88.792	87.079	82.594	76.857	71.369
0.480	51.994	50.412	47.139	43.853	41.396	87.727	86.055	81.679	76.084	70.725
0.500	51.382	49.824	46.608	43.385	40.971	86.603	84.973	80.712	75.264	70.038
0.520	50.737	49.203	46.046	42.889	40.520	85.417	83.832	79.689	74.394	69.306
0.540	50.054	48.546	45.451	42.364	40.041	84.167	82.628	78.609	73.471	68.526
0.560	49.833	47.852	44.823	41.808	39.531	82.849	81.359	77.467	72.494	67.694
0.580	48.571	47.119	44.159	41.219	38.989	81.462	80.021	76.262	71.457	66.808
0.600	47.767	46.345	43.456	40.595	38.413	80.000	78.611	74.989	70.358	65.863
0.610	47.348	45.941	43.090	40.269	38.112	79.240	77.878	74.325	69.764	65.367
0.620	46.917	45.526	42.714	39.933	37.801	78.460	77.125	73.643	69.192	64.855
0.630	46.474	45.100	42.326	39.587	37.479	77.660	76.351	72.942	68.582	64.325
0.640	46.019	44.661	41.928	39.231	37.148	76.837	75.557	72.221	67.954	63.778
0.650	45.550	44.210	41.518	38.864	36.806	75.993	74.741	71.480	67.307	63.212
0.660	45.068	43.745	41.095	38.485	36.452	75.127	73.903	71.717	66.639	62.627
0.670	44.572	43.268	40.661	38.095	36.087	74.236	73.041	69.932	65.951	62.022
0.680	44.062	42.776	40.213	37.692	35.709	73.321	72.156	69.124	65.240	61.395
0.690	43.536	42.269	39.752	37.277	35.318	72.381	71.245	68.293	64.507	60.746
0.700	42.995	41.748	39.276	36.848	34.914	71.414	70.309	67.436	63.750	60.075
0.710	42.437	41.210	38.786	36.405	34.496	70.420	69.346	66.554	62.968	59.378
0.720	41.861	40.656	37.280	35.947	34.063	69.397	68.354	65.644	62.160	58.657
0.730	41.268	40.084	37.758	35.474	33.614	68.345	67.333	64.706	61.325	57.908
0.740	40.656	39.494	37.219	34.984	33.148	67.261	66.281	63.738	60.460	57.131
0.750	40.024	38.885	36.661	34.476	32.665	66.144	65.197	62.739	59.565	56.323
0.760	39.371	38.255	36.085	33.950	32.163	64.992	64.078	61.706	58.638	55.464
0.770	38.695	37.603	35.488	33.405	31.641	53.804	62.924	60.639	57.676	54.611
0.780	37.996	36.929	34.870	32.838	31.098	62.578	61.731	59.534	56.678	53.702
0.790	37.272	36.230	34.229	32.249	30.533	61.311	60.498	58.390	55.642	52.755
0.800	36.521	35.506	33.564	31.636	29.943	60.000	59.222	57.204	54.564	51.766
0.810	35.741	34.754	32.872	30.998	29.328	58.643	57.900	55.973	53.441	50.734
0.820	34.931	33.972	32.152	30.331	28.684	57.236	56.529	54.693	52.271	49.654
0.830	34.087	33.157	31.401	29.635	28.011	55.776	55.105	53.362	51.049	48.524
0.840	33.207	32.308	30.617	28.905	27.305	54.259	53.623	51.973	49.771	47.337
0.850	32.288	31.421	29.797	28.139	26.563	52.678	52.079	50.524	48.431	46.090
0.860	31.326	30.492	28.937	27.334	25.782	51.029	50.468	49.007	47.025	44.777
0.870	30.317	29.517	28.032	26.484	24.958	49.305	48.781	47.416	45.544	43.391
0.880	29.255	28.491	27.079	25.586	24.087	47.497	47.011	45.742	39.639	41.923
0.890	28.134	27.407	26.069	24.632	23.163	45.596	45.148	43.975	37.690	40.364
0.900	26.946	26.259	24.997	23.615	22.179	43.589	43.180	42.103	44.773	38.703
0.905	26.324	25.657	24.434	23.081	21.662	42.541	42.152	41.124	43.980	37.829
0.910	25.682	25.036	23.852	22.527	21.127	41.461	41.091	40.111	43.165	36.924
0.915	25.018	24.393	23.248	21.952	20.573	40.345	39.995	39.064	42.324	35.985
0.920	24.329	23.727	22.621	21.355	19.997	39.192	38.861	37.979	41.458	35.009
0.925	23.615	23.036	21.969	20.733	19.399	37.997	37.686	36.852	35.589	33.993
0.930	22.872	22.317	21.289	20.083	18.776	36.756	36.465	35.680	34.473	32.933
0.935	22.098	21.568	20.579	19.405	18.126	35.465	35.194	34.457	33.307	31.825
0.940	21.291	20.785	19.834	18.693	17.447	34.117	33.867	33.178	32.085	30.663
0.945	20.445	19.967	19.051	17.944	16.734	32.707	32.477	31.836	30.800	29.441
0.950	19.559	19.107	18.225	17.155	15.984	31.225	31.015	30.422	29.445	28.150
0.955	18.626	18.204	17.349	16.319	15.193	29.661	29.471	28.926	28.008	26.782
0.960	17.564	17.171	16.417	15.430	14.355	28.000	27.831	27.334	26.477	25.322
0.965	16.488	16.127	15.420	14.481	13.464	26.225	26.076	25.626	24.833	23.754
0.970	15.334	15.006	14.347	13.464	12.513	24.311	24.182	23.780	23.052	22.055
0.975	14.089	13.796	13.190	12.370	11.497	22.221	22.112	21.758	21.100	20.191
0.980	12.746	12.490	11.941	11.200	10.421	19.900	19.812	19.506	18.923	18.111
0.985	11.318	11.104	10.622	9.979	9.322	17.256	17.187	16.932	16.431	15.731
0.990	9.922	9.752	9.359	8.853	8.380	14.107	14.058	13.857	13.451	12.889
0.995	9.279	9.166	8.915	8.654	8.552	9.988	9.959	9.820	9.536	9.178
1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

$$_BR_1(y) = 2 - 2\left[E(\sigma_A) - \frac{\sigma_B^2}{2}K(\sigma_A)\right]. \qquad (9)$$

Index $[_BR_1(z)]_t$. Equation (33) of part I is valid for this case as well. Substituting for $\langle y_N^4\rangle_t$, $\langle (y_P^c)^4\rangle_t$ and $\langle y_N^2(y_P^c)^2\rangle_t$ from (*A*-13), (*A*-15) and (*A*-17) respectively and simplifying the result by using (16) of part I, we obtain

$$[_BR_1(z)]_t = \frac{(_BR_1(z) + \sigma_B^2 + 2\sigma_A^2\sigma_B^2 y_t^2 + \sigma_B^4 y_t^4)}{(y_t^4 + 2y_t^2 + 2)}, \qquad (10)$$

where $_BR_1(z)$ is known to be (SP, 1976)

$$_BR_1(z) = \sigma_B^2. \qquad (11)$$

Index $[R_1^c(y)]_t$. Equation (37) of part I is valid for this case as well, provided β_C is replaced by β_{NC} and $P(y_N, y_P^c)$ is taken to be the function in (1) of this part. Following the method used for this index in part I, the final expression can be shown to be

$$[R_1^c(y)]_t = \frac{1}{\beta_{NC}}\left[R_1^c(y) - 2\int_0^{y_t/(1+y_t)}\int_0^1 \left|\left[\left(\frac{u}{1-u}\right) - \left(\frac{v}{1-v}\right)\right]\right. \right.$$
$$\times \left[\left(\frac{u}{1-u}\right) + \left(\frac{u}{1-v}\right)\right]^{-1}\Bigg|$$
$$\times P\left(\frac{u}{1-u}, \frac{v}{1-v}\right)$$
$$\left. \times \frac{\mathrm{d}u\mathrm{d}v}{(1-u)^2(1-v)^2}\right], \qquad (12)$$

Table 2. *Values of* $[_BR_1(y)]_t$ *and* $[_BR_1(z)]_t$ *as functions of* σ_A *and* y_t *for the non-centrosymmetric case*

σ_A ↓	$[_BR_1(y)]_t$ y_t → 0.00	0.15	0.30	0.45	0.60	$[_BR_1(z)]_t$ y_t → 0.00	0.15	0.30	0.45	0.60
0.000	42.920	41.074	37.096	32.931	29.740	100.000	97.800	91.774	83.442	74.733
0.040	42.852	41.008	37.037	32.881	29.696	99.840	97.647	91.639	83.333	74.647
0.080	42.645	40.812	36.863	32.731	29.564	99.360	97.188	91.236	83.003	74.387
0.120	42.303	40.485	36.574	32.482	29.345	98.560	96.423	90.564	82.452	73.951
0.160	41.826	40.030	36.171	32.137	29.041	97.440	95.351	89.620	81.677	73.337
0.200	41.216	39.449	35.657	31.695	28.654	96.000	93.972	88.404	80.676	72.540
0.240	40.475	38.743	35.033	31.161	28.184	94.240	92.285	86.914	79.444	71.553
0.280	39.606	37.916	34.301	30.534	27.635	92.160	90.290	85.146	77.976	70.371
0.320	38.612	36.969	33.465	29.819	27.007	89.760	87.985	83.098	76.266	68.985
0.360	37.493	35.904	32.525	29.014	26.302	87.040	85.371	80.766	74.307	67.385
0.400	36.251	34.722	31.482	28.122	25.520	84.000	82.444	78.146	72.092	65.561
0.420	35.583	34.088	30.922	27.643	25.099	82.360	80.864	76.726	70.885	64.560
0.440	34.886	33.424	30.337	27.142	24.659	80.640	79.206	75.233	69.611	63.500
0.460	34.157	32.731	29.725	26.618	24.198	78.840	77.468	73.665	68.269	62.376
0.480	33.397	32.008	29.087	26.071	23.717	76.960	75.653	72.022	66.856	61.188
0.500	32.606	31.255	28.423	25.501	23.215	75.000	73.758	70.303	65.372	59.935
0.520	31.783	30.472	27.731	24.907	22.691	72.960	71.784	68.508	63.815	58.613
0.540	30.927	29.658	27.012	24.289	22.144	70.840	69.731	66.635	62.185	57.221
0.560	30.039	28.813	26.264	23.645	21.574	68.640	67.598	64.685	60.478	55.757
0.580	29.117	27.936	25.488	22.975	20.979	66.360	65.386	62.655	58.694	54.218
0.600	28.161	27.026	24.682	22.278	20.359	64.000	63.093	60.545	56.832	52.603
0.610	27.670	26.558	24.267	21.918	20.038	62.790	61.917	59.460	55.870	51.766
0.620	27.170	26.082	23.845	21.552	19.711	61.560	60.720	58.355	54.889	50.909
0.630	26.661	25.598	23.415	21.178	19.377	60.310	59.504	57.229	53.886	50.031
0.640	26.143	25.104	22.976	20.797	19.036	59.040	58.267	56.083	52.863	49.133
0.650	25.616	24.602	22.530	20.408	18.687	57.750	57.010	54.916	51.819	48.214
0.660	25.079	24.091	22.075	20.012	18.331	56.440	55.733	53.729	50.753	47.273
0.670	24.533	23.570	21.612	19.607	17.966	55.110	54.436	52.520	49.667	46.311
0.680	23.977	23.041	21.139	19.194	17.594	53.760	53.118	51.290	48.558	45.327
0.690	23.412	22.501	20.658	18.772	17.213	52.390	51.780	50.040	47.427	44.321
0.700	22.836	21.953	20.169	18.342	16.824	51.000	50.422	48.768	46.274	43.292
0.710	22.251	21.394	19.669	17.903	16.427	49.590	49.043	47.474	45.099	42.240
0.720	21.655	20.826	19.161	17.455	16.020	48.160	47.644	46.160	43.901	41.164
0.730	21.049	20.247	18.643	16.998	15.604	46.710	46.224	44.823	42.680	40.065
0.740	20.432	19.659	18.115	16.531	15.179	45.240	44.784	43.465	41.436	38.942
0.750	19.805	19.059	17.577	16.055	14.744	43.750	43.323	42.084	40.168	37.795
0.760	19.166	18.450	17.029	15.568	14.298	42.240	41.841	40.682	38.877	36.622
0.770	18.517	17.829	16.471	15.071	13.843	40.710	40.339	39.257	37.561	35.425
0.780	17.857	17.198	15.902	14.563	13.377	39.160	38.817	37.810	36.221	34.202
0.790	17.185	16.556	15.322	14.045	12.900	37.590	37.273	36.341	34.857	32.953
0.800	16.501	15.902	14.731	13.516	12.413	36.000	35.709	34.849	33.468	31.678
0.810	15.806	15.237	14.129	12.975	11.913	34.390	34.124	33.334	32.054	30.376
0.820	15.098	14.560	13.516	12.422	11.402	32.760	32.518	31.796	30.614	29.047
0.830	14.379	13.871	12.890	11.857	10.879	31.110	30.892	30.235	29.148	27.690
0.840	13.647	13.170	12.252	11.280	10.344	29.440	29.244	28.650	27.657	26.305
0.850	12.903	12.456	11.602	10.689	9.796	27.750	27.576	27.042	26.139	24.892
0.860	12.146	11.730	10.939	10.086	9.236	26.040	25.886	25.411	24.594	23.451
0.870	11.375	10.991	10.263	9.469	8.662	24.310	24.175	23.756	23.023	21.980
0.880	10.592	10.239	9.573	8.838	8.074	22.560	22.444	22.077	21.424	20.479
0.890	9.795	9.474	8.870	8.192	7.473	20.790	20.691	20.373	19.798	18.949
0.900	8.984	8.694	8.151	7.531	6.858	19.000	18.917	18.646	18.144	17.388
0.905	8.573	8.299	7.787	7.194	6.545	18.098	18.022	17.773	17.307	16.596
0.910	8.158	7.901	7.418	6.854	6.229	17.190	17.121	16.894	16.462	15.796
0.915	7.740	7.498	7.046	6.510	5.909	16.278	16.216	16.009	15.610	14.988
0.920	7.319	7.092	6.669	6.161	5.586	15.360	15.305	15.118	14.751	14.173
0.925	6.893	6.683	6.289	5.808	5.259	14.438	14.389	14.220	13.885	13.349
0.930	6.464	6.269	5.904	5.451	4.929	13.510	13.467	13.317	13.012	12.517
0.935	6.031	5.852	5.515	5.090	4.595	12.578	12.540	12.407	12.131	11.678
0.940	5.594	5.430	5.122	4.724	4.258	11.640	11.608	11.490	11.243	10.830
0.945	5.153	5.005	4.723	4.354	3.918	10.698	10.670	10.568	10.348	9.974
0.950	4.708	4.575	4.321	3.979	3.574	9.750	9.727	9.639	9.445	9.110
0.955	4.258	4.140	3.913	3.600	3.228	8.798	8.779	8.704	8.535	8.237
0.960	3.805	3.702	3.500	3.217	2.878	7.840	7.825	7.763	7.617	7.356
0.965	3.347	3.259	3.082	2.828	2.526	6.878	6.866	6.815	6.692	6.467
0.970	2.884	2.810	2.659	2.436	2.171	5.910	5.901	5.861	5.759	5.569
0.975	2.417	2.357	2.230	2.039	1.814	4.938	4.931	4.900	4.818	4.662
0.980	1.945	1.899	1.795	1.638	1.455	3.960	3.956	3.933	3.870	3.747
0.985	1.467	1.434	1.354	1.233	1.094	2.978	2.975	2.960	2.914	2.824
0.990	0.985	0.963	0.908	0.825	0.730	1.990	1.989	1.980	1.951	1.891
0.995	0.496	0.486	0.456	0.414	0.366	0.998	0.997	0.993	0.979	0.950
1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

where $R_1^f(y)$ is known to be (Parthasarathi & Parthasarathy, 1977; hereafter PP, 1977)

$$R_1^f(y) = 2 - \frac{2}{\sigma_B}\ln(1+\sigma_B). \qquad (13)$$

Index $[R_1^f(z)]_t$. Equation (40) of part I is valid for this case as well. In this case the final expression can be shown to be

$$[R_1^f(z)]_t = \frac{1}{\beta_{NC}}\Bigg[R_1^f(z) - 2\int_0^{y_t/(1+y_t)}\int_0^1 \Bigg|\left[\left(\frac{u}{1-u}\right)^2 - \left(\frac{v}{1-v}\right)^2\right] \times\left[\left(\frac{u}{1-u}\right)^2 + \left(\frac{v}{1-v}\right)^2\right]^{-1}\Bigg| \times P\left(\frac{u}{1-u},\frac{v}{1-v}\right)\frac{\mathrm{d}u\mathrm{d}v}{(1-u)^2(1-v)^2}\Bigg], \qquad (14)$$

where $R_1^f(z)$ is known to be (PP, 1977)

$$R_1^f(z) = 2\sigma_B/(1+\sigma_B). \qquad (15)$$

3. Discussion of the theoretical results

The theoretical expression for the six different normalized R indices valid for truncated data have been derived in (4), (6), (8), (10), (12) and (14). As in the C case, these indices depend on the parameters y_t and σ_A.

Table 3. *Values of* $[R_1^f(y)_t]$ *and* $[R_1^f(z)]_t$ *as functions of* σ_A *and* y_1 *for the non-centrosymmetric case*

	$[R_1^f(y)]_t$					$[R_1^f(z)]_t$				
σ_A ↓ y_t →	0.00	0.15	0.30	0.45	0.60	y_t → 0.00	0.15	0.30	0.45	0.60
0.000	61.371	59.387	56.213	53.963	53.376	100.000	98.071	94.184	90.853	89.518
0.040	61.340	59.356	56.183	53.934	53.347	99.960	98.030	94.144	90.813	89.479
0.080	61.247	59.263	56.093	53.847	53.259	99.839	97.908	94.022	90.694	89.359
0.120	61.091	59.107	55.942	53.702	53.111	99.637	97.704	93.817	90.495	89.158
0.160	60.871	58.887	55.729	53.497	52.902	99.352	97.414	93.528	90.213	88.873
0.200	60.585	58.601	55.452	53.230	52.631	98.980	97.037	93.152	89.846	88.502
0.240	60.230	58.247	55.109	52.900	52.294	98.517	96.569	92.685	89.379	88.040
0.280	59.803	57.821	54.696	52.503	51.888	97.959	96.004	92.122	88.839	87.483
0.320	59.301	57.319	54.210	52.035	51.409	97.300	95.337	91.457	81.169	86.823
0.360	58.718	56.737	53.647	51.492	50.851	96.531	94.559	90.682	87.432	86.051
0.400	58.047	56.068	53.000	50.868	50.209	95.644	93.661	89.789	86.556	85.156
0.420	57.677	55.699	52.644	50.523	49.853	95.152	93.164	89.294	86.074	84.662
0.440	57.283	55.305	52.263	50.156	49.473	94.626	92.631	88.765	85.555	84.130
0.460	56.862	54.885	51.858	49.764	49.067	94.063	92.062	88.199	85.002	83.561
0.480	56.414	54.439	51.427	49.346	48.634	93.462	91.454	87.596	84.410	82.951
0.500	55.937	53.963	50.968	48.902	48.171	92.820	90.805	86.951	83.776	82.296
0.520	55.430	53.458	50.481	48.430	47.678	92.135	90.112	86.264	83.104	81.600
0.540	54.890	52.920	49.962	47.926	47.152	91.403	89.372	85.530	82.363	80.852
0.560	54.316	52.348	49.411	47.391	46.591	90.620	88.582	84.747	81.613	80.051
0.580	53.704	51.739	48.825	46.821	4 .992	89.784	87.737	83.910	80.790	79.192
0.600	53.053	51.092	48.202	46.213	45.352	88.889	86.833	83.015	79.909	78.270
0.610	52.712	50.752	47.875	45.894	45.015	88.418	86.357	82.545	79.445	77.754
0.620	52.359	50.401	47.538	45.565	44.667	87.930	85.865	82.058	78.965	77.280
0.630	51.995	50.039	47.190	45.224	44.306	87.425	85.355	81.554	78.466	76.757
0.640	51.619	49.665	46.830	44.873	43.934	86.902	84.827	81.032	77.952	76.214
0.650	51.230	49.279	46.458	44.509	43.547	86.359	84.280	80.492	77.416	75.650
0.660	50.828	48.879	46.074	44.132	43.147	85.797	83.712	79.931	76.863	75.064
0.670	50.412	48.466	45.678	43.743	42.732	85.213	83.124	79.350	76.288	74.456
0.680	49.982	48.039	45.267	43.339	42.302	84.607	82.513	78.748	75.690	73.822
0.690	49.536	47.596	44.842	42.921	41.856	83.978	81.878	78.122	75.069	73.164
0.700	49.074	47.138	44.402	42.488	41.393	83.324	81.218	77.472	74.424	72.4[illegible]7
0.710	48.595	46.663	43.946	42.039	40.911	82.643	80.532	76.796	73.752	71.762
0.720	48.099	46.171	43.474	41.572	40.411	81.934	79.819	76.093	73.052	71.016
0.730	47.583	45.660	42.984	41.087	39.891	81.196	79.075	75.361	72.322	70.238
0.740	47.048	45.129	42.474	40.583	39.349	80.426	78.300	74.596	71.560	69.424
0.750	46.491	44.578	41.946	40.058	38.785	79.622	77.490	73.802	70.765	68.574
0.760	45.911	44.004	41.396	39.511	38.196	78.782	76.645	72.971	69.933	67.663
0.770	45.308	43.407	40.823	38.940	37.582	77.903	75.761	72.102	69.061	66.750
0.780	44.678	42.784	40.226	38.344	36.940	76.982	74.834	71.192	68.147	65.770
0.790	44.020	42.134	39.602	37.721	36.269	76.016	73.863	70.237	67.188	64.741
0.800	43.332	41.454	38.951	37.068	35.566	75.000	72.842	69.236	66.178	63.659
0.810	42.612	40.743	38.269	36.383	34.828	73.931	71.768	68.182	65.114	62.518
0.820	41.856	39.997	37.554	35.663	34.054	72.803	70.636	67.071	63.990	61.315
0.830	41.061	39.214	36.803	34.905	33.241	71.611	69.440	65.897	62.800	60.042
0.840	40.224	38.389	36.012	34.105	32.384	70.348	68.173	64.655	61.539	58.695
0.850	39.341	37.519	35.177	33.259	31.479	69.006	66.829	63.336	60.196	57.264
0.860	38.405	36.599	34.293	32.362	30.524	67.575	65.396	61.931	58.765	55.743
0.870	37.412	35.623	33.355	31.407	29.512	66.046	63.866	60.430	57.232	54.120
0.880	36.353	34.584	32.355	30.388	28.438	64.404	62.225	58.819	55.504	52.384
0.890	35.220	33.473	31.285	29.296	27.295	62.634	60.456	57.083	53.807	50.522
0.900	34.002	32.280	30.134	28.121	26.076	60.714	58.540	55.201	51.879	48.517
0.905	33.356	31.649	29.524	27.499	25.435	59.690	57.519	54.198	50.852	47.455
0.910	32.684	30.992	28.889	26.851	24.771	58.618	56.452	53.148	49.777	46.349
0.915	31.983	30.307	28.226	26.175	24.083	57.494	55.333	52.047	48.651	45.196
0.920	31.249	29.591	27.532	25.469	23.369	56.313	54.158	50.890	47.469	43.993
0.925	30.480	28.842	26.804	24.730	22.627	55.069	52.920	49.671	46.226	42.734
0.930	29.672	28.054	26.040	23.955	21.855	53.754	51.614	48.383	44.915	41.416
0.935	28.821	27.226	25.233	23.141	21.052	52.360	50.230	47.017	43.530	40.032
0.940	27.920	26.350	24.380	22.283	20.212	50.877	48.759	45.565	42.061	38.575
0.945	26.965	25.422	23.474	21.376	19.335	49.292	47.189	44.013	40.498	37.036
0.950	25.945	24.433	22.507	20.416	18.414	47.590	45.505	42.347	38.830	35.411
0.955	24.852	23.373	21.471	19.394	17.445	45.751	43.687	40.549	37.040	33.680
0.960	23.671	22.230	20.352	18.302	16.420	43.750	41.711	38.594	35.110	31.831
0.965	22.386	20.988	19.137	17.129	15.331	41.553	39.544	36.451	33.014	29.843
0.970	20.973	19.622	17.803	15.859	14.165	39.113	37.140	34.079	30.719	27.686
0.975	19.395	18.100	16.322	14.471	12.902	36.361	34.434	31.418	28.177	25.321
0.980	17.600	16.369	14.650	12.931	11.513	33.194	31.323	28.379	25.315	22.688
0.985	15.496	14.343	12.720	11.181	9.951	29.432	27.633	24.816	22.011	19.687
0.990	12.906	11.850	10.399	9.108	8.122	24.726	23.026	20.450	18.026	16.129
0.995	9.369	8.4[illegible]2	7.348	6.420	5.801	18.161	16.636	14.571	12.771	11.556
1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

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.

References

PARTHASARATHI, V. & PARTHASARATHY, S. (1977). *Pramana*, **9**, 61–69.

PARTHASARATHY, S. & VELMURUGEN, D. (1981). *Acta Cryst.* A**37**, 472–480.

SRINIVASAN, R. & PARTHASARATHY, S. (1976). *Statistical Applications in X-ray Crystallography*. Oxford: Pergamon Press.

WILSON, A. J. C. (1949). *Acta Cryst.* **2**, 318–321.

Acta Cryst. (1981). A**37**, 485–488

Absorption Coefficients of Electrons in Crystals

BY Y. KAMIYA, Y. NAKAI AND E. MASUDA*

Department of Physics, Nagoya University, Nagoya, Japan 464

(*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

* Present address: Transistor Works, Tokyo Shibaura Electric Co. Ltd, Saiwai-ku, Kawasaki, 210, Japan.

0567-7394/81/040485-04$01.00