(i) intensities measured quantitatively and with sufficient accuracy are needed for a reliable determination of a polytype unless its period is quite small (systematic errors have to be allowed for);

(ii) a method is needed which gives all polytypes in reasonable agreement with the observed data.

We believe that our method meets this requirement. These views are confirmed by Gomes de Mesquita (1969) who successfully applied our method to the determination of a 120*R* polytype of SiC. In this case the *R* value obtained was 6·6% and was further reduced to 5·9% by allowing for secondary extinction. For comparison, the observed and calculated intensities obtained by Tokonami (1966) in his test example of a 96*R* polytype are given in Table 10, with the intensities again arranged in order of decreasing observed values.

Table 10. *Intensity values observed and calculated by Tokonami* (1966) *for his test example, arranged in order of decreasing* I_{obs} *values*

l	I_{obs}	I_{calc}	l	I_{obs}	I_{calc}
22	128	22	28	16	8
31	96	60	82	16	6
79	96	72	88	16	1
46	64	31	40	8	11
64	64	289	43	8	0
49	64	256	67	8	0·6
34	64	126	73	8	0·4
37	64	36	85	8	0
16	64	27	91	8	1
70	64	0	1	0	0·1
10	32	5	4	0	0·2
25	32	19	52	0	12
67	32	4	55	0	0·9
19	32	21	58	0	0·1
7	16	2	61	0	0·7
13	16	11	94	0	0·7

We would like to express our thanks to Mr P. Kovács and Mr E. Lendvay who kindly supplied the crystals used in our experiments.

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Complex Lattice Potentials in Electron Diffraction Calculated for a Number of Crystals

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(*Received* 29 *January* 1969)

Structure potentials, V_g, and absorption potentials for 100 keV-electrons are given in tabulated form for almost all monatomic crystals with elements $Z=3$ to 90 and for a number of crystals of the rock-salt type. The absorption potentials are given in the form of the Fourier coefficients C'_{0g} of the Yoshioka imaginary potential for excitation of crystal electrons and excitation of phonons at the temperatures 20, 93 and 293 °K. All computations are based on numerical Hartree–Fock–Slater atomic radial functions by Herman & Skillman (*Atomic Structure Calculations*. Englewood Cliffs: Prentice Hall, 1963). The calculations show that the ratio $C'_{0g}(\text{el})/V_g$, where $C'_{0g}(\text{el})$ refers to excitation of single crystal electrons, lies between 0·005 and 0·012 for the lower reflexion vectors **g** and practically all Z. In contrast to this the ratio $C'_{0g}(\text{phonon})/V_g$ is much larger and increases about linearly with Z, for a given **g**.

1. Introduction

The scattering of fast electrons in crystals can be understood in terms of a complex periodic potential by which the electrons are supposed to be diffracted. Its real part consists of the electrical potential of the crystal atoms plus their dynamical polarization induced by the passing external electrons, while the imaginary part represents the inelastic scattering suffered by these electrons during passage (Yoshioka, 1957).

Calculations of the imaginary crystal potentials have been done on the basis of the Thomas–Fermi atomic model for MgO (Yoshioka, 1957) and later, for Li, Be, Ne, Al and Cu by use of Hartree–Fock atomic functions (Whelan, 1956*a*). In these two papers the excitation of the tightly bound crystal electrons was dealt with. This mechanism, however, proved to be too weak to fully account for the experimental anomalous absorption effects, and it was soon found that the thermal diffuse scattering (phonon excitation) is the

main contributon to the total imaginary potential. Imaginary potentials due to phonon excitation have been calculated by Yoshioka & Kainuma (1962) and by Whelan (1965*b*) for several crystals, and, on the basis of a different theoretical approach by Hall & Hirsch (1965), and using the same theory by Humphreys & Hirsch (1968). All these computations, as far as they involve atomic numbers $Z>28$, rely on Thomas–Fermi–Dirac electron scattering factors. Meanwhile new Hartree–Fock–Slater (HFS) atomic radial functions have become available for all elements of the periodic system. These functions are needed for the calculation of both the real and imaginary lattice potentials. On the other hand more experimental results have been reported which should be compared with theory.

In the present paper a table of the complex lattice potentials is given which has been computed with the use of the HFS atomic functions by Herman & Skillman (1963). The evaluation of the imaginary potentials has been shortened by an analytical solution of an angle integration previously done numerically or substituted by a mean value. The Table contains the imaginary potentials due to the excitation of core electrons, plasma electrons and phonons, together with the structure potentials, for a number of crystals. The dependences on the reflexion vector **g**, the temperature and the atomic weight are discussed.

2. Complex lattice potential

On transmission through a perfect crystal the high energy electrons can be described as being diffracted by the crystal potential

$$V(\mathbf{r})=\sum_{g}(V_g+iV_g^i)\exp(-i\mathbf{g}\,.\,\mathbf{r})\,. \qquad (1)$$

The sum is over all reciprocal lattice vectors **g**. V_g is the usual structure potential. V_g^i represents the imaginary potential which accounts for the inelastic scattering. The most important mechanisms of inelastic scattering are the excitation of phonons, the excitation of plasmons and of (tightly bound) core electrons. Each one of these mechanisms contributes a part to V_g^i denoted by C_{0g}^i. Other processes of minor importance including the production of Bremsstrahlung are omitted.

Virtual inelastic scattering gives rise to a small addition to the real potential (Yoshioka, 1957) which will be ignored. In the following a number of formulae are compiled which are relevant for the understanding of the Tables.

3. Structure potentials V_g

The Fourier coefficient of the crystal potential is given by

$$V_g=-\frac{e^2}{\varepsilon_0 V_c g^2}\sum_{\alpha}[Z^{(\alpha)}-f^{(\alpha)}(g)]\exp(-i\mathbf{g}\,.\,\mathbf{R}_\alpha) \qquad (2)$$

$f^{(\alpha)}(g)$ is the atomic X-ray scattering amplitude for the atom located at R_α ($\alpha=1,\ \ldots,\ r$) in the unit cell of volume V_c . $f(s)=\sum_j f_j(s)$ is a sum over the subshells of the atom. The functions $f_j^{(\alpha)}(s)$ have been calculated from the tabulated atomic radial wave functions published by Herman & Skillman (1963).

Comments on the evaluation of V_0

As is well known, the value of the mean inner potential V_0 depends much on the outer electrons of the crystal atoms.

One way of calculating V_0 would be to assume the crystal to consist of free neutral atoms. Another extreme way is to take ions to be at the lattice points and the remaining electrons to be distributed uniformly. The contribution of p perfectly free electrons to V_0 is (Bethe, 1928):

$$V_0=-\frac{3}{10}\frac{e^2p}{4\pi\varepsilon_0 r_0}\,; \qquad (3)$$

r_0 is chosen so that a sphere of radius r_0 has the same volume as the crystal atom.

In the table two values of V_0 are given for each elementary crystal which may be considered as the upper and lower limits of the actual values. The upper value listed as the first number in the row designated by V_g is based on the assumption of free neutral atoms in the crystal. The lower limit given in the (000)-line and V_g-row has been calculated in the following way: V_0 of the p-times ionized free atom (*i.e.* the p outermost electrons of the neutral atom are missing) plus the V_0 of p free electrons from equation (3). This procedure is different from, and believed to be more appropriate than, taking *free* ions plus p free electrons.

4. Imaginary structure potentials C_{0g}^i

The imaginary structure potentials incorporate the absorption properties of the crystal with respect to the incident electrons. They therefore depend on their energy, $E_0=\hbar^2k_0^2/2m$.

4·1. *Excitation of electrons*

Calculating the absorption due to excitation of core electrons gives (Yoshioka, 1957; see also Whelan, 1965*a*)

$$C_{0g}^i(\text{core})=-\frac{\hbar^2}{2m}\frac{4}{a_0^{*2}k_0V_c}\int\frac{S(\mathbf{s},\mathbf{s}-\mathbf{g})}{\mathbf{s}^2(\mathbf{s}-\mathbf{g})^2}\,d\sigma\,, \qquad (4)$$

where

$$S(\mathbf{s},\mathbf{s}-\mathbf{g})=\sum_{\alpha}\exp(-i\mathbf{g}\mathbf{R}_\alpha)\,(f^{(\alpha)}(g)-\sum_j f_j^{(\alpha)}(\mathbf{s})f_j^{(\alpha)}(\mathbf{s}-\mathbf{g}))$$

$a_0^*=a_0m_0/m$ is the relativistic Bohr radius.

An exchange term in $S(\mathbf{s},\mathbf{s}-\mathbf{g})$ which arises from overlapping of the subshells in an atom has been ignored in the course of the derivation of this formula as has any overlapping of neighbouring crystal atoms. Furthermore, this formula must be applied only to

closed-shell structures of atoms. This restriction, however, is not severe since the inner electrons contribute the main share and the outermost electrons contribute almost nothing to the value of C^i_{0g}(core), in contrast to C^i_{00} where this question will be considered in more detail (§4·2). We therefore include the non-closed outer shells in the sum of equation (5) by assuming them to be spherically symmetric, which also leads to $S(\mathbf{s},\mathbf{s}-\mathbf{g}) = S(s,|\mathbf{s}-\mathbf{g}|)$.

The coordinate system used for the integration of the absorption potentials is shown in Fig. 1. In this coordinate system expression (4) reads

$$C^i_{0g}(\text{core}) = -\frac{\hbar^2}{2m}\frac{4}{a_0^{*2}k_0V_c}\sum_\alpha \exp(-i\mathbf{g}\mathbf{R}_\alpha) \times \int_0^{2k_0}\int_0^{2\pi} \frac{[f^{(\alpha)}(2a) - \sum_j f_j^{(\alpha)}(\sqrt{a^2+r^2+2ar\cos\varphi}) f_j^{(\alpha)}(\sqrt{a^2+r^2-2ar\cos\varphi}]\, r\,dr\,d\varphi}{(a^2+r^2)^2-(2ar\cos\varphi)^2} \tag{6}$$

$$= -\frac{\hbar^2}{2m}\frac{4}{a_0^{*2}k_0V_c}\sum_\alpha \exp(-i\mathbf{g}\mathbf{R}_\alpha) \times \int_0^{2k_0} \frac{f^{(\alpha)}(2a) - \sum_j f_j^{(\alpha)}(\sqrt{|a^2-r^2|}) f^{(\alpha)}(\sqrt{2(a^2+r^2)-|a^2-r^2|})}{(a^2+r^2)\,|a^2-r^2|}\, r\,dr\,. \tag{7}$$

The φ-integration has been performed with the help of the integration procedure given in the Appendix.

The imaginary potential due to crystal electron excitation is then given by

$$C^i_{0g}(\text{el}) = C^i_{0g}(\text{core}) + C^i_{0g}(\text{plasmon})\,.$$

In addition collective and single-electron excitation give rise to a another contribution to C^i_{0g} which is of opposite sign. These contributions have not been calculated here (see Radi, 1968).

For $\mathbf{g}=0$ the electronic absorption consists of the core part alone, as will be seen in the next section.

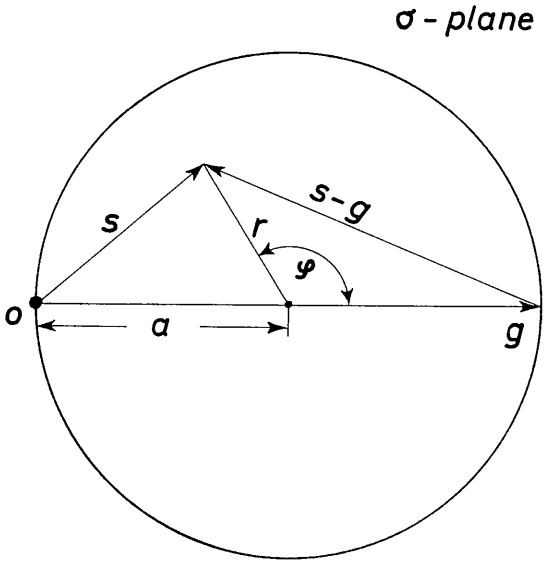


Fig. 1. Coordinate system used for integration of C^i_{0g} potentials. s, scattering vector, g, reciprocal lattice vector.

4·2. *Plasmon excitation*

In the case of plasmon excitation (Ferrell, 1956):

$$C^i_{00}(\text{plasmon}) = -\frac{\hbar\omega_p}{2a_0k_0}\ln\frac{s_c}{s_{\min}} \tag{8}$$

and (Radi, 1968)

$$C^i_{0g}(\text{plasmon}) = 0 \quad (\mathbf{g}\neq 0)\,. \tag{9}$$

For C^i_{00}(plasmon) the problem is to determine the number, p, of free electrons per atom taking part in collective oscillations. This is easily done in cases where the crystal absorption spectrum shows a definite plasmon peak which is in agreement with

$$\omega_p = \sqrt{\frac{e^2n}{m_0\varepsilon_0}}\,, \tag{10}$$

where $n = pA(0)/V_c$, the density of the plasma electrons, and p is a natural number; $A(0)$ = number of atoms in the unit cell. In the other cases, p had to be chosen by arguments of chemical valence, *i.e.* p = the number of electrons in the outmost subshell. Although this is somewhat arbitrary, the consequences are not too critical in our application to the estimation of the mean electronic absorption.

Introducing $s_c \simeq \omega_p/v_F$ as the maximum wave number of a plasmon, with $v_F = (\hbar/m_0)\sqrt[3]{3\pi^2n} = \hbar k_F/m_0$, the Fermi velocity, and $s_{\min} = \omega_p m/(\hbar k_0)$, we can rewrite (8):

$$C^i_{00}(\text{plasmon}) = -\frac{\hbar\omega_p}{2a_0k_0}\ln\frac{k_0}{k_F\sqrt{1+E_0/m_0c^2)}}\,. \tag{11}$$

With p given, this C^i_{00} is determined entirely. p, $\hbar\omega_p$ and C^i_{00}(plasmon) are listed in the C^i_{0g}(el) rows of the Tables.

Since C^i_{00}(core) depends on $s_{\min} = \overline{\Delta E}m/(\hbar^2k_0)$ one must choose a realistic $\overline{\Delta E}$, which ought to be done by consideration of the experimental energy losses for core electron excitation. We shall use a universal $s_{\min} = 0{\cdot}02$ Å^{-1} instead, because this value corresponds to the usual aperture size and only electrons scattered into

Table 1. *Monatomic crystals. Theoretical structure potentials V_g and Yoshioka absorption potentials for* 100 keV-*electrons due to the excitation of crystal electrons C_g^i(el) and excitation of phonons C_g^i(phonon) at $T=20°K$, 93°K and 293°K*

V_g^i in the last row represents the total imaginary potential coefficient at 293°K, being the sum of the third and the sixth row

For every particular lattice type (dia, b.c.c., f.c.c., h.c.p.) a set of reflections, g, have been chosen (indices g_i in the first row) The V_0 value in the (000, V_g) spot represents a lower limit and the number immediately above this represents an upper limit for the mean inner potential V_0. On top of the C_g^i (el) row, C_{00}^i (plasmon) is shown separately. This is calculated on the basis of p free electrons per atom. The number p is indicated above the third row together with the plasmon energy EP. Above the rows designated by C_g^i (phonon) the absolute temperature and mean-square vibration amplitude, u_6^2 (denoted by U2), pertaining to the three rows are given. DT is the Debye temperature of the crystal. DT = 300** means a dummy number, used in cases where no DT was available. The corresponding absorption potentials are irrelevant.

All real and imaginary lattice potentials are given in eV and with opposite signs as they are usually negative quantities. Absorption potentials at electron energies other than 100 keV may be obtained with the help of the conversion factors given in Table 3

DIA C 6
A =3.56 P= 4
EP=31.3 DT= 2020
T= 20 93 293
U2=.0013 .0017 .0020

G	VG	CIG(EL)	CIG(PHONON)			VIG
	19.75	.686				
000	15.93	.733	.033	.040	.045	.78
111	6.96	.029	.022	.027	.030	.06
220	5.11	.006	.028	.034	.038	.04
311	2.78	.003	.019	.023	.025	.03
400	2.83	.003	.025	.029	.032	.03
331	1.71	.002	.017	.020	.022	.02
422	1.95	.003	.022	.026	.028	.03
511	1.24	.002	.015	.018	.019	.02
440	1.50	.002	.021	.024	.026	.03
620	1.23	.002	.019	.022	.023	.03
444	1.04	.002	.018	.020	.021	.02
553	.61	.001	.012	.013	.014	.01
733	.55	.001	.011	.012	.013	.01
555	.49	.000	.010	.011	.012	.01
840	.66	.001	.014	.016	.016	.02
664	.61	.001	.014	.015	.015	.02
933	.39	.000	.009	.010	.010	.01

DIA SI 14
A =5.42 P= 4
EP=16.6 DT= 580
T= 20 93 293
U2=.0020 .0024 .0045

G	VG	CIG(EL)	CIG(PHONON)			VIG
	12.20	.404				
000	11.47	.604	.058	.066	.097	.70
111	5.25	.038	.041	.046	.067	.10
220	4.36	.018	.055	.062	.089	.11
311	2.49	.010	.038	.043	.061	.07
400	2.71	.011	.052	.058	.082	.09
331	1.70	.007	.036	.040	.056	.06
422	2.03	.008	.050	.056	.077	.08
511	1.32	.005	.035	.038	.053	.06
440	1.66	.007	.048	.053	.072	.08
620	1.42	.005	.046	.051	.067	.07
444	1.26	.004	.044	.048	.063	.07
553	.77	.002	.030	.032	.041	.04
733	.70	.002	.029	.031	.039	.04
555	.65	.001	.028	.030	.037	.04
840	.87	.002	.038	.041	.050	.05
664	.81	.001	.037	.040	.047	.05
933	.52	.000	.025	.027	.031	.03

DIA GE 32
A =5.66 P= 4
EP=15.6 DT= 366
T= 20 93 293
U2=.0019 .0038 .0091

G	VG	CIG(EL)	CIG(PHONON)			VIG
	13.82	.383				
000	13.69	1.038	.222	.335	.527	1.56
111	6.72	.087	.158	.236	.367	.45
220	6.45	.054	.214	.318	.487	.54
311	3.92	.029	.150	.221	.334	.36
400	4.59	.029	.210	.307	.451	.48
331	2.96	.017	.146	.212	.308	.32
422	3.69	.019	.203	.293	.415	.43
511	2.45	.012	.143	.204	.285	.30
440	3.14	.013	.195	.277	.379	.39
620	2.76	.010	.190	.265	.349	.36
444	2.47	.007	.184	.253	.320	.33
553	1.53	.003	.125	.168	.202	.20
733	1.40	.003	.121	.160	.185	.19
555	1.29	.002	.117	.153	.170	.17
840	1.75	.002	.163	.211	.229	.23
664	1.63	.002	.158	.201	.210	.21
933	1.05	.000	.107	.133	.132	.13

DIA SN 50
A =6.49 P= 4
EP=12.7 DT= 260
T= 20 93 293
U2=.0008 .0016 .0049

G	VG	CIG(EL)	CIG(PHONON)			VIG
	13.69	.321				
000	14.03	1.268	.193	.302	.571	1.84
111	7.29	.104	.136	.212	.400	.50
220	7.38	.064	.192	.299	.555	.62
311	4.56	.033	.133	.207	.383	.42
400	5.42	.032	.192	.297	.540	.57
331	3.52	.018	.133	.205	.370	.39
422	4.41	.019	.182	.279	.500	.52
511	2.93	.011	.129	.198	.351	.36
440	3.76	.013	.181	.277	.484	.50
620	3.29	.009	.177	.269	.461	.47
444	2.93	.007	.174	.263	.441	.45
553	1.80	.003	.121	.181	.294	.30
733	1.65	.003	.119	.177	.283	.29
555	1.52	.002	.118	.174	.271	.27
840	2.05	.003	.164	.241	.372	.37
664	1.90	.003	.161	.236	.357	.36
933	1.23	.002	.112	.162	.239	.24

BCC LI 3
A =3.46 P= 1
EP= 8.2 DT= 316
T= 20 93 293
U2=.0182 .0247 .0562

G	VG	CIG(EL)	CIG(PHONON)			VIG
	6.16	.220				
000	2.88	.279	.013	.015	.023	.30
110	1.66	.005	.011	.012	.015	.02
200	.96	.004	.009	.010	.011	.01
211	.70	.003	.008	.008	.008	.00
220	.57	.003	.007	.007	.006	.00
310	.49	.002	.006	.006	.004	.00
222	.43	.002	.006	.005	.003	.00
400	.35	.001	.004	.004	.002	.00
332	.27	.000	.003	.003	.000	.00
521	.22	.000	.002	.001	.000	.00
611	.18	.000	.001	.000	.000	.00
444	.15	.000	.000	.000	.000	.00
642	.13	.000	.000	.000	.000	.00
820	.11	.000	.000	.000	.000	.00
840	.09	.000	.000	.000	.000	.00
763	.08	.000	.000	.000	.000	.00
961	.07	.000	.000	.000	.000	.00

BCC NA 11
A =4.30 P= 1
EP= 5.9 DT= 163
T= 20 93 293
U2=.0108 .0254 .0726

G	VG	CIG(EL)	CIG(PHONON)			VIG
	4.66	.166				
000	3.30	.386	.050	.073	.106	.49
110	2.22	.025	.048	.068	.088	.11
200	1.60	.016	.046	.063	.072	.08
211	1.33	.011	.044	.058	.059	.07
220	1.17	.008	.042	.054	.048	.05
310	1.05	.006	.040	.049	.039	.04
222	.96	.005	.038	.045	.032	.03
400	.82	.003	.035	.038	.021	.02
332	.68	.002	.030	.029	.010	.01
521	.55	.001	.025	.020	.004	.00
611	.46	.000	.021	.014	.000	.00
444	.38	.000	.017	.009	.000	.00
642	.34	.000	.014	.006	.000	.00
820	.29	.000	.011	.003	.000	.00
840	.25	.000	.008	.001	.000	.00
763	.21	.000	.006	.000	.000	.00
961	.17	.000	.003	.000	.000	.00

BCC K 19
A =5.33 P= 1
EP= 4.3 DT= 132
T= 20 93 293
U2=.0088 .0230 .0705

G	VG	CIG(EL)	CIG(PHONON)			VIG
	4.46	.125				
000	3.62	.504	.066	.107	.167	.67
110	2.64	.031	.064	.102	.150	.18
200	2.01	.017	.062	.096	.131	.14
211	1.70	.011	.061	.091	.114	.12
220	1.48	.007	.059	.086	.099	.10
310	1.32	.005	.057	.081	.086	.09
222	1.20	.004	.055	.076	.074	.08
400	1.01	.002	.051	.067	.055	.06
332	.81	.001	.047	.056	.035	.04
521	.64	.000	.042	.045	.019	.02
611	.53	.000	.038	.035	.009	.00
444	.43	.000	.033	.026	.003	.00
642	.38	.000	.030	.021	.000	.00
820	.33	.000	.025	.015	.000	.00
840	.28	.000	.022	.010	-.001	.00
763	.25	.000	.019	.007	-.001	.00
961	.21	.000	.014	.003	.000	.00

BCC V 23
A =3.03 P= 2
EP=14.1 DT= 356
T= 20 93 293
U2=.0021 .0031 .0075

G	VG	CIG(EL)	CIG(PHONON)			VIG
	23.93	.350				
000	15.43	2.202	.218	.278	.464	2.67
110	10.27	.073	.210	.266	.432	.50
200	7.21	.033	.203	.255	.401	.43
211	5.71	.017	.193	.241	.367	.38
220	4.76	.010	.187	.231	.340	.35
310	4.08	.006	.179	.219	.313	.32
222	3.57	.004	.173	.210	.291	.29
400	2.86	.003	.161	.193	.250	.25
332	2.19	.002	.146	.170	.201	.20
521	1.67	.003	.130	.147	.154	.16
611	1.36	.002	.117	.129	.119	.12
444	1.11	.002	.104	.111	.087	.09
642	.97	.002	.094	.097	.067	.07
820	.82	.002	.083	.082	.046	.05
840	.72	.002	.074	.070	.032	.03
763	.62	.001	.064	.058	.020	.02
961	.51	.001	.051	.042	.008	.00

BCC CR 24
A =2.89 P= 1
EP=10.7 DT= 445
T= 20 93 293
U2=.0018 .0020 .0045

G	VG	CIG(EL)	CIG(PHONON)			VIG
	23.84	.278				
000	17.55	3.413	.245	.262	.430	3.84
110	11.07	.094	.236	.252	.406	.50
200	8.01	.040	.229	.244	.385	.42
211	6.39	.020	.218	.232	.358	.38
220	5.33	.011	.211	.224	.338	.35
310	4.57	.007	.204	.216	.319	.32
222	4.00	.005	.196	.208	.300	.30
400	3.19	.003	.183	.193	.267	.27
332	2.44	.002	.166	.174	.227	.23
521	1.86	.003	.148	.154	.185	.19
611	1.51	.003	.134	.138	.153	.16
444	1.23	.002	.119	.122	.123	.12
642	1.08	.002	.109	.111	.103	.10
820	.91	.002	.096	.097	.080	.08
840	.79	.002	.085	.085	.062	.06
763	.69	.002	.075	.074	.047	.05
961	.56	.002	.061	.059	.029	.03

Table 1 (*cont.*)

BCC FE 26
A =2.86 P= 2
EP=15.3 DT= 411
T= 20 93 293
U2=.001 .0022 .0050

G	VG	CIG(EL)	CIG(PHONON)			VIG
	25.03	.377				
000	17.23	2.430	.280	.330	.538	2.97
110	11.68	.096	.269	.316	.506	.60
200	8.39	.045	.262	.306	.479	.52
211	6.73	.025	.250	.291	.445	.47
220	5.66	.015	.242	.281	.419	.43
310	4.89	.010	.235	.271	.395	.40
222	4.31	.006	.227	.260	.370	.38
400	3.48	.003	.213	.242	.329	.33
332	2.68	.002	.193	.217	.275	.28
521	2.06	.002	.173	.190	.221	.22
611	1.67	.002	.157	.170	.180	.18
444	1.35	.002	.139	.148	.140	.14
642	1.18	.002	.128	.133	.115	.12
820	.99	.002	.113	.115	.087	.09
840	.86	.002	.101	.100	.065	.07
763	.75	.002	.089	.086	.047	.05
961	.61	.003	.072	.067	.027	.03

BCC RB 37
A =5.62 P= 1
EP= 3.9 DT= 72
T= 20 93 293
U2=.0095 .0350 .1087

G	VG	CIG(EL)	CIG(PHONON)			VIG
	5.08	.117				
000	4.31	.668	.177	.304	.425	1.09
110	3.29	.046	.176	.290	.370	.41
200	2.60	.027	.170	.272	.314	.33
211	2.22	.018	.168	.257	.267	.28
220	1.97	.013	.162	.240	.224	.23
310	1.77	.010	.159	.226	.189	.19
222	1.62	.008	.159	.214	.160	.16
400	1.38	.006	.149	.186	.111	.11
332	1.14	.004	.138	.153	.064	.06
521	.93	.003	.127	.118	.029	.03
611	.80	.003	.116	.092	.012	.01
444	.68	.002	.104	.066	.003	.00
642	.61	.002	.095	.050	.000	.00
820	.54	.002	.084	.033	-.002	.00
840	.48	.001	.074	.022	-.001	.00
763	.43	.000	.064	.012	-.001	.00
961	.36	.000	.049	.004	.000	.00

BCC NB 41
A =3.30 P= 1
EP= 8.8 DT= 276
T= 20 93 293
U2=.0021 .0030 .0074

G	VG	CIG(EL)	CIG(PHONON)			VIG
	24.38	.233				
000	19.83	4.194	.470	.580	.939	5.13
110	12.61	.104	.465	.570	.901	1.00
200	9.15	.046	.441	.538	.836	.88
211	7.31	.027	.432	.523	.791	.82
220	6.13	.019	.419	.505	.744	.76
310	5.29	.015	.413	.494	.708	.72
222	4.67	.013	.402	.479	.669	.68
400	3.80	.011	.382	.450	.600	.61
332	3.01	.008	.357	.414	.513	.52
521	2.40	.006	.327	.371	.418	.42
611	2.01	.005	.301	.335	.343	.35
444	1.69	.003	.273	.296	.269	.27
642	1.50	.002	.254	.270	.222	.22
820	1.29	.002	.230	.237	.168	.17
840	1.13	.001	.207	.207	.125	.13
763	.98	.000	.182	.175	.087	.09
961	.81	.000	.151	.137	.047	.05

BCC MO 42
A =3.15 P= 1
EP= 9.4 DT= 374
T= 20 93 293
U2=.0010 .0014 .0033

G	VG	CIG(EL)	CIG(PHONON)			VIG
	27.27	.248				
000	22.22	4.548	.355	.441	.737	5.29
110	14.19	.113	.350	.434	.717	.83
200	10.27	.049	.348	.430	.699	.75
211	8.18	.028	.336	.414	.664	.69
220	6.83	.020	.331	.407	.643	.66
310	5.88	.016	.321	.392	.612	.63
222	5.17	.013	.315	.384	.591	.60
400	4.20	.011	.304	.368	.552	.56
332	3.31	.009	.289	.347	.501	.51
521	2.63	.007	.271	.321	.441	.45
611	2.20	.005	.255	.299	.392	.40
444	1.84	.004	.239	.277	.341	.34
642	1.63	.003	.228	.261	.307	.31
820	1.40	.002	.210	.237	.260	.26
840	1.22	.001	.197	.219	.224	.22
763	1.07	.001	.181	.198	.186	.19
961	.87	.001	.161	.170	.139	.14

BCC CS 55
A =6.13 P= 1
EP= 3.5 DT= 48
T= 20 93 293
U2=.0114 .0470 .1440

G	VG	CIG(EL)	CIG(PHONON)			VIG
	5.58	.144				
000	4.91	.842	.309	.541	.735	1.58
110	3.89	.058	.310	.519	.636	.69
200	3.13	.034	.299	.484	.532	.56
211	2.70	.023	.297	.457	.447	.46
220	2.41	.017	.285	.422	.369	.38
310	2.17	.013	.281	.396	.307	.31
222	1.99	.011	.272	.367	.253	.26
400	1.71	.008	.263	.322	.173	.17
332	1.42	.006	.243	.259	.094	.09
521	1.17	.004	.225	.196	.040	.04
611	1.01	.003	.204	.146	.014	.01
444	.87	.002	.182	.101	.002	.00
642	.78	.002	.167	.075	-.001	.00
820	.68	.001	.147	.047	-.002	.00
840	.61	.001	.129	.028	-.002	.00
763	.54	.000	.112	.015	-.001	.00
961	.45	.000	.087	.003	.000	.00

BCC BA 56
A =5.02 P= 2
EP= 6.6 DT= 115
T= 20 93 293
U2=.0024 .0067 .0204

G	VG	CIG(EL)	CIG(PHONON)			VIG
	11.40	.183				
000	9.11	1.313	.259	.452	.754	2.07
110	6.73	.075	.254	.442	.721	.79
200	5.10	.042	.261	.444	.698	.74
211	4.26	.028	.247	.421	.650	.68
220	3.70	.020	.246	.413	.619	.64
310	3.29	.016	.250	.412	.595	.61
222	2.98	.013	.242	.396	.558	.57
400	2.51	.009	.235	.377	.502	.51
332	2.06	.007	.228	.354	.430	.43
521	1.68	.005	.217	.322	.348	.35
611	1.43	.003	.206	.294	.282	.28
444	1.21	.002	.194	.263	.217	.22
642	1.09	.002	.188	.244	.177	.18
820	.94	.001	.175	.214	.128	.13
840	.83	.001	.167	.191	.093	.09
763	.73	.001	.154	.165	.062	.06
961	.60	.000	.140	.131	.030	.03

BCC TA 73
A =3.30 P= 2
EP=12.4 DT= 238
T= 20 93 293
U2=.0009 .0016 .0043

G	VG	CIG(EL)	CIG(PHONON)			VIG
	31.08	.314				
000	24.07	4.113	.792	1.130	1.939	6.05
110	16.80	.180	.797	1.133	1.917	2.09
200	12.64	.097	.758	1.073	1.800	1.89
211	10.46	.064	.756	1.065	1.756	1.82
220	9.03	.046	.743	1.043	1.694	1.74
310	7.99	.036	.745	1.040	1.662	1.69
222	7.20	.029	.733	1.020	1.605	1.63
400	6.05	.021	.714	.984	1.502	1.52
332	4.93	.014	.687	.935	1.365	1.38
521	4.01	.009	.652	.872	1.200	1.21
611	3.39	.006	.622	.816	1.059	1.06
444	2.85	.004	.587	.754	.908	.91
642	2.53	.003	.565	.714	.810	.81
820	2.17	.002	.530	.654	.680	.68
840	1.90	.002	.502	.606	.577	.58
763	1.65	.002	.467	.547	.467	.47
961	1.35	.003	.424	.475	.340	.34

BCC W 74
A =3.16 P= 2
EP=13.2 DT= 327
T= 20 93 293
U2=.0007 .0010 .0024

G	VG	CIG(EL)	CIG(PHONON)			VIG
	34.80	.331				
000	27.12	4.628	.776	.978	1.643	6.27
110	18.76	.190	.774	.973	1.623	1.81
200	14.04	.101	.782	.982	1.626	1.72
211	11.54	.066	.757	.949	1.555	1.62
220	9.91	.048	.756	.945	1.535	1.58
310	8.74	.037	.727	.906	1.457	1.49
222	7.85	.030	.724	.900	1.433	1.46
400	6.57	.021	.707	.875	1.368	1.39
332	5.34	.014	.680	.836	1.272	1.28
521	4.33	.009	.647	.789	1.156	1.16
611	3.65	.006	.613	.740	1.046	1.05
444	3.07	.004	.588	.703	.952	.95
642	2.72	.003	.560	.664	.866	.87
820	2.33	.002	.534	.625	.776	.78
840	2.03	.002	.508	.588	.695	.70
763	1.77	.002	.476	.543	.604	.61
961	1.37	.010	.433	.484	.489	.50

BCC TL 81
A =3.88 P= 3
EP=11.9 DT= 98
T= 20 93 293
U2=.0023 .0071 .0217

G	VG	CIG(EL)	CIG(PHONON)			VIG
	19.25	.303				
000	17.26	2.166	1.031	1.812	2.829	5.00
110	12.46	.156	1.002	1.745	2.634	2.78
200	9.78	.085	1.019	1.732	2.477	2.55
211	8.27	.056	1.019	1.694	2.304	2.35
220	7.23	.041	.968	1.594	2.085	2.12
310	6.46	.031	.956	1.544	1.923	1.95
222	5.86	.025	.963	1.519	1.791	1.81
400	4.97	.018	.908	1.389	1.493	1.50
332	4.07	.012	.872	1.260	1.163	1.17
521	3.31	.009	.822	1.104	.830	.83
611	2.81	.007	.775	.969	.589	.59
444	2.38	.006	.722	.824	.379	.38
642	2.13	.005	.676	.718	.260	.26
820	1.85	.004	.627	.598	.145	.15
840	1.64	.003	.582	.496	.075	.08
763	1.45	.002	.536	.400	.029	.03
961	1.21	.002	.454	.269	-.006	.00

larger angles are lost for image formation by inelastic interaction. This $s_{\min}$ will be used throughout the Tables. It would correspond to $\overline{\Delta E} \simeq 70$ eV for $E_0 =$ 100 keV.

4·3. *Phonon excitation*

For the imaginary potential due to phonon excitation we use the result given by Hall & Hirsch, 1965:

$$C^I_{0g}(\text{phonon}) = -\frac{\hbar^2}{2m}\frac{4}{a_0^{*2}k_0V_c}\sum_\alpha \exp(-i\mathbf{g}\mathbf{R}_\alpha) \times \int \frac{[Z^{(\alpha)}-f^{(\alpha)}(\mathbf{s})]\,[Z^{(\alpha)}-f^{(\alpha)}(\mathbf{s}-\mathbf{g})]}{\mathbf{s}^2(\mathbf{s}-\mathbf{g})^2} \times \{\exp[-M(\mathbf{g})]-\exp[-M(\mathbf{s})-M(\mathbf{s}-\mathbf{g})]\}d\sigma\,, \quad (12)$$

Table 1 (*cont.*)

FCC NE 10
A =4.52 P= 0
EP= 0.0 DT= 63
T= 20 93 293
U2=.0454 .0000 .0000

G	VG	CIG(EL)	CIG(PHONON)			VIG
	3.22	.000				
000	3.22	.607	.132	.000	.000	.61
111	2.65	.042	.116	.000	.000	.04
200	2.49	.033	.109	.000	.000	.03
220	2.01	.016	.087	.000	.000	.02
311	1.75	.010	.072	.000	.000	.01
222	1.68	.009	.068	.000	.000	.00
400	1.45	.006	.053	.000	.000	.00
331	1.31	.004	.043	.000	.000	.00
422	1.12	.003	.031	.000	.000	.00
440	.92	.002	.017	.000	.000	.00
620	.77	.001	.009	.000	.000	.00
444	.66	.000	.005	.000	.000	.00
642	.58	.000	.002	.000	.000	.00
733	.50	.000	.000	.000	.000	.00
662	.44	.000	.000	.000	.000	.00
664	.39	.000	-.001	.000	.000	.00
933	.35	.000	-.001	.000	.000	.00

FCC AL 13
A =4.04 P= 3
EP=15.8 DT= 390
T= 20 93 293
U2=.0035 .0046 .0105

G	VG	CIG(EL)	CIG(PHONON)			VIG
	14.91	.387				
000	10.00	.690	.087	.103	.162	.85
111	5.93	.033	.084	.098	.149	.18
200	4.98	.026	.081	.095	.144	.17
220	3.17	.016	.077	.089	.129	.14
311	2.57	.013	.074	.085	.119	.13
222	2.43	.012	.073	.083	.115	.13
400	2.02	.009	.069	.079	.104	.11
331	1.81	.007	.067	.075	.097	.10
422	1.55	.005	.063	.070	.085	.09
440	1.27	.003	.057	.063	.070	.07
620	1.08	.002	.052	.056	.058	.06
444	.94	.001	.048	.051	.048	.05
642	.84	.000	.044	.046	.039	.04
733	.72	.000	.039	.040	.030	.03
662	.65	.000	.035	.035	.024	.02
664	.57	.000	.031	.031	.018	.02
933	.51	.000	.028	.027	.013	.01

FCC AR 18
A =5.43 P= 0
EP= 0.0 DT= 85
T= 20 93 293
U2=.0144 .0000 .0000

G	VG	CIG(EL)	CIG(PHONON)			VIG
	4.96	.000				
000	4.96	1.063	.144	.000	.000	1.06
111	3.92	.046	.138	.000	.000	.05
200	3.63	.033	.135	.000	.000	.03
220	2.78	.012	.125	.000	.000	.01
311	2.35	.007	.118	.000	.000	.00
222	2.24	.006	.115	.000	.000	.00
400	1.87	.004	.105	.000	.000	.00
331	1.66	.003	.099	.000	.000	.00
422	1.39	.002	.090	.000	.000	.00
440	1.11	.002	.076	.000	.000	.00
620	.93	.002	.066	.000	.000	.00
444	.80	.002	.056	.000	.000	.00
642	.70	.002	.049	.000	.000	.00
733	.61	.002	.040	.000	.000	.00
662	.55	.002	.034	.000	.000	.00
664	.49	.001	.028	.000	.000	.00
933	.44	.001	.023	.000	.000	.00

FCC CA 20
A =5.58 P= 2
EP= 8.0 DT= 225
T= 20 93 293
U2=.0043 .0076 .0213

G	VG	CIG(EL)	CIG(PHONON)			VIG
	8.87	.215				
000	6.75	.726	.084	.117	.200	.93
111	4.65	.038	.083	.114	.188	.22
200	4.04	.030	.081	.112	.182	.21
220	2.84	.015	.078	.105	.164	.18
311	2.39	.010	.076	.101	.152	.16
222	2.28	.009	.076	.102	.149	.16
400	1.92	.005	.073	.095	.133	.14
331	1.73	.004	.071	.092	.124	.13
422	1.48	.003	.068	.086	.109	.11
440	1.20	.002	.063	.078	.089	.09
620	1.01	.001	.059	.071	.073	.07
444	.87	.001	.055	.065	.060	.06
642	.76	.001	.052	.060	.049	.05
733	.66	.001	.048	.053	.037	.04
662	.59	.001	.045	.048	.030	.03
664	.52	.001	.042	.043	.022	.02
933	.47	.001	.039	.039	.017	.02

FCC MN 25
A =3.70 P= 2
EP=14.8 DT= 380
T= 20 93 293
U2=.0018 .0024 .0057

G	VG	CIG(EL)	CIG(PHONON)			VIG
	24.08	.365				
000	16.38	2.305	.251	.301	.502	2.81
111	11.34	.092	.243	.290	.475	.56
200	9.93	.069	.241	.288	.467	.53
220	6.96	.029	.229	.272	.427	.45
311	5.79	.017	.224	.264	.404	.42
222	5.48	.015	.220	.259	.393	.41
400	4.54	.008	.209	.244	.359	.37
331	4.03	.006	.203	.236	.338	.34
422	3.38	.003	.193	.223	.307	.31
440	2.68	.002	.178	.202	.261	.26
620	2.22	.002	.166	.186	.225	.23
444	1.89	.002	.154	.171	.195	.20
642	1.65	.002	.145	.159	.170	.17
733	1.41	.002	.133	.143	.140	.14
662	1.26	.002	.125	.133	.121	.12
664	1.11	.002	.115	.121	.100	.10
933	1.00	.002	.107	.110	.083	.08

FCC FE 26
A =3.63 P= 2
EP=15.2 DT= 411
T= 20 93 293
U2=.0017 .0022 .0050

G	VG	CIG(EL)	CIG(PHONON)			VIG
	24.51	.374				
000	16.95	2.384	.274	.323	.526	2.91
111	11.80	.100	.265	.312	.500	.60
200	10.37	.076	.263	.309	.492	.56
220	7.32	.033	.253	.295	.455	.49
311	6.11	.020	.246	.285	.430	.45
222	5.79	.017	.241	.279	.419	.43
400	4.81	.009	.231	.266	.387	.40
331	4.27	.006	.223	.256	.365	.37
422	3.59	.004	.212	.241	.332	.34
440	2.86	.002	.196	.221	.287	.29
620	2.37	.002	.182	.203	.249	.25
444	2.02	.002	.170	.187	.217	.22
642	1.77	.002	.160	.174	.191	.19
733	1.51	.002	.146	.157	.160	.16
662	1.35	.002	.138	.146	.140	.14
664	1.18	.002	.127	.133	.117	.12
933	1.06	.002	.118	.122	.099	.10

FCC CO 27
A =3.54 P= 2
EP=15.7 DT= 385
T= 20 93 293
U2=.0014 .0022 .0051

G	VG	CIG(EL)	CIG(PHONON)			VIG
	25.28	.385				
000	17.70	2.478	.302	.370	.607	3.09
111	12.38	.109	.292	.356	.575	.68
200	10.91	.083	.290	.353	.565	.65
220	7.75	.036	.279	.337	.523	.56
311	6.48	.022	.271	.325	.493	.51
222	6.15	.019	.266	.319	.480	.50
400	5.13	.011	.254	.303	.442	.45
331	4.56	.007	.246	.292	.416	.42
422	3.84	.004	.234	.274	.377	.38
440	3.06	.002	.218	.252	.325	.33
620	2.54	.002	.203	.231	.281	.28
444	2.17	.002	.189	.212	.243	.24
642	1.89	.002	.178	.197	.212	.21
733	1.61	.002	.164	.179	.177	.18
662	1.44	.002	.152	.164	.151	.15
664	1.26	.002	.141	.149	.125	.13
933	1.14	.002	.132	.137	.106	.11

FCC NI 28
A =3.52 P= 2
EP=15.9 DT= 425
T= 20 93 293
U2=.0015 .0020 .0046

G	VG	CIG(EL)	CIG(PHONON)			VIG
	24.90	.389				
000	17.78	2.466	.315	.378	.620	3.09
111	12.51	.116	.304	.364	.588	.70
200	11.06	.089	.303	.362	.580	.67
220	7.93	.040	.292	.347	.540	.58
311	6.66	.025	.284	.335	.511	.53
222	6.33	.021	.279	.329	.499	.52
400	5.29	.012	.270	.317	.466	.48
331	4.72	.009	.259	.303	.437	.44
422	3.99	.005	.248	.288	.401	.40
440	3.20	.003	.230	.264	.347	.35
620	2.66	.002	.215	.243	.303	.30
444	2.27	.002	.200	.224	.265	.27
642	1.99	.002	.189	.209	.233	.23
733	1.69	.002	.175	.190	.197	.20
662	1.51	.002	.164	.177	.172	.17
664	1.32	.002	.151	.160	.143	.14
933	1.19	.002	.142	.148	.123	.12

FCC CU 29
A =3.61 P= 1
EP=10.8 DT= 320
T= 20 93 293
U2=.0018 .0027 .0069

G	VG	CIG(EL)	CIG(PHONON)			VIG
	19.98	.280				
000	15.82	2.738	.345	.443	.746	3.48
111	11.24	.131	.336	.429	.708	.83
200	10.12	.101	.335	.426	.696	.79
220	7.53	.046	.323	.408	.641	.68
311	6.40	.029	.315	.394	.602	.63
222	6.11	.025	.309	.386	.585	.61
400	5.16	.015	.297	.367	.535	.55
331	4.62	.011	.288	.353	.500	.51
422	3.94	.006	.273	.332	.446	.45
440	3.17	.003	.254	.302	.375	.38
620	2.65	.002	.235	.274	.314	.32
444	2.28	.002	.219	.251	.265	.27
642	1.99	.001	.205	.231	.224	.23
733	1.70	.001	.189	.207	.179	.18
662	1.52	.002	.176	.189	.149	.15
664	1.33	.002	.162	.169	.117	.12
933	1.20	.002	.150	.153	.093	.09

with

$$M(\mathbf{s}) = \tfrac{1}{2}\overline{u_s^2}s^2\,, \tag{13}$$

the exponent of the Debye–Waller factor. $\overline{u_s^2}$ is the mean-square vibration amplitude. It depends on the index α of the atomic number.

The absorption potential (12) is based on the rigid-ion model (adiabatic approximation). For the lattice vibrations an Einstein model has been assumed, *i.e.* correlation between atoms at different sites is being neglected. Thereby also the orientation dependence of C_{0g}^{i} is averaged out.

For evaluation of the integral in (12), the coordinate system of Fig. 1 is used and again the azimuthal integration is performed as given in the Appendix. This leads to

Table 1 (*cont.*)

FCC KR 36
A =5.59 P= 0
EP= 0.0 DT= 63
T= 20 93 293
U2=.0109 .0410 .0000

G	VG	CIG(EL)	CIG(PHONON)			VIG
	6.87	.000				
000	6.87	1.521	.365	.614	.000	1.52
111	5.41	.072	.358	.567	.000	.07
200	5.03	.054	.349	.545	.000	.05
220	3.89	.025	.332	.472	.000	.03
311	3.33	.018	.320	.424	.000	.02
222	3.19	.016	.322	.414	.000	.02
400	2.71	.012	.301	.353	.000	.01
331	2.45	.011	.291	.317	.000	.01
422	2.11	.009	.272	.262	.000	.00
440	1.76	.007	.246	.194	.000	.00
620	1.52	.006	.222	.143	.000	.00
444	1.34	.005	.201	.105	.000	.00
642	1.21	.004	.183	.077	.000	.00
733	1.08	.003	.160	.048	.000	.00
662	.99	.002	.144	.033	.000	.00
664	.89	.002	.124	.018	.000	.00
933	.82	.001	.109	.010	.000	.00

FCC SR 38
A =6.08 P= 2
EP= 7.0 DT= 160
T= 20 93 293
U2=.0029 .0068 .0209

G	VG	CIG(EL)	CIG(PHONON)			VIG
	9.09	.192				
000	7.35	.897	.158	.250	.417	1.31
111	5.31	.057	.155	.244	.398	.45
200	4.71	.046	.156	.244	.393	.44
220	3.46	.025	.152	.236	.365	.39
311	2.97	.018	.150	.231	.346	.36
222	2.84	.017	.149	.228	.339	.35
400	2.44	.012	.149	.223	.318	.33
331	2.22	.010	.144	.216	.299	.31
422	1.93	.008	.141	.208	.273	.28
440	1.61	.006	.137	.196	.237	.24
620	1.39	.005	.132	.184	.205	.21
444	1.23	.004	.128	.174	.178	.18
642	1.10	.003	.123	.163	.154	.16
733	.97	.003	.118	.151	.127	.13
662	.89	.003	.113	.141	.108	.11
664	.80	.002	.108	.130	.087	.09
933	.74	.002	.103	.120	.072	.07

FCC RH 45
A =3.80 P= 1
EP=10.0 DT= 343
T= 20 93 293
U2=.0010 .0015 .0037

G	VG	CIG(EL)	CIG(PHONON)			VIG
	28.55	.263				
000	23.68	4.421	.459	.596	1.012	5.43
111	16.34	.142	.453	.585	.981	1.12
200	14.59	.102	.451	.583	.972	1.07
220	10.45	.039	.432	.555	.907	.94
311	8.67	.024	.427	.546	.877	.90
222	8.21	.021	.428	.546	.872	.89
400	6.78	.015	.412	.522	.817	.83
331	6.00	.012	.406	.513	.789	.80
422	5.05	.011	.391	.491	.736	.74
440	4.05	.009	.374	.465	.669	.68
620	3.40	.008	.357	.438	.607	.61
444	2.95	.007	.344	.419	.558	.56
642	2.62	.007	.329	.396	.508	.51
733	2.28	.005	.314	.374	.455	.46
662	2.06	.005	.303	.357	.417	.42
664	1.84	.004	.287	.334	.369	.37
933	1.68	.003	.273	.314	.329	.33

FCC PD 46
A =3.89 P= 0
EP= 0.0 DT= 271
T= 20 93 293
U2=.0013 .0021 .0055

G	VG	CIG(EL)	CIG(PHONON)			VIG
	22.37	.000				
000	22.37	4.773	.526	.707	1.207	5.98
111	15.24	.154	.521	.696	1.167	1.32
200	13.81	.111	.520	.694	1.155	1.26
220	10.15	.042	.497	.658	1.066	1.11
311	8.49	.025	.483	.636	1.009	1.03
222	8.06	.022	.491	.645	1.012	1.03
400	6.68	.014	.468	.609	.931	.94
331	5.93	.011	.459	.594	.888	.90
422	4.99	.010	.446	.571	.822	.83
440	4.00	.008	.420	.530	.722	.73
620	3.36	.008	.401	.499	.642	.65
444	2.91	.007	.385	.472	.575	.58
642	2.58	.006	.366	.443	.510	.51
733	2.24	.006	.348	.413	.442	.45
662	2.03	.005	.331	.387	.389	.39
664	1.81	.004	.314	.360	.333	.34
933	1.65	.003	.299	.336	.289	.29

FCC AG 47
A =4.08 P= 1
EP= 9.0 DT= 216
T= 20 93 293
U2=.0016 .0030 .0084

G	VG	CIG(EL)	CIG(PHONON)			VIG
	21.87	.239				
000	18.74	3.325	.541	.784	1.344	4.67
111	13.82	.145	.540	.777	1.296	1.44
200	12.53	.107	.523	.753	1.254	1.36
220	9.34	.043	.515	.731	1.167	1.21
311	7.90	.026	.501	.704	1.094	1.12
222	7.51	.023	.493	.692	1.067	1.09
400	6.29	.014	.482	.667	.986	1.00
331	5.61	.011	.471	.647	.928	.94
422	4.76	.009	.457	.617	.842	.85
440	3.83	.007	.433	.572	.721	.73
620	3.21	.007	.409	.528	.616	.62
444	2.78	.006	.393	.496	.535	.54
642	2.46	.006	.375	.463	.462	.47
733	2.13	.005	.354	.425	.380	.38
662	1.93	.005	.336	.394	.323	.33
664	1.72	.004	.318	.362	.263	.26
933	1.56	.004	.300	.331	.215	.22

FCC XE 54
A =6.24 P= 0
EP= 0.0 DT= 55
T= 20 93 293
U2=.0088 .0344 .0000

G	VG	CIG(EL)	CIG(PHONON)			VIG
	7.77	.000				
000	7.77	1.814	.500	.885	.000	1.81
111	6.26	.084	.489	.835	.000	.08
200	5.80	.066	.489	.820	.000	.07
220	4.54	.032	.471	.742	.000	.03
311	3.93	.022	.460	.689	.000	.02
222	3.76	.020	.453	.670	.000	.02
400	3.23	.015	.444	.609	.000	.02
331	2.93	.013	.426	.560	.000	.01
422	2.56	.010	.408	.492	.000	.01
440	2.14	.007	.382	.401	.000	.00
620	1.86	.006	.352	.323	.000	.00
444	1.65	.004	.329	.262	.000	.00
642	1.49	.004	.307	.211	.000	.00
733	1.32	.003	.278	.156	.000	.00
662	1.21	.002	.259	.122	.000	.00
664	1.08	.002	.234	.086	.000	.00
933	.99	.002	.214	.062	.000	.00

FCC IR 77
A =3.84 P= 2
EP=14.0 DT= 285
T= 20 93 293
U2=.0004 .0010 .0028

G	VG	CIG(EL)	CIG(PHONON)			VIG
	37.24	.348				
000	30.07	4.986	.850	1.188	2.168	7.15
111	21.54	.216	.847	1.180	2.131	2.34
200	19.30	.166	.848	1.181	2.127	2.29
220	14.14	.080	.819	1.135	2.011	2.09
311	11.97	.056	.818	1.131	1.982	2.04
222	11.41	.051	.825	1.140	1.988	2.04
400	9.65	.037	.800	1.100	1.887	1.92
331	8.69	.030	.796	1.092	1.851	1.88
422	7.49	.024	.775	1.055	1.754	1.78
440	6.19	.017	.747	1.010	1.627	1.64
620	5.32	.013	.725	.971	1.516	1.53
444	4.68	.010	.708	.942	1.427	1.44
642	4.19	.008	.683	.901	1.323	1.33
733	3.68	.006	.663	.866	1.222	1.23
662	3.34	.005	.645	.836	1.139	1.14
664	2.99	.004	.620	.794	1.035	1.04
933	2.72	.003	.604	.766	.961	.96

FCC PT 78
A =3.92 P= 1
EP= 9.6 DT= 236
T= 20 93 293
U2=.0008 .0015 .0040

G	VG	CIG(EL)	CIG(PHONON)			VIG
	32.14	.252				
000	26.14	5.200	.987	1.460	2.498	7.70
111	20.31	.221	.987	1.455	2.457	2.67
200	18.40	.168	.970	1.427	2.404	2.57
220	13.73	.078	.953	1.394	2.300	2.37
311	11.67	.053	.934	1.358	2.211	2.26
222	11.12	.048	.939	1.364	2.207	2.25
400	9.42	.035	.920	1.327	2.104	2.14
331	8.47	.029	.911	1.308	2.042	2.07
422	7.30	.023	.885	1.260	1.919	1.94
440	6.03	.017	.859	1.208	1.769	1.78
620	5.18	.013	.834	1.158	1.631	1.64
444	4.56	.011	.813	1.116	1.512	1.52
642	4.09	.009	.782	1.059	1.380	1.39
733	3.59	.006	.752	1.002	1.238	1.24
662	3.27	.005	.728	.958	1.134	1.14
664	2.92	.004	.703	.908	1.016	1.02
933	2.66	.003	.679	.864	.917	.92

FCC AU 79
A =4.08 P= 1
EP= 9.0 DT= 175
T= 20 93 293
U2=.0017 .0026 .0074

G	VG	CIG(EL)	CIG(PHONON)			VIG
	28.20	.239				
000	25.02	4.523	1.432	1.817	3.042	7.57
111	18.59	.215	1.441	1.820	2.976	3.19
200	16.95	.164	1.388	1.752	2.867	3.03
220	12.83	.076	1.381	1.730	2.730	2.80
311	10.96	.052	1.345	1.678	2.589	2.64
222	10.47	.047	1.324	1.649	2.529	2.57
400	8.90	.033	1.303	1.611	2.385	2.41
331	8.02	.027	1.279	1.573	2.273	2.30
422	6.92	.022	1.249	1.522	2.109	2.13
440	5.72	.016	1.192	1.434	1.861	1.87
620	4.91	.013	1.130	1.341	1.633	1.64
444	4.32	.011	1.093	1.280	1.457	1.46
642	3.88	.008	1.045	1.208	1.289	1.29
733	3.37	.010	.990	1.124	1.095	1.10
662	3.11	.005	.940	1.052	.952	.95
664	2.78	.004	.892	.979	.801	.80
933	2.54	.003	.840	.905	.673	.67

$$C^I_{0g}(\text{phonon}) = -\frac{\hbar^2}{2m}\frac{8\pi}{a_0^{*2}k_0V_c}\sum_\alpha \exp(-i\mathbf{g}\mathbf{R}_\alpha)$$
$$\times\int_0^{2k_0}$$
$$\frac{[Z^{(\alpha)}-f^{(\alpha)}(\sqrt{|a^2-r^2|})]\,[Z^{(\alpha)}-f^{(\alpha)}(\sqrt{2(a^2+r^2)-|a^2-r^2|})]}{(a^2+r^2)\,|a^2-r^2|}$$
$$\times\{\exp(-2\overline{u_s^2}a^2)-\exp[-\overline{u_s^2}(r^2+a^2)]\}rdr\,. \qquad (14)$$

In order to compute this one requires the mean-square vibration displacement $\overline{u_s^2}$; this can hardly be determined theoretically and therefore must be taken from measurements of related quantities, such as the intensity variation of X-ray diffraction reflexions with temperature (Debye–Waller factor), or from the specific heat, elastic constants or electrical resistance. We use an average of the measured values as compiled in

Table 1 (*cont.*)

FCC PB 82
A =4.95 P= 4
EP=13.5 DT= 85
T= 20 93 293
U2=.0030 .0105 .0320

G	VG	CIG(EL)	CIG(PHONON)			VIG
	19.41	.338				
000	18.25	1.959	1.174	2.117	3.177	5.14
111	12.76	.158	1.149	2.040	2.910	3.06
200	11.58	.126	1.189	2.067	2.867	2.98
220	8.82	.067	1.119	1.910	2.462	2.52
311	7.64	.048	1.124	1.857	2.239	2.27
222	7.33	.044	1.107	1.818	2.151	2.18
400	6.35	.031	1.077	1.714	1.863	1.88
331	5.79	.026	1.059	1.644	1.675	1.69
422	5.07	.019	1.023	1.524	1.393	1.40
440	4.26	.014	.991	1.374	1.048	1.05
620	3.69	.011	.940	1.221	.776	.78
444	3.26	.009	.902	1.094	.575	.58
642	2.93	.008	.860	.976	.420	.42
733	2.59	.006	.810	.837	.270	.27
662	2.36	.006	.779	.745	.186	.19
664	2.13	.005	.726	.627	.106	.11
933	1.95	.004	.691	.541	.060	.06

FCC TH 90
A =5.08 P= 2
EP= 9.2 DT= 157
T= 20 93 293
U2=.0011 .0026 .0076

G	VG	CIG(EL)	CIG(PHONON)			VIG
	26.58	.243				
000	20.91	3.910	.728	1.198	2.036	5.95
111	15.01	.149	.719	1.178	1.977	2.12
200	13.37	.117	.748	1.224	2.020	2.13
220	9.74	.061	.708	1.148	1.872	1.93
311	8.25	.045	.718	1.157	1.843	1.88
222	7.87	.041	.708	1.138	1.807	1.85
400	6.69	.032	.695	1.109	1.724	1.75
331	6.04	.027	.676	1.071	1.644	1.67
422	5.24	.022	.675	1.059	1.575	1.59
440	4.38	.016	.657	1.016	1.445	1.46
620	3.80	.012	.638	.970	1.322	1.33
444	3.37	.010	.626	.938	1.222	1.23
642	3.04	.008	.611	.902	1.125	1.13
733	2.68	.006	.595	.861	1.009	1.01
662	2.45	.006	.582	.828	.923	.93
664	2.21	.005	.563	.784	.819	.82
933	2.02	.004	.545	.745	.733	.74

HCP BE 4
A =2.28 P= 2
A3=3.59 EP=18.5 DT= 1188
T= 20 93 293
U2=.0030 .0031 .0049

G	VG	CIG(EL)	CIG(PHONON)			VIG
	16.32	.441				
000	7.41	.522	.019	.020	.027	.55
002	4.07	.006	.017	.017	.023	.03
100	2.38	.003	.009	.009	.012	.01
101	3.32	.005	.014	.015	.019	.02
102	1.21	.003	.008	.008	.010	.01
110	1.86	.005	.014	.015	.018	.02
112	1.39	.004	.013	.013	.017	.02
201	1.19	.004	.011	.012	.014	.02
104	.53	.002	.006	.006	.007	.00
203	.82	.003	.010	.010	.012	.01
114	.84	.003	.011	.011	.013	.02
211	.77	.003	.010	.010	.012	.01
006	.64	.002	.009	.010	.011	.01
123	.61	.002	.009	.009	.010	.01
205	.53	.002	.008	.008	.009	.00
220	.59	.002	.009	.009	.010	.01
132	.26	.000	.004	.004	.004	.00

HCP MG 12
A =3.20 P= 2
A3=5.20 EP=10.9 DT= 316
T= 20 93 293
U2=.0049 .0073 .0185

G	VG	CIG(EL)	CIG(PHONON)			VIG
	9.24	.282				
000	6.53	.558	.065	.082	.130	.69
002	4.09	.031	.064	.079	.120	.15
100	2.19	.017	.031	.039	.060	.08
101	3.31	.024	.055	.068	.102	.12
102	1.42	.010	.030	.037	.055	.06
110	2.34	.015	.059	.072	.102	.12
112	1.94	.011	.056	.068	.092	.10
201	1.65	.010	.048	.058	.079	.09
104	.82	.004	.027	.032	.041	.04
203	1.29	.006	.045	.053	.066	.07
114	1.37	.006	.050	.059	.070	.07
211	1.21	.005	.044	.051	.062	.07
006	1.13	.003	.046	.053	.056	.06
123	1.02	.003	.041	.047	.051	.05
205	.93	.003	.039	.044	.045	.05
220	1.02	.003	.044	.049	.049	.05
132	.45	.000	.020	.022	.020	.02

HCP SC 21
A =3.31 P= 2
A3=5.27 EP=10.5 DT= 300**
T= 20 93 293
U2=.0031 .0043 .0108

G	VG	CIG(EL)	CIG(PHONON)			VIG
	14.69	.273				
000	9.99	1.284	.132	.160	.270	1.55
002	6.82	.051	.127	.153	.253	.30
100	3.69	.030	.064	.077	.128	.16
101	5.65	.041	.112	.135	.220	.26
102	2.51	.014	.063	.075	.120	.13
110	4.22	.018	.120	.143	.226	.24
112	3.49	.011	.117	.138	.211	.22
201	2.98	.009	.101	.119	.181	.19
104	1.43	.003	.056	.065	.096	.10
203	2.25	.004	.095	.111	.159	.16
114	2.33	.004	.106	.123	.171	.17
211	2.11	.003	.093	.108	.152	.16
006	1.83	.002	.098	.113	.145	.15
123	1.71	.002	.087	.100	.132	.13
205	1.51	.002	.083	.095	.120	.12
220	1.67	.002	.095	.108	.134	.14
132	.73	.000	.045	.051	.060	.06

HCP TI 22
A =2.95 P= 2
A3=4.68 EP=12.5 DT= 388
T= 20 93 293
U2=.0021 .0028 .0065

G	VG	CIG(EL)	CIG(PHONON)			VIG
	19.77	.317				
000	12.92	1.782	.159	.190	.313	2.09
002	8.73	.063	.155	.185	.298	.36
100	4.74	.037	.079	.094	.152	.19
101	7.26	.050	.133	.159	.256	.30
102	3.21	.016	.074	.088	.140	.16
110	5.40	.021	.146	.173	.269	.29
112	4.43	.012	.140	.165	.252	.26
201	3.77	.010	.121	.143	.216	.23
104	1.80	.003	.067	.079	.116	.12
203	2.81	.004	.113	.132	.191	.19
114	2.90	.004	.127	.148	.209	.21
211	2.63	.004	.111	.129	.185	.19
006	2.25	.002	.118	.135	.181	.18
123	2.12	.002	.105	.121	.165	.17
205	1.85	.002	.101	.115	.152	.15
220	2.06	.002	.114	.131	.171	.17
132	.89	.001	.054	.061	.077	.08

HCP CO 27
A =2.51 P= 2
A3=4.07 EP=15.8 DT= 385
T= 20 93 293
U2=.0016 .0022 .0051

G	VG	CIG(EL)	CIG(PHONON)			VIG
	25.44	.386				
000	17.77	2.489	.304	.372	.610	3.10
002	12.38	.109	.293	.357	.577	.68
100	6.54	.061	.148	.181	.292	.35
101	10.18	.084	.257	.313	.502	.58
102	4.64	.028	.145	.175	.277	.30
110	7.80	.036	.280	.338	.525	.56
112	6.50	.022	.272	.327	.495	.51
201	5.52	.018	.234	.280	.424	.44
104	2.71	.006	.129	.154	.227	.23
203	4.20	.008	.219	.259	.374	.38
114	4.39	.006	.246	.290	.411	.42
211	3.91	.006	.213	.252	.359	.36
006	3.49	.003	.228	.266	.356	.36
123	3.19	.003	.201	.236	.320	.32
205	2.84	.002	.193	.224	.295	.30
220	3.08	.002	.219	.253	.327	.33
132	1.34	.001	.104	.119	.147	.15

HCP ZN 30
A =2.66 P= 2
A3=4.95 EP=13.5 DT= 320
T= 20 93 293
U2=.0020 .0060 .0110

G	VG	CIG(EL)	CIG(PHONON)			VIG
	16.64	.337				
000	13.55	1.741	.304	.569	.768	2.51
002	10.22	.126	.305	.561	.741	.86
100	4.87	.056	.151	.277	.365	.42
101	7.84	.083	.256	.470	.618	.70
102	3.80	.033	.145	.262	.340	.37
110	6.15	.039	.282	.497	.628	.66
112	5.42	.029	.275	.477	.589	.61
201	4.49	.022	.242	.413	.504	.52
104	2.51	.012	.138	.234	.284	.29
203	3.70	.013	.228	.375	.438	.45
114	4.07	.013	.260	.422	.487	.50
211	3.30	.009	.221	.353	.399	.41
006	3.61	.009	.251	.395	.440	.45
123	2.87	.006	.211	.323	.349	.35
205	2.76	.005	.209	.317	.338	.34
220	2.69	.003	.226	.323	.322	.32
132	1.21	.001	.108	.147	.139	.14

HCP Y 39
A =3.65 P= 2
A3=5.73 EP= 9.1 DT= 300**
T= 20 93 293
U2=.0016 .0022 .0055

G	VG	CIG(EL)	CIG(PHONON)			VIG
	15.22	.242				
000	11.49	1.755	.196	.238	.402	2.16
002	7.96	.073	.192	.233	.390	.46
100	4.32	.043	.098	.118	.198	.24
101	6.68	.060	.166	.200	.335	.39
102	3.03	.021	.095	.115	.190	.21
110	5.21	.031	.189	.228	.373	.40
112	4.35	.021	.189	.227	.366	.39
201	3.73	.018	.163	.196	.316	.33
104	1.80	.007	.091	.109	.173	.18
203	2.87	.011	.156	.186	.292	.30
114	3.00	.011	.180	.215	.333	.34
211	2.72	.010	.153	.183	.287	.30
006	2.41	.008	.171	.203	.305	.31
123	2.26	.007	.150	.178	.271	.28
205	2.01	.006	.147	.173	.259	.26
220	2.26	.007	.170	.200	.298	.30
132	1.01	.003	.083	.097	.141	.14

International Tables for X-ray Crystallography (1962). For those elements, where u_s^2 is not listed but only a Debye temperature Θ_D given, the expression

$$\overline{u_s^2} = \frac{\hbar^2}{k_B M_a \Theta_E} \left\{ \frac{1}{\exp(\Theta_E/T) - 1} + \frac{1}{2} \right\} \quad (15)$$

is used with an Einstein temperature $\Theta_E = \Theta_D/\sqrt{3}$.

In general, an analytical expression for u_s^2 such as that above does not cover the temperature range between 20°K and 300°K with a single Debye temperature. We, therefore, compute directly from the measured vibration amplitudes if possible.

In the case of compounds a unique Debye temperature is even more questionable for several reasons. But in the absence of something better, we use a Debye temperature and an atomic mass averaged over the

Table 1 (*cont.*)

HCP ZR 40
A =3.23 P= 2
A3=5.14 EP=10.9 DT= 269
T= 20 93 293
U2=.0015 .0025 .0067

G	VG	CIG(EL)	CIG(PHONON)			VIG
	21.01	.282				
000	15.49	2.516	.283	.386	.662	3.18
002	10.58	.088	.287	.389	.651	.74
100	5.69	.051	.138	.188	.319	.37
101	8.80	.070	.246	.333	.558	.63
102	3.97	.024	.138	.186	.308	.33
110	6.72	.034	.277	.372	.605	.64
112	5.57	.023	.264	.353	.566	.59
201	4.75	.019	.228	.304	.487	.50
104	2.30	.008	.128	.170	.266	.27
203	3.61	.012	.223	.294	.451	.46
114	3.78	.012	.250	.329	.496	.51
211	3.40	.011	.219	.288	.438	.45
006	3.02	.009	.241	.313	.449	.46
123	2.81	.008	.211	.276	.402	.41
205	2.50	.007	.206	.267	.379	.38
220	2.78	.008	.235	.304	.427	.43
132	1.23	.004	.115	.147	.199	.20

HCP TC 43
A =2.73 P= 2
A3=4.39 EP=13.9 DT= 300**
T= 20 93 293
U2=.0014 .0019 .0049

G	VG	CIG(EL)	CIG(PHONON)			VIG
	31.54	.347				
000	23.38	3.826	.509	.618	1.051	4.88
002	15.82	.118	.500	.604	1.008	1.12
100	8.44	.069	.254	.307	.513	.58
101	13.09	.092	.428	.517	.863	.95
102	5.89	.029	.250	.301	.491	.52
110	9.85	.038	.476	.572	.924	.96
112	8.08	.025	.462	.552	.875	.90
201	6.87	.021	.403	.482	.761	.78
104	3.30	.009	.226	.269	.414	.42
203	5.13	.013	.382	.453	.686	.70
114	5.34	.013	.435	.514	.764	.78
211	4.79	.012	.381	.451	.675	.68
006	4.23	.011	.412	.482	.682	.69
123	3.91	.010	.361	.424	.610	.62
205	3.47	.009	.352	.411	.575	.58
220	3.82	.010	.399	.465	.643	.65
132	1.68	.004	.194	.224	.299	.30

HCP RU 44
A =2.71 P= 1
A3=4.28 EP=10.1 DT= 413
T= 20 93 293
U2=.0008 .0011 .0025

G	VG	CIG(EL)	CIG(PHONON)			VIG
	29.55	.263				
000	24.30	4.660	.382	.472	.785	5.44
002	16.09	.130	.376	.463	.761	.89
100	8.61	.079	.191	.236	.388	.47
101	13.49	.102	.323	.398	.653	.75
102	6.15	.031	.189	.232	.378	.41
110	10.43	.039	.362	.444	.718	.76
112	8.54	.024	.358	.438	.699	.72
201	7.28	.020	.314	.384	.612	.63
104	3.45	.008	.173	.211	.332	.34
203	5.40	.012	.297	.361	.563	.57
114	5.58	.012	.338	.410	.632	.64
211	5.07	.011	.295	.359	.556	.57
006	4.37	.010	.324	.390	.586	.59
123	4.11	.009	.285	.344	.521	.53
205	3.61	.009	.276	.332	.495	.50
220	4.03	.010	.317	.380	.565	.57
132	1.77	.005	.154	.185	.269	.27

HCP CD 48
A =2.98 P= 2
A3=5.62 EP=11.3 DT= 146
T= 20 93 293
U2=.0027 .0066 .0200

G	VG	CIG(EL)	CIG(PHONON)			VIG
	18.29	.291				
000	15.92	2.278	.604	.976	1.613	3.89
002	12.49	.153	.590	.946	1.514	1.66
100	5.92	.066	.306	.485	.761	.82
101	9.63	.096	.518	.820	1.282	1.37
102	4.75	.036	.293	.460	.698	.73
110	7.67	.039	.571	.877	1.252	1.28
112	6.76	.027	.553	.839	1.149	1.17
201	5.58	.020	.476	.717	.962	.98
104	3.15	.011	.273	.410	.546	.55
203	4.58	.012	.458	.667	.816	.82
114	5.04	.012	.519	.751	.897	.90
211	4.03	.009	.442	.630	.717	.72
006	4.49	.009	.504	.713	.796	.80
123	3.49	.006	.426	.587	.608	.61
205	3.39	.006	.420	.576	.585	.59
220	3.23	.006	.457	.596	.517	.52
132	1.45	.003	.218	.276	.215	.22

HCP LA 57
A =3.75 P= 2
A3=6.06 EP= 8.6 DT= 142
T= 20 93 293
U2=.0018 .0044 .0145

G	VG	CIG(EL)	CIG(PHONON)			VIG
	19.31	.231				
000	14.60	2.477	.387	.645	1.159	3.64
002	10.56	.100	.383	.633	1.108	1.21
100	5.58	.057	.195	.321	.562	.62
101	8.73	.079	.328	.542	.949	1.02
102	4.04	.028	.189	.310	.528	.55
110	6.87	.039	.375	.610	1.014	1.05
112	5.80	.027	.377	.606	.970	.99
201	4.93	.023	.325	.521	.832	.85
104	2.45	.010	.179	.285	.444	.45
203	3.84	.014	.309	.488	.736	.75
114	4.06	.014	.348	.545	.803	.81
211	3.61	.012	.303	.476	.707	.72
006	3.32	.010	.338	.517	.706	.71
123	3.03	.009	.298	.458	.636	.64
205	2.73	.008	.290	.440	.587	.59
220	3.01	.009	.332	.500	.653	.66
132	1.35	.004	.163	.241	.297	.30

HCP CE 58
A =3.65 P= 2
A3=5.96 EP= 9.0 DT= 140
T= 20 93 293
U2=.0022 .0052 .0156

G	VG	CIG(EL)	CIG(PHONON)			VIG
	20.22	.238				
000	14.32	2.217	.484	.778	1.309	3.53
002	10.72	.111	.477	.761	1.247	1.35
100	5.61	.061	.242	.385	.631	.69
101	8.82	.087	.408	.651	1.066	1.15
102	4.13	.031	.235	.371	.592	.62
110	7.06	.043	.465	.727	1.132	1.17
112	6.01	.030	.467	.720	1.077	1.10
201	5.10	.025	.401	.619	.923	.94
104	2.57	.011	.222	.339	.493	.50
203	4.02	.015	.381	.576	.811	.82
114	4.27	.015	.436	.653	.892	.90
211	3.76	.014	.373	.561	.775	.79
006	3.53	.011	.418	.611	.775	.78
123	3.18	.010	.365	.535	.691	.70
205	2.89	.008	.358	.518	.640	.65
220	3.15	.009	.409	.586	.704	.71
132	1.41	.004	.198	.278	.314	.32

HCP PR 59
A =3.66 P= 2
A3=5.91 EP= 9.0 DT= 300**
T= 20 93 293
U2=.0010 .0014 .0035

G	VG	CIG(EL)	CIG(PHONON)			VIG
	19.93	.238				
000	14.20	2.178	.304	.372	.643	2.82
002	10.62	.113	.301	.367	.631	.74
100	5.60	.063	.153	.186	.320	.38
101	8.81	.089	.258	.314	.541	.63
102	4.13	.032	.149	.182	.310	.34
110	7.11	.046	.296	.361	.612	.66
112	6.06	.032	.299	.364	.611	.64
201	5.16	.026	.258	.313	.526	.55
104	2.57	.011	.143	.173	.289	.30
203	4.06	.016	.247	.299	.495	.51
114	4.30	.016	.284	.343	.563	.58
211	3.82	.014	.243	.294	.484	.50
006	3.54	.011	.276	.331	.533	.54
123	3.22	.010	.240	.289	.468	.48
205	2.92	.009	.237	.285	.455	.46
220	3.22	.009	.273	.328	.521	.53
132	1.44	.004	.133	.160	.250	.25

HCP ND 60
A =3.65 P= 2
A3=5.89 EP= 9.0 DT= 300**
T= 20 93 293
U2=.0010 .0013 .0034

G	VG	CIG(EL)	CIG(PHONON)			VIG
	19.90	.239				
000	14.27	2.251	.311	.381	.659	2.91
002	10.62	.118	.308	.376	.647	.76
100	5.61	.065	.156	.191	.328	.39
101	8.80	.094	.264	.322	.554	.65
102	4.13	.034	.153	.186	.318	.35
110	7.14	.048	.304	.369	.628	.68
112	6.10	.034	.307	.373	.627	.66
201	5.19	.028	.264	.321	.540	.57
104	2.60	.012	.146	.178	.296	.31
203	4.11	.017	.254	.307	.508	.52
114	4.36	.016	.291	.352	.579	.59
211	3.87	.015	.250	.302	.497	.51
006	3.60	.011	.283	.340	.548	.56
123	3.27	.011	.247	.297	.481	.49
205	2.96	.009	.243	.293	.468	.48
220	3.27	.010	.280	.337	.536	.54
132	1.47	.004	.137	.164	.257	.26

HCP GD 64
A =3.63 P= 2
A3=5.78 EP= 9.1 DT= 152
T= 20 93 293
U2=.0015 .0032 .0103

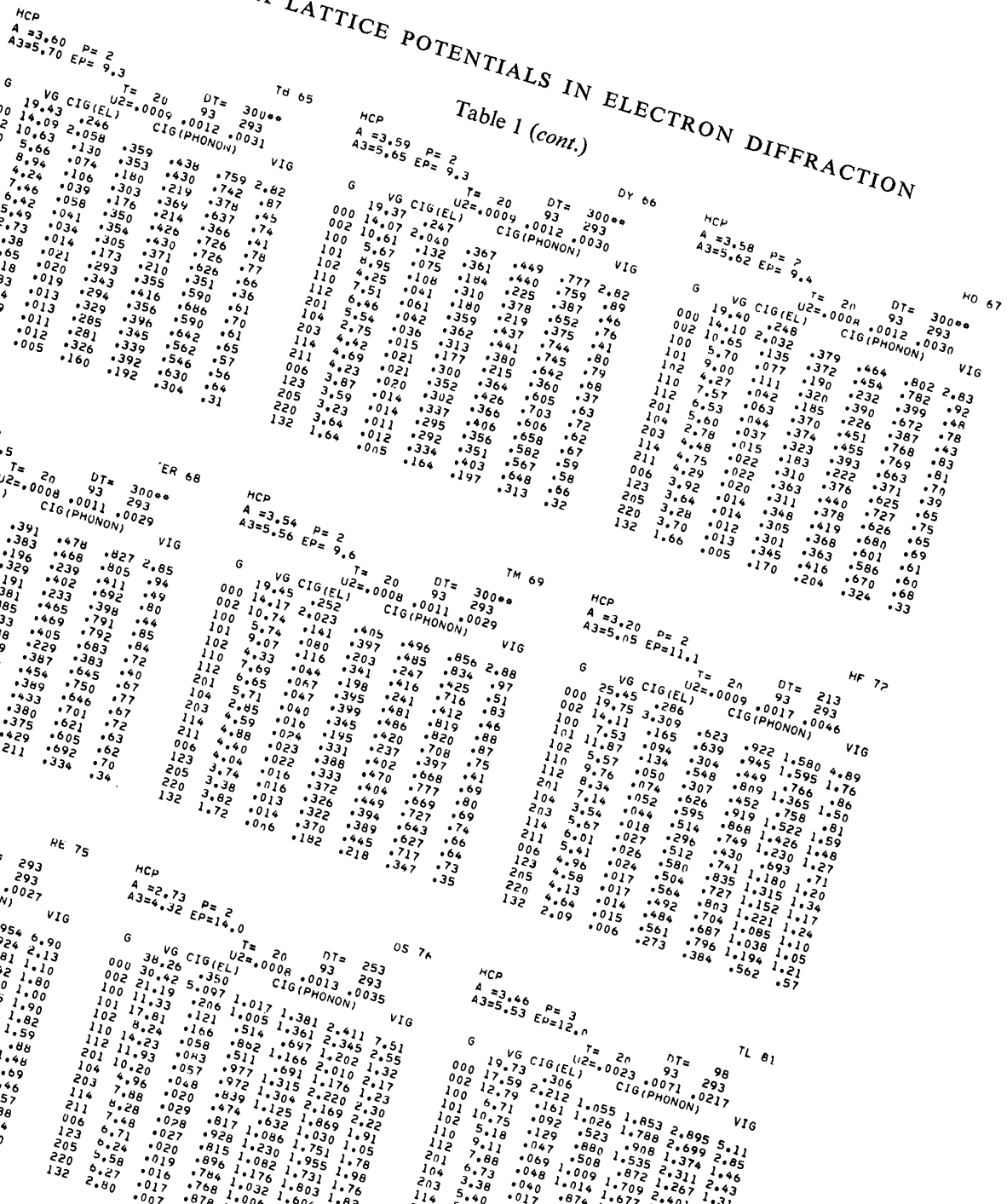
G	VG	CIG(EL)	CIG(PHONON)			VIG
	19.21	.242				
000	14.81	2.391	.474	.736	1.317	3.71
002	10.84	.123	.466	.720	1.269	1.39
100	5.77	.070	.238	.367	.645	.71
101	9.08	.099	.400	.618	1.089	1.19
102	4.26	.037	.232	.355	.613	.65
110	7.44	.054	.460	.703	1.193	1.24
112	6.36	.037	.464	.703	1.157	1.19
201	5.43	.031	.400	.606	.996	1.02
104	2.70	.013	.223	.335	.538	.55
203	4.31	.019	.381	.570	.900	.92
114	4.57	.018	.447	.663	1.015	1.03
211	4.09	.017	.375	.560	.874	.89
006	3.76	.013	.425	.620	.900	.91
123	3.46	.012	.369	.542	.804	.81
205	3.12	.010	.362	.527	.754	.76
220	3.49	.011	.418	.606	.856	.86
132	1.57	.004	.205	.293	.395	.40

constituents of the compound (of Na–Cl type) to compute $\overline{u_s^2}$ from equation (15). The Debye temperature is taken from *International Tables* (1962).

5. Discussion

For the purpose of the discussion of some general aspects of the complex lattice potentials in Tables 1 and 2 it is useful to divide the absorption potentials, V_g', by the structure potential V_g, whereby the structure effects (lattice type) and the dependence on the degree of close packing, *i.e.* on the value of the lattice constants, are cancelled out. Furthermore, only these ratios, V_g'/V_g and V_g'/V_0', enter the formulae of electron diffraction theory to any great extent.

Table 1 (*cont.*)



V_g itself represents the elastic scattering power of crystal in scattering electrons into the reflection **g**; depends on the lattice constant and on the atomic tering power of the atoms comprising the crystal. ly packed crystals (small a) have larger structure tials than loosely packed crystals. el)/V_g (see Tables and Fig. 2) decreases with in- g **g**, for a given substance. The main point is, however, that for a given **g**, C'_{0g}(el)/V_g does not vary noticeably with Z, being between 0·005 and 0·012 for practically all crystals in the lower range of reflections, which experimentally are the only important ones, the ratio does depend somewhat on the atom's place in the periodic system, as for alkali and rare gas crystals the values are highest (max. 0·016 for Ne–111), but it does not vary systemati-

Table 2. *Compound crystals (rock-salt type). Theoretical structure potentials, V_g, and Yoshioka absorption potentials, for* 100 keV *electrons, due to the excitation of crystal electrons* C_g^i(el) *and excitation of phonons* C_g^i(phonon) *at* $T=20°K$, 93 °K *and* 293 °K

V_g^i in the last row represents the total imaginary potential coefficient at 293 °K being the sum of the third and the sixth row.

Above the rows designated by C_g^i (phonon) the absolute temperature and mean-square vibration amplitude, u_g^2 (denoted by U2), pertaining to the three rows are given.

All real and imaginary lattice potentials are given in eV and with opposite signs, as they usually are negative quantities.

Absorption potentials and coefficients at electron energies other than 100 keV may be obtained with the help of the conversion factors given in Table 3.

3 LI +1 — 9 F -1 — LIF — A= 4.02 — DT= 650

G	VG	CIG(EL)	CIG(PHONON) T= 20 U2=.0050	CIG(PHONON) 93 .0052	CIG(PHONON) 293 .0088	VIG
000	13,61	1.202	.076	.077	.105	1.31
111	-3,87	-.041	-.069	-.070	-.095	-.14
200	4,29	.044	.071	.073	.098	.14
220	3,26	.019	.067	.068	.089	.11
311	-2,15	-.006	-.059	-.060	-.077	-.08
222	2,63	.010	.062	.063	.080	.09
400	2,20	.007	.057	.058	.072	.08
331	-1,46	-.001	-.050	-.051	-.062	-.06
422	1,65	.003	.049	.050	.058	.06
440	1,32	.002	.043	.043	.048	.05
620	1,10	.001	.037	.038	.039	.04
444	,94	.001	.033	.033	.032	.03
642	,82	.000	.029	.029	.027	.03
733	-,47	.000	-.023	-.023	-.019	-.02
662	,62	.000	.021	.021	.017	.02
664	,54	.000	.018	.018	.013	.01
933	-,32	.000	-.014	-.014	-.009	.00

3 LI +1 — 17 CL -1 — LICL — A= 5.14 — DT= 463

G	VG	CIG(EL)	CIG(PHONON) T= 20 U2=.0043	CIG(PHONON) 93 .0048	CIG(PHONON) 293 .0100	VIG
000	10,82	1.654	.094	.100	.153	1.81
111	-4,95	-.040	-.089	-.095	-.144	-.18
200	4,86	.036	.091	.098	.145	.18
220	3,55	.013	.086	.091	.133	.15
311	-2,61	-.003	-.081	-.086	-.123	-.13
222	2,78	.007	.082	.087	.123	.13
400	2,29	.005	.078	.083	.114	.12
331	-1,73	-.002	-.073	-.077	-.104	-.11
422	1,69	.004	.071	.075	.098	.10
440	1,35	.004	.066	.069	.085	.09
620	1,13	.003	.061	.063	.075	.08
444	,98	.003	.057	.059	.066	.07
642	,86	.003	.053	.055	.058	.06
733	-,60	-.002	-.047	-.049	-.048	-.05
662	,68	.002	.046	.046	.044	.05
664	,61	.002	.042	.042	.037	.04
933	-,43	-.001	-.037	-.037	-.030	-.03

3 LI +1 — 35 BR -1 — LIBR — A= 5.49 — DT= 387

G	VG	CIG(EL)	CIG(PHONON) T= 20 U2=.0025	CIG(PHONON) 93 .0030	CIG(PHONON) 293 .0069	VIG
000	11,40	1.980	.184	.205	.323	2.30
111	-6,09	-.068	-.182	-.203	-.316	-.38
200	5,89	.058	.179	.199	.311	.37
220	4,44	.028	.179	.198	.303	.33
311	-3,49	-.016	-.171	-.189	-.288	-.30
222	3,60	.019	.177	.195	.293	.31
400	3,04	.014	.169	.186	.277	.29
331	-2,50	-.010	-.166	-.183	-.268	-.28
422	2,37	.010	.164	.181	.259	.27
440	1,97	.008	.155	.170	.237	.24
620	1,71	.006	.150	.164	.221	.23
444	1,51	.005	.144	.156	.205	.21
642	1,36	.004	.138	.149	.190	.19
733	-1,07	-.002	-.131	-.141	-.171	-.17
662	1,11	.002	.127	.135	.159	.16
664	1,00	.002	.120	.127	.143	.14
933	-,81	.000	-.113	-.119	-.129	-.13

3 LI +1 — 53 I -1 — LII — A= 6.00 — DT= 331

G	VG	CIG(EL)	CIG(PHONON) T= 20 U2=.0019	CIG(PHONON) 93 .0025	CIG(PHONON) 293 .0060	VIG
000	12,12	2.432	.250	.292	.479	2.91
111	-7,33	-.084	-.245	-.285	-.466	-.55
200	6,95	.071	.247	.288	.469	.54
220	5,30	.034	.242	.282	.452	.49
311	-4,31	-.021	-.239	-.277	-.442	-.46
222	4,33	.023	.238	.275	.437	.46
400	3,69	.017	.238	.275	.430	.45
331	-3,15	-.012	-.231	-.267	-.413	-.43
422	2,91	.011	.228	.262	.399	.41
440	2,44	.008	.222	.255	.378	.39
620	2,12	.006	.215	.245	.354	.36
444	1,88	.005	.209	.238	.336	.34
642	1,69	.004	.201	.228	.314	.32
733	-1,37	-.002	-.194	-.218	-.290	-.29
662	1,36	.002	.189	.211	.273	.28
664	1,21	.002	.183	.203	.253	.25
933	-1,02	-.001	-.175	-.194	-.233	-.23

11 NA +1 — 9 F -1 — NAF — A= 4.61 — DT= 439

G	VG	CIG(EL)	CIG(PHONON) T= 20 U2=.0046	CIG(PHONON) 93 .0052	CIG(PHONON) 293 .0112	VIG
000	11,34	1.100	.083	.090	.136	1.24
111	-1,20	-.006	-.008	-.009	-.016	-.02
200	4,55	.062	.081	.087	.130	.19
220	3,71	.031	.078	.083	.120	.15
311	-,52	.002	-.006	-.007	-.011	.00
222	3,14	.018	.074	.079	.110	.13
400	2,71	.011	.071	.075	.102	.11
331	-,28	.001	-.004	-.005	-.008	.00
422	2,13	.005	.064	.067	.086	.09
440	1,75	.003	.058	.061	.072	.08
620	1,48	.002	.053	.055	.061	.06
444	1,28	.001	.048	.050	.051	.05
642	1,13	.000	.044	.045	.043	.04
733	-,03	.000	.000	.000	.000	.00
662	,86	.000	.035	.036	.028	.03
664	,75	.000	.031	.031	.022	.02
933	-,01	.000	.000	.000	.000	.00

11 NA +1 — 17 CL -1 — NACL — A= 5.63 — DT= 281

G	VG	CIG(EL)	CIG(PHONON) T= 20 U2=.0051	CIG(PHONON) 93 .0073	CIG(PHONON) 293 .0190	VIG
000	9,54	1.430	.101	.123	.202	1.63
111	-3,08	-.018	-.055	-.068	-.113	-.13
200	4,81	.052	.098	.119	.188	.24
220	3,75	.024	.094	.113	.172	.20
311	-1,52	.004	-.049	-.059	-.090	-.09
222	3,08	.014	.091	.109	.158	.17
400	2,62	.009	.087	.102	.143	.15
331	-,92	.002	-.045	-.053	-.072	-.07
422	2,02	.006	.080	.093	.119	.12
440	1,65	.004	.074	.085	.099	.10
620	1,40	.004	.069	.078	.083	.09
444	1,22	.003	.065	.071	.070	.07
642	1,09	.003	.061	.066	.059	.06
733	-,24	-.001	-.028	-.030	-.023	-.02
662	,86	.002	.052	.054	.039	.04
664	,76	.002	.048	.048	.030	.03
933	-,17	-.001	-.023	-.022	-.011	-.01

11 NA +1 — 35 BR -1 — NABR — A= 5.95 — DT= 200

G	VG	CIG(EL)	CIG(PHONON) T= 20 U2=.0041	CIG(PHONON) 93 .0074	CIG(PHONON) 293 .0210	VIG
000	10,06	1.698	.208	.285	.459	2.16
111	-4,24	-.043	-.172	-.234	-.369	-.41
200	5,61	.070	.205	.278	.433	.50
220	4,43	.036	.199	.268	.402	.44
311	-2,37	-.008	-.164	-.219	-.318	-.33
222	3,70	.023	.194	.258	.372	.40
400	3,19	.018	.192	.251	.347	.36
331	-1,64	-.005	-.156	-.203	-.271	-.28
422	2,54	.012	.181	.232	.296	.31
440	2,14	.009	.173	.217	.256	.26
620	1,86	.007	.165	.202	.219	.23
444	1,65	.005	.158	.190	.189	.19
642	1,49	.004	.151	.178	.163	.17
733	-,68	-.002	-.119	-.135	-.109	-.11
662	1,21	.003	.135	.150	.111	.11
664	1,09	.002	.127	.137	.088	.09
933	-,52	-.001	-.100	-.105	-.059	-.06

11 NA +1 — 53 I -1 — NAI — A= 6.46 — DT= 198

G	VG	CIG(EL)	CIG(PHONON) T= 20 U2=.0028	CIG(PHONON) 93 .0052	CIG(PHONON) 293 .0147	VIG
000	10,56	2.058	.265	.369	.614	2.67
111	-5,51	-.061	-.242	-.335	-.550	-.61
200	6,41	.080	.265	.366	.596	.68
220	5,07	.041	.260	.356	.567	.61
311	-3,22	-.013	-.237	-.322	-.502	-.52
222	4,24	.027	.254	.346	.538	.57
400	3,68	.020	.255	.344	.518	.54
331	-2,31	-.008	-.228	-.306	-.453	-.46
422	2,95	.013	.240	.320	.462	.47
440	2,50	.009	.233	.306	.419	.43
620	2,18	.007	.224	.291	.378	.39
444	1,94	.005	.217	.277	.343	.35
642	1,76	.004	.212	.267	.312	.32
733	-,99	-.002	-.186	-.230	-.249	-.25
662	1,42	.002	.196	.238	.244	.25
664	1,28	.002	.186	.222	.211	.21
933	-,74	-.001	-.165	-.192	-.169	-.17

19 K +1 — 9 F -1 — K F — A= 5.33 — DT= 333

G	VG	CIG(EL)	CIG(PHONON) T= 20 U2=.0044	CIG(PHONON) 93 .0056	CIG(PHONON) 293 .0137	VIG
000	11,38	1.242	.103	.119	.192	1.43
111	1,26	.012	.045	.051	.077	.09
200	5,10	.062	.100	.115	.181	.24
220	4,14	.027	.097	.112	.170	.20
311	,80	-.001	.042	.047	.068	.07
222	3,47	.015	.094	.107	.158	.17
400	2,97	.009	.090	.102	.145	.15
331	,55	-.001	.039	.043	.057	.06
422	2,30	.005	.084	.094	.125	.13
440	1,87	.003	.077	.086	.106	.11
620	1,57	.003	.072	.079	.091	.09
444	1,35	.002	.067	.073	.079	.08
642	1,19	.002	.063	.068	.068	.07
733	,19	.001	.027	.028	.025	.03
662	,92	.002	.054	.056	.047	.05
664	,81	.002	.050	.051	.038	.04
933	,15	.001	.022	.022	.015	.02

Table 2 (*cont.*)

19 K +1 — K CL
17 CL −1
A= 6.28 DT= 218
T= 20 93 293
U2=.0052 .0088 .0244

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	9.33	1.352	.107	.143	.239	1.59
111	-1.00	-.001	-.007	-.010	-.021	-.02
200	4.97	.059	.105	.140	.225	.28
220	4.01	.025	.102	.134	.206	.23
311	-.38	.002	-.005	-.008	-.014	-.01
222	3.35	.013	.098	.128	.189	.20
400	2.87	.008	.096	.123	.173	.18
331	-.18	.000	-.004	-.006	-.010	.00
422	2.22	.004	.089	.112	.144	.15
440	1.80	.003	.084	.103	.120	.12
620	1.52	.003	.079	.094	.100	.10
444	1.31	.003	.074	.087	.084	.09
642	1.15	.002	.070	.080	.071	.07
733	-.02	.000	-.002	-.002	-.002	.00
662	.90	.002	.062	.066	.046	.05
664	.80	.002	.057	.060	.035	.04
933	-.02	.000	-.001	-.002	.000	.00

19 K +1 — K BR
35 BR −1
A= 6.58 DT= 152
T= 20 93 293
U2=.0048 .0106 .0313

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	9.57	1.536	.195	.295	.469	2.00
111	-2.09	-.023	-.112	-.165	-.250	-.27
200	5.51	.074	.190	.285	.438	.51
220	4.49	.036	.190	.279	.407	.44
311	-1.15	-.007	-.106	-.152	-.210	-.22
222	3.80	.032	.185	.268	.373	.39
400	3.29	.015	.181	.257	.341	.36
331	-.80	-.006	-.103	-.143	-.179	-.18
422	2.61	.009	.171	.236	.285	.29
440	2.18	.007	.163	.218	.238	.24
620	1.87	.006	.157	.204	.200	.21
444	1.65	.005	.150	.189	.168	.17
642	1.48	.004	.145	.176	.141	.14
733	-.39	-.002	-.080	-.094	-.065	-.07
662	1.19	.003	.131	.147	.090	.09
664	1.07	.003	.123	.132	.068	.07
933	-.32	.000	-.069	-.072	-.032	-.03

19 K +1 — K I
53 I −1
A= 7.05 DT= 158
T= 20 93 293
U2=.0033 .0070 .0207

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	9.86	1.812	.239	.362	.597	2.41
111	-3.41	-.041	-.186	-.278	-.446	-.49
200	6.14	.081	.235	.353	.572	.65
220	4.99	.041	.239	.353	.552	.59
311	-2.00	-.011	-.177	-.261	-.398	-.41
222	4.23	.026	.227	.336	.515	.54
400	3.69	.018	.225	.329	.488	.51
331	-1.45	-.008	-.178	-.254	-.363	-.37
422	2.96	.011	.219	.314	.438	.45
440	2.49	.008	.212	.298	.392	.40
620	2.16	.006	.208	.286	.353	.36
444	1.91	.005	.198	.269	.313	.32
642	1.72	.004	.193	.256	.281	.28
733	-.69	-.002	-.145	-.187	-.188	-.19
662	1.39	.003	.179	.227	.213	.22
664	1.24	.002	.173	.213	.182	.18
933	-.54	.000	-.130	-.156	-.122	-.12

37 RB +1 — RBF
9 F −1
A= 5.63 DT= 238
T= 20 93 293
U2=.0034 .0054 .0147

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	12.19	1.506	.210	.270	.434	1.94
111	2.81	.039	.169	.214	.329	.37
200	6.04	.080	.206	.263	.414	.49
220	4.93	.039	.201	.255	.390	.43
311	1.83	.009	.159	.199	.290	.30
222	4.16	.024	.203	.255	.375	.40
400	3.61	.017	.194	.242	.347	.36
331	1.36	.006	.155	.191	.260	.27
422	2.86	.011	.186	.228	.307	.32
440	2.38	.008	.177	.214	.270	.28
620	2.05	.006	.169	.202	.239	.25
444	1.80	.005	.162	.190	.211	.22
642	1.62	.004	.156	.180	.187	.19
733	.64	.003	.121	.136	.128	.13
662	1.30	.003	.139	.156	.137	.14
664	1.16	.002	.132	.143	.114	.12
933	.51	.001	.105	.112	.081	.08

37 RB +1 — RBCL
17 CL −1
A= 6.56 DT= 176
T= 20 93 293
U2=.0040 .0079 .0230

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	9.78	1.471	.174	.249	.402	1.87
111	.25	.019	.088	.121	.175	.19
200	5.53	.074	.169	.242	.380	.45
220	4.54	.035	.170	.239	.361	.40
311	.43	.010	.085	.115	.158	.17
222	3.84	.020	.166	.231	.337	.36
400	3.32	.014	.162	.223	.314	.33
331	.45	.006	.085	.113	.145	.15
422	2.62	.009	.154	.208	.272	.28
440	2.17	.007	.149	.197	.238	.24
620	1.86	.006	.143	.185	.207	.21
444	1.63	.005	.138	.174	.181	.19
642	1.46	.005	.134	.165	.159	.16
733	.32	.002	.070	.083	.072	.07
662	1.17	.004	.122	.143	.113	.12
664	1.05	.003	.115	.131	.092	.10
933	.27	.000	.062	.068	.044	.05

37 RB +1 — RBBR
35 BR −1
A= 6.86 DT= 128
T= 20 93 293
U2=.0042 .0105 .0316

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	9.85	1.606	.244	.388	.608	2.21
111	-.86	-.002	-.009	-.018	-.037	-.04
200	5.94	.086	.239	.377	.572	.66
220	4.90	.044	.241	.372	.538	.58
311	-.34	.001	-.008	-.016	-.028	-.03
222	4.18	.028	.230	.354	.493	.52
400	3.65	.020	.227	.343	.457	.48
331	-.17	.000	-.007	-.013	-.021	-.02
422	2.93	.013	.220	.322	.391	.40
440	2.47	.010	.212	.301	.334	.34
620	2.15	.009	.207	.284	.287	.30
444	1.91	.007	.198	.265	.244	.25
642	1.72	.006	.193	.249	.208	.21
733	-.05	.000	-.004	-.006	-.005	.00
662	1.41	.005	.177	.212	.139	.14
664	1.28	.004	.168	.193	.109	.11
933	-.03	.000	-.003	-.004	-.002	.00

37 RB +1 — RBI
53 I −1
A= 7.32 DT= 108
T= 20 93 293
U2=.0040 .0113 .0346

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	9.95	1.822	.306	.516	.813	2.64
111	-2.24	-.022	-.119	-.202	-.321	-.34
200	6.41	.092	.302	.505	.769	.86
220	5.27	.048	.308	.501	.728	.78
311	-1.23	-.004	-.112	-.186	-.273	-.28
222	4.51	.031	.293	.475	.668	.70
400	3.95	.023	.290	.462	.621	.64
331	-.86	-.003	-.107	-.172	-.231	-.23
422	3.20	.015	.283	.436	.537	.55
440	2.71	.011	.273	.409	.461	.47
620	2.37	.009	.264	.383	.395	.40
444	2.11	.007	.256	.360	.339	.35
642	1.92	.006	.247	.337	.290	.30
733	-.37	.000	-.088	-.115	-.088	-.09
662	1.56	.004	.230	.290	.197	.20
664	1.42	.004	.220	.265	.156	.16
933	-.28	.000	-.078	-.089	-.045	-.04

47 AG +1 — AGCL
17 CL −1
A= 5.55 DT= 136
T= 20 93 293
U2=.0045 .0108 .0324

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	14.32	2.515	.438	.681	1.070	3.59
111	1.23	.055	.287	.425	.609	.66
200	9.18	.109	.426	.653	.973	1.08
220	7.33	.050	.417	.624	.870	.92
311	1.52	.021	.269	.388	.497	.52
222	6.13	.029	.414	.601	.778	.81
400	5.26	.019	.393	.560	.680	.70
331	1.41	.009	.261	.358	.402	.41
422	4.12	.010	.371	.504	.528	.54
440	3.38	.007	.349	.452	.408	.42
620	2.88	.006	.332	.409	.316	.32
444	2.51	.005	.312	.367	.243	.25
642	2.23	.005	.296	.331	.186	.19
733	.73	.001	.191	.199	.091	.09
662	1.76	.004	.260	.258	.093	.10
664	1.56	.004	.242	.223	.059	.06
933	.54	.001	.158	.136	.029	.03

47 AG +1 — AGBR
35 BR −1
A= 5.76 DT= 140
T= 20 93 293
U2=.0033 .0078 .0233

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	15.01	2.792	.463	.726	1.169	3.96
111	-.59	.025	.086	.127	.187	.21
200	9.89	.127	.454	.705	1.095	1.22
220	7.94	.063	.443	.679	1.009	1.07
311	.32	.009	.085	.123	.171	.18
222	6.68	.039	.433	.652	.927	.97
400	5.80	.027	.430	.635	.856	.88
331	.46	.001	.083	.117	.149	.15
422	4.62	.016	.406	.583	.715	.73
440	3.86	.012	.391	.542	.601	.61
620	3.33	.009	.376	.504	.506	.51
444	2.94	.007	.360	.468	.423	.43
642	2.64	.006	.345	.434	.354	.36
733	.21	.000	.066	.076	.052	.05
662	2.11	.004	.313	.363	.226	.23
664	1.89	.004	.295	.326	.172	.18
933	.13	.001	.057	.058	.025	.03

cally as a function of Z. This feature is remarkable since $C^I_{0g}(\mathrm{el})$ is a function of the inelastic atomic scattering factors, while V_g is proportional to the elastic scattering factors. Usually the ratio of total inelastic over elastic scattering cross sections decreases with the atomic number Z (Lenz, 1954).

As to the absolute values, $C^I_{0g}(\mathrm{el})$ $(\mathbf{g}\neq 0)$ gives only a small contribution to V^I_g at normal temperatures. It is more important for the lighter elements than for the heavy ones and it becomes more important at low temperatures where the phonon scattering is fading out.

APPENDIX

Evaluation of the integral

The integral

$$\mathscr{I} = \int_0^{2\pi} \frac{B(d\cos\varphi)}{c^2 - d^2\cos^2\varphi}\, d\varphi$$

Table 2 (*cont.*)

55 CS +1 — 9 F −1 — CSF — A= 6.01 DT= 184 — T= 20 93 293 — U2=.0030 .0058 .0168

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	13.55	1.904	.329	.467	.763	2.67
111	4.66	.061	.291	.409	.652	.71
200	7.21	.093	.325	.458	.731	.82
220	5.85	.045	.318	.444	.688	.73
311	2.96	.014	.284	.391	.586	.60
222	4.93	.029	.311	.430	.647	.68
400	4.28	.021	.311	.425	.615	.64
331	2.20	.009	.273	.369	.518	.53
422	3.41	.013	.295	.396	.539	.55
440	2.86	.009	.286	.376	.479	.49
620	2.48	.007	.274	.354	.422	.43
444	2.19	.005	.266	.337	.374	.38
642	1.97	.004	.254	.315	.329	.33
733	1.02	.003	.221	.267	.252	.25
662	1.58	.003	.233	.276	.242	.24
664	1.41	.002	.223	.257	.202	.20
933	.78	.001	.195	.218	.156	.16

12 MG +0 — 8 O +0 — MGO — A= 4.21 DT= 820 — T= 20 93 293 — U2=.0025 .0026 .0038

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	16.23	4.967	.081	.082	.104	5.07
111	1.26	−.002	.027	.027	.033	.03
200	7.11	.054	.077	.078	.099	.15
220	4.95	.026	.074	.075	.094	.12
311	.32	.007	.025	.025	.031	.04
222	3.90	.016	.070	.071	.088	.10
400	3.25	.010	.068	.068	.084	.09
331	.31	.004	.024	.024	.029	.03
422	2.46	.005	.062	.062	.075	.08
440	1.98	.003	.057	.057	.068	.07
620	1.66	.002	.053	.053	.062	.06
444	1.43	.001	.049	.049	.056	.06
642	1.25	.001	.046	.046	.051	.05
733	.21	.000	.016	.016	.018	.02
662	.96	.000	.038	.039	.041	.04
664	.84	.000	.035	.035	.036	.04
933	.15	.000	.013	.013	.013	.01

12 MG +2 — 8 O −2 — MGO — A= 4.21 DT= 820 — T= 20 93 293 — U2=.0025 .0026 .0038

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	17.94	1.703	.077	.078	.099	1.80
111	−2.78	−.008	−.012	−.012	−.017	−.03
200	5.95	.066	.074	.075	.095	.16
220	4.59	.030	.072	.072	.091	.12
311	−1.09	.005	−.009	−.009	−.012	.00
222	3.76	.017	.068	.069	.086	.10
400	3.18	.011	.065	.066	.081	.09
331	−.55	.003	−.006	−.006	−.008	.00
422	2.44	.005	.060	.060	.073	.08
440	1.98	.003	.055	.055	.066	.07
620	1.66	.002	.051	.051	.059	.06
444	1.43	.001	.047	.047	.054	.06
642	1.25	.001	.044	.044	.049	.05
733	−.05	.000	.000	.000	.000	.00
662	.96	.000	.037	.037	.040	.04
664	.84	.000	.034	.034	.035	.04
933	−.02	.000	.000	.000	.000	.00

82 PB +2 — 16 S −2 — PBS — A= 5.94 DT= 230 — T= 20 93 293 — U2=.0015 .0025 .0069

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	16.88	2.976	.466	.614	1.014	3.99
111	2.19	.042	.393	.512	.824	.91
200	9.95	.128	.462	.607	.994	1.12
220	7.94	.065	.456	.597	.965	1.03
311	2.31	.036	.393	.509	.799	.84
222	6.68	.042	.448	.585	.935	.98
400	5.81	.031	.455	.591	.926	.96
331	2.15	.020	.384	.496	.759	.78
422	4.65	.019	.437	.565	.863	.88
440	3.92	.014	.432	.553	.821	.83
620	3.40	.011	.420	.534	.771	.78
444	3.02	.009	.414	.523	.733	.74
642	2.72	.008	.406	.509	.694	.70
733	1.27	.004	.344	.427	.555	.56
662	2.20	.006	.383	.473	.601	.61
664	1.98	.005	.375	.458	.558	.56
933	.99	.003	.320	.386	.450	.45

82 PB +2 — 34 SE −2 — PBSE — A= 6.14 DT= 168 — T= 20 93 293 — U2=.0018 .0036 .0107

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	17.11	3.169	.537	.797	1.312	4.48
111	.58	.052	.314	.450	.696	.75
200	10.44	.143	.536	.791	1.283	1.43
220	8.39	.077	.528	.775	1.235	1.31
311	1.19	.024	.315	.448	.670	.69
222	7.11	.051	.519	.759	1.188	1.24
400	6.22	.038	.527	.764	1.164	1.20
331	1.23	.013	.309	.435	.629	.64
422	5.05	.025	.506	.726	1.068	1.09
440	4.30	.018	.500	.707	.997	1.01
620	3.77	.014	.480	.672	.914	.93
444	3.37	.011	.471	.651	.849	.86
642	3.05	.009	.462	.630	.789	.80
733	.76	.002	.278	.367	.422	.42
662	2.49	.007	.439	.581	.657	.66
664	2.26	.005	.424	.551	.586	.59
933	.59	.002	.257	.324	.320	.32

82 PB +2 — 52 TE −2 — PBTE — A= 6.44 DT= 139 — T= 20 93 293 — U2=.0019 .0044 .0133

G	VG	CIG(EL)	CIG(PHONON)			VIG
000	17.74	3.588	.586	.936	1.544	5.13
111	−1.64	.026	.177	.259	.362	.39
200	11.15	.150	.591	.937	1.513	1.66
220	8.92	.081	.582	.916	1.450	1.53
311	−.18	.017	.181	.263	.360	.38
222	7.55	.054	.572	.895	1.389	1.44
400	6.61	.041	.582	.901	1.355	1.40
331	.19	.009	.179	.259	.345	.35
422	5.39	.026	.550	.841	1.222	1.25
440	4.60	.019	.540	.813	1.126	1.14
620	4.04	.014	.526	.779	1.032	1.05
444	3.61	.011	.514	.749	.948	.96
642	3.27	.009	.507	.728	.877	.89
733	.30	.002	.165	.223	.240	.24
662	2.66	.006	.480	.663	.711	.72
664	2.40	.005	.463	.625	.626	.63
933	.26	.002	.155	.199	.183	.18

Table 3. *Conversion factors*

Conversion of absorption potentials for primary electron energies other than 100 keV is done by multiplying the tabulated values by the factor $v(100\text{ keV})/v(E)$. (v is the velocity of an electron of energy E.)

In order to obtain the frequently used absorption coefficients, $\mu_0 = -2m/(\hbar^2 k) \cdot C^i_{00}$ and $\Delta\mu_g = -2m/(\hbar^2 k) \cdot C_{0g}{}^i$, the Table also contains the factor by which the $C^i(100\text{ keV})$-values of Tables 1 and 2 must be multiplied to give the absorption coefficients at the required energy E.

E (keV)	$\frac{v(100\text{keV})}{v(E)}$	$\frac{\mu(E)}{C^i(100\text{ keV})}$ (10^5 cm^{-1}eV^{-1})
20	2·017	7·511
30	1·669	5·148
40	1·466	3·968
50	1·328	3·260
60	1·229	2·788
70	1·152	2·452
80	1·091	2·199
90	1·041	2·004
100	1·000	1·847
200	0·788	1·148
300	0·706	0·921
400	0·662	0·810
500	0·635	0·746

can be calculated in the closed form. Supposing $B(d\cos\varphi) = B(-d\cos\varphi)$, which is true for our application, the integral becomes

$$\mathcal{I} = \frac{1}{c}\int_0^{2\pi} \frac{B(d\cos\varphi)}{c + d\cos\varphi}\, d\varphi\,.$$

On introduction of the complex variable

$$z = \exp i\varphi;\quad \cos\varphi = (z+\bar{z})/2\,,$$

the integral is written as

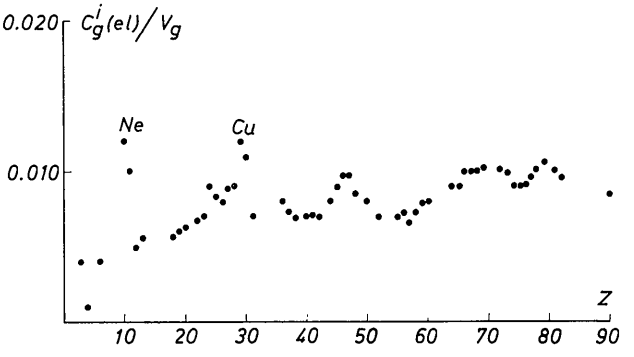


Fig. 2. $C^i{}_{0g}(\text{el})/V_g$ for the fixed value $|g| = 3.$ plotted *versus* Z.

$$\mathscr{I} = \frac{1}{ic}\oint \frac{B[d(z+\bar{z})/2]dz}{z[c+d(z+\bar{z})/2]} = \frac{2}{icd}\oint \frac{B[d(z+\bar{z})/2]dz}{z^2+2(c/d)z+1} .$$

Integration over the unit circle is carried out by means of the residue theorem. The zeros of the denominator

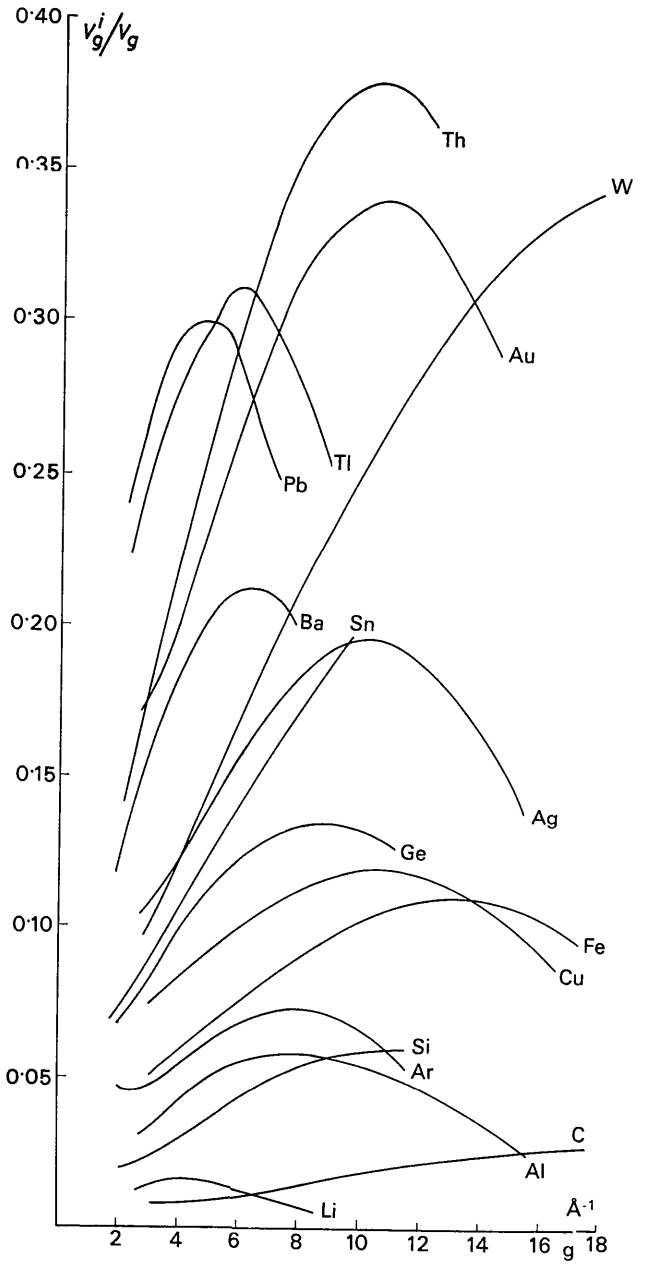


Fig. 3. V^i_g/V_g as a function of g for a number of monatomic crystals. The curves start at the lowest reflection g. The values at g = 0 are not drawn because the curves would overlap here, since C^i_{00} (plasmon) makes a δ-shaped contribution to V^i_g at g = 0.

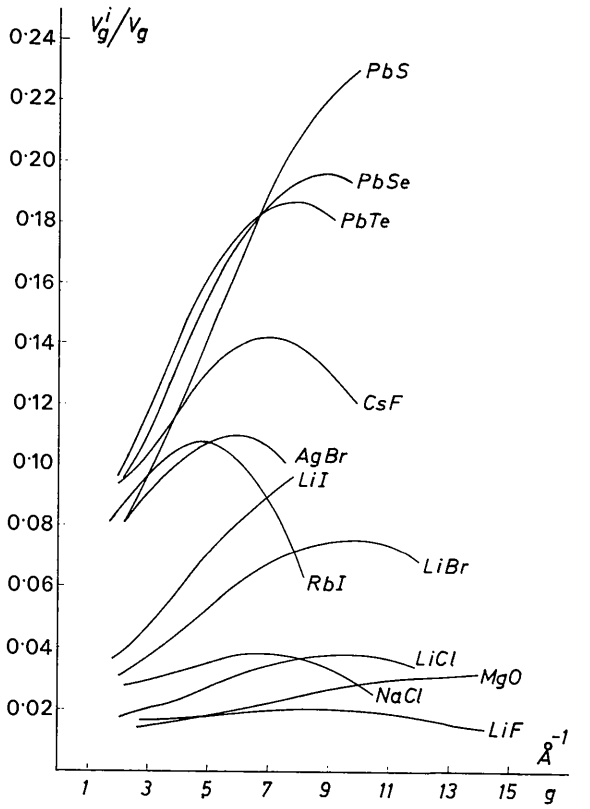


Fig. 4. As Fig. 3, but showing compounds of the NaCl-type.

occur at

$$z_\pm = -\frac{c}{d} \pm \sqrt{c^2/d^2-1}$$

assuming $c \geq d$. Of the two poles of the integrand only z_+ lies within the unit circle (on the real axis). This gives

$$\mathscr{I} = \frac{4\pi}{cd}\frac{B(dz_+)}{2z_+ + 2c/d} = \frac{2\pi}{c}\frac{B(-c+\sqrt{c^2-d^2})}{\sqrt{c^2-d^2}}$$

In our application

$$c = a^2+r^2$$
$$d = 2ar \quad (c \geq d)$$
$$\sqrt{c^2-d^2} = |a^2-r^2| ,$$

then

$$\mathscr{I} = \frac{2\pi B[-(a^2+r^2)+|a^2-r^2|]}{(a^2+r^2)\,|a^2-r^2|} .$$

The computations were carried out on the CDC 3300 at the Zentrum für Datenverarbeitung der Universität Tübingen.

The temperature dependence of V_g and C^i_{0g}(el) can be described in a satisfactory way (exact for a rigid-ion Einstein model) by multiplying the required potential

Table 4. *Comparison of theoretical and experimental values of* V_g^i *at* 300°K

The data refer to 100 keV electrons. Some of the experimental values have been extrapolated to 100 keV.

	g	V_g^i theor. (eV)	V_g^i exp. (eV)	References
MgO	000	1·80	1·50	Goodman & Lehmpfuhl (1967).
	200	0·16	{0·13 0·55	Authors referenced in Goodman & Lehmpfuhl.
Al	000	0·85	0·50	Hashimoto (1964). See also Metherell & Whelan (1967) and Watanabe (1965).
	111	0·18	0·23	
Cu	000	3·48	1·35	Goringe & Whelan (1966).
	111	0·83	0·81	
	200	0·79	0·92	
Si	000	0·70	0·68	Meyer-Ehmsen (1969).
	220	0·11	0·11	
	311	0·07	0·08	
	422	0·08	0·08	
Ge	000	1·56	1·25	Meyer-Ehmsen (1969).
	220	0·54	0·52	
	422	0·43	0·36	
NaCl	000	1·63		Graff & Gaukler (1969).
	220	0·20	0·21	
	420	0·14	0·15	

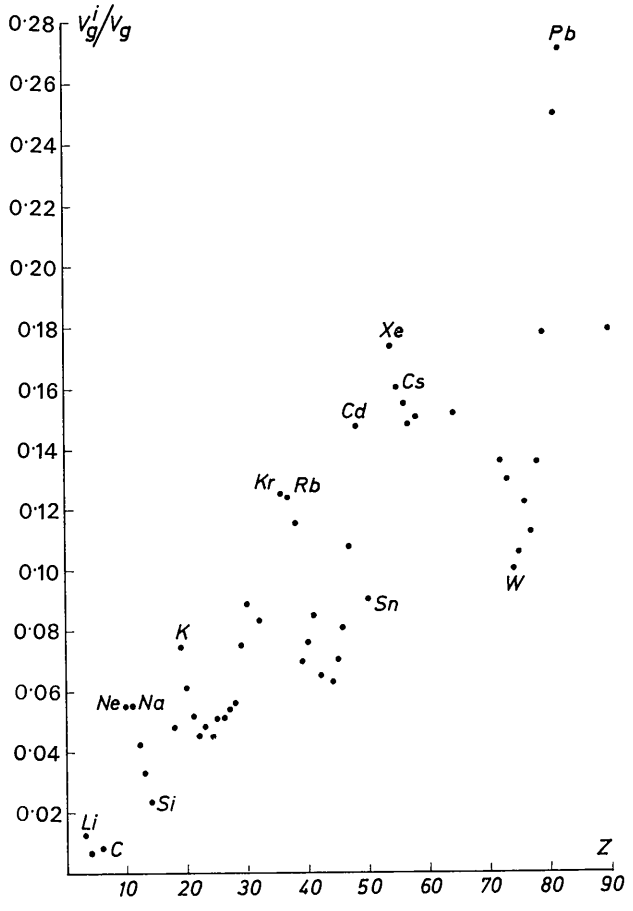


Fig. 5. V^i_g/V_g for the fixed value $|\mathbf{g}| = 3$ plotted *versus* Z.

with the corresponding Debye–Waller factor, exp $[-M(g)]$, as shown by Ohtsuki 1966).

The main contribution to V_g^i is from C^i_{0g} (phonon). Because of the properties of $C^i_{0g}(\text{el})/V_g$, the curves V_g^i/V_g given in Figs. 3, 4 and 5 can approximately be taken to be qualitatively the same as that for C^i_{0g} (phonon)$/V_g$ or, with an appropriate factor, $C^i_{0g}(\text{phonon})/C^i_{0g}(\text{el})$. The values of $C^i_{0g}(\text{phonon})/V_g$ increase with $\mathbf{g}$, with atomic weight and with temperature (see also Whelan, 1965*b* and Humphreys & Hirsch, 1968).

For a given crystal (Figs. 4 and 5), V_g^i/V_g increases approximately linearly with g (in the region of practical interest), goes through a maximum and falls again (to negative values at very high g).

For a given $\mathbf{g}$, the absorption parameter V_g^i/V_g increases in a rough linear way with the atomic weight, and therefore also with Z (see Fig. 5). The form of the plot is not as simple to explain as that of atomic radii, since the phonon scattering depends on the Debye temperature and therefore on structure effects. Crystals of the diamond type, for instance, are on the lower fringe, whereas alkali and rare gas crystals appear on the upper fringe of the plot. Nevertheless, a variation with position in the periodic system is evident.

The parameter V_g^i/V_0 (see Fig. 6 for some examples) is a measure of the 'localization' of the inelastic scattering probability at the atomic planes. Phonon scattering is strongly, and electron excitation weakly, localized (see also Whelan, 1965*a*,*b*). The parameter V_g^i/V_0^i determines the strength of the anomalous transmission effects.

A large part of V_0^i consists of the plasmon contribution, which is shown separately in Tables 1 and 2. It is not meant to represent an actual plasmon excitation of energy, EP, in every case, but rather to indicate the contribution, C^i_{00}(plasmon), of the 'free' electrons to C^i_{0g}(el) which also contains the contribution from single electron excitations.

In Table 2 the crystal MgO is listed twice, with different assumptions about the electron distributions within the crystal.

In Table 4 theoretical values in Tables 1 and 2 are compared with experimental values of V_g^i. Agreement is satisfactory in most cases. Exceptions at V_0^i may be due to theoretical assumptions about the minimum scattering wave vector while slight deviations at V_g^i may be partly explained on the experimental side, where evaluation is rendered difficult by complications such as, for instance, many-beam effects.

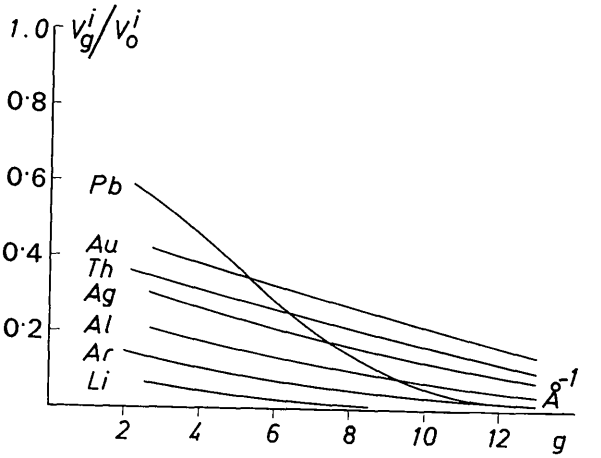


Fig. 6. V^i_g/V^i_0 as a function of g for some crystals.

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The Dynamical Scattering Amplitude of an Imperfect Crystal

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(*Received* 21 *February* 1969)

A formal expression for the X-ray dynamical scattering amplitude of an imperfect crystal is obtained. The resultant expression includes the dynamical line broadening effect on the diffracted X-rays caused by imperfections. The effects due to absorption in the crystal are also taken into account.

1. Introduction

In studying the problems of diffraction by crystals it is desirable to have a dynamical solution for diffracted beams because, even under a single Bragg condition, there are strong interactions between the crystal electrons and the beams. When the crystal is perfect, one uses the two-wave approximation to derive an approximate dynamical solution for a single Bragg reflection. When an incident beam satisfies several Bragg conditions simultaneously, one needs to employ 'more than two'-wave approximations which are sometimes only solvable by numerical computations.

There is no true dynamical theory for diffraction unless the multiple interaction is correctly treated. Since difficulty is encountered in obtaining dynamical solutions for a perfect crystal, greater difficulty is expected in seeking completely dynamical solutions for an imperfect crystal.

In electron diffraction where the multiple scattering is essential, a formal theory of dynamical diffraction has been formulated by Niehrs (1959*a*,*b*) and Fujimoto (1959, 1960). In this theory the scattering amplitude is completely dynamical in form. In practice, it is admittedly tedious to calculate the scattering amplitude to a great degree of accuracy. Nevertheless this am-