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Electron Scattering Factors of Ions and their Parameterization

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Abstract

Elastic electron scattering factors of 106 ions are represented in a parameterized form that separates the diverging Coulomb term due to ionic charge from the finite contribution of the remaining screened atomic field. This parameterization is shown to be very convenient for many-beam analysis of electron diffraction data and numerically more accurate for interpolating the electron scattering factors of ions in the region of small angles of scattering than the conventional methods of interpolation. Absorptive electron scattering factors have also been calculated numerically for a wide range of ions. It is found that these factors differ from those of the corresponding neutral atoms only for small angles of scattering with $s < 0.3$ Å^{-1}. For most applications of transmission electron diffraction, the effects of crystal ionicity on the absorptive crystal structure factors may therefore be neglected and the corresponding factors of neutral atoms may be used.

1. Introduction

For general dynamical electron diffraction calculations and in particular for reflection high-energy electron diffraction (RHEED) calculations, the most convenient way of representing electron atomic scattering factors is to fit the numerical values of these factors into a sum of Gaussians (Doyle &Turner, 1968):

$$f^{(e)}(s) = \sum_j a_j \exp(-b_j s^2), \tag{1}$$

where $s = \sin\theta/\lambda$, θ being the angle of scattering and λ being the electron wavelength, and a_j and b_j are fitting parameters. For the case of neutral atoms, these parameters have been tabulated for all the elements of the Periodic Table (Peng *et al.*, 1996). It is the purpose of the present paper to give such a table for ions and to investigate the effects of crystal ionicity on the absorptive crystal structure factors.

2. Electron scattering factors of ions and parameterization

The electron scattering amplitude of an ion is very different from that of a neutral atom. For X-ray diffraction, the atomic scattering factors of both neutral atoms and ions satisfy the condition (James, 1965)

$$Z_0 = \lim_{s\to 0} f^{(X)}(s), \tag{2}$$

where Z_0 is the number of electrons associated with each atom that can either be in a neutral or in a charged ionic state. For a neutral atom, $Z_0 = Z$, Z being the atomic number of the atom. For an ion, $Z_0 \neq Z$ and the difference between the two quantities represents the excess or deficiency of charge on the nucleus resulting from charge transfer associated with the formation of chemical bonds in the crystal (Cowley, 1992; Spence, 1993). The atomic scattering factor for electron diffraction is related to that for X-ray diffraction by the Mott formula (Mott & Massey, 1965):

$$f^{(e)}(s) = (m_0 e^2/8\pi^2\hbar^2)\{[Z - f^{(X)}(s)]/s^2\}, \tag{3}$$

where e is the electron charge, m_0 is the electron mass and $\hbar = h/(2\pi)$, with h being Planck's constant. For an ion where the number of electrons associated with the ion is not equal to the charge of the nucleus, $Z \neq Z_0$, it follows from equation (3) that as s approaches zero the scattering factor diverges as $\sim (Z - Z_0)/s^2$. It has been known for some years, see for example Doyle & Turner (1968), that the divergence of the electron scattering factor of an ion arises from the contribution of the unscreened long-range Coulomb potential of the ionic charge on the nucleus. This may be readily demonstrated by rearranging (3) as

$$\begin{aligned} f^{(e)}(s) &= (m_0 e^2/8\pi^2\hbar^2)\{[Z_0 - f^{(X)}(s)]/s^2\} \\ &\quad + (m_0 e^2/8\pi^2\hbar^2)(\Delta Z/s^2) \\ &= f_0^{(e)}(s) + (m_0 e^2/8\pi^2\hbar^2)(\Delta Z/s^2), \end{aligned} \tag{4}$$

where $\Delta Z = Z - Z_0$ represents the ionic charge and the second term on the right-hand side represents the divergent contribution from the unscreened Coulomb potential of the ionic charge. The first term on the right-hand side [*i.e.* $f_0^{(e)}(s)$] results from scattering of electrons by the screened atomic field. Condition (2) ensures that $f_0^{(e)}(s)$ remains finite in the limit $s \to 0$.

Electron scattering factors of ions have been calculated numerically and tabulated by several authors including Doyle & Turner (1968) and Rez *et al.* (1994).

Table 1. *Parameterization of the electron atomic scattering factors of ions*

Ion	Z	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	R (%)
H^{1-}	1	0.140E+0	0.649E+0	0.137E+1	0.337E+0	0.787E+0	0.984E+0	0.867E+1	0.389E+2	0.111E+3	0.166E+3	0.046
Li^{1+}	3	0.460E−2	0.165E−1	0.435E−1	0.649E−1	0.270E−1	0.358E−1	0.239E+0	0.879E+0	0.264E+1	0.709E+1	0.031
Be^{2+}	4	0.340E−2	0.103E−1	0.233E−1	0.325E−1	0.120E−1	0.267E−1	0.162E+0	0.531E+0	0.148E+1	0.388E+1	0.022
O^{1-}	8	0.205E+0	0.628E+0	0.117E+1	0.103E+1	0.290E+0	0.397E+0	0.264E+1	0.880E+1	0.271E+2	0.918E+2	0.012
O^{2-}	8	0.421E−1	0.210E+0	0.852E+0	0.182E+1	0.117E+1	0.609E−1	0.559E+0	0.296E+1	0.115E+2	0.377E+2	0.037
F^{1-}	9	0.134E+0	0.391E+0	0.814E+0	0.928E+0	0.347E+0	0.228E+0	0.147E+1	0.468E+1	0.132E+2	0.360E+2	0.013
Na^{1+}	11	0.256E−1	0.919E−1	0.297E+0	0.514E+0	0.199E+0	0.397E−1	0.287E+0	0.118E+1	0.375E+1	0.108E+2	0.018
Mg^{2+}	12	0.210E−1	0.672E−1	0.198E+0	0.368E+0	0.174E+0	0.331E−1	0.222E+0	0.838E+0	0.248E+1	0.675E+1	0.019
Al^{3+}	13	0.192E−1	0.579E−1	0.163E+0	0.284E+0	0.114E+0	0.306E−1	0.198E+0	0.713E+0	0.204E+1	0.525E+1	0.029
Si^{4+}	14	0.192E+0	0.289E+0	0.100E+0	−0.728E−1	0.120E−2	0.359E+0	0.196E+1	0.934E+1	0.111E+2	0.134E+2	0.055
Cl^{1-}	17	0.265E+0	0.596E+0	0.160E+1	0.269E+1	0.123E+1	0.252E+0	0.156E+1	0.621E+1	0.178E+2	0.478E+2	0.010
K^{1+}	19	0.199E+0	0.396E+0	0.928E+0	0.145E+1	0.450E+0	0.192E+0	0.110E+1	0.391E+1	0.975E+1	0.234E+2	0.013
Ca^{2+}	20	0.164E+0	0.327E+0	0.743E+0	0.116E+1	0.307E+0	0.157E+0	0.894E+0	0.315E+1	0.767E+1	0.177E+2	0.013
Sc^{3+}	21	0.163E+0	0.307E+0	0.716E+0	0.880E+0	0.139E+0	0.157E+0	0.899E+0	0.306E+1	0.705E+1	0.161E+2	0.013
Ti^{2+}	22	0.399E+0	0.104E+1	0.121E+1	−0.797E−1	0.352E+0	0.376E+0	0.274E+1	0.810E+1	0.142E+2	0.232E+2	0.009
Ti^{3+}	22	0.364E+0	0.919E+0	0.135E+1	−0.933E+0	0.589E+0	0.364E+0	0.267E+1	0.818E+1	0.118E+2	0.149E+2	0.013
Ti^{4+}	22	0.116E+0	0.256E+0	0.565E+0	0.772E+0	0.132E+0	0.108E+0	0.655E+0	0.238E+1	0.551E+1	0.123E+2	0.015
V^{2+}	23	0.317E+0	0.939E+0	0.149E+1	−0.131E+1	0.147E+1	0.269E+0	0.209E+1	0.722E+1	0.152E+2	0.176E+2	0.009
V^{3+}	23	0.341E+0	0.805E+0	0.942E+0	0.783E−1	0.156E+0	0.321E+0	0.223E+1	0.599E+1	0.134E+2	0.169E+2	0.020
V^{5+}	23	0.367E−1	0.124E+0	0.244E+0	0.723E+0	0.435E+0	0.330E−1	0.222E+0	0.824E+0	0.280E+1	0.670E+1	0.017
Cr^{2+}	24	0.237E+0	0.634E+0	0.123E+1	0.713E+0	0.859E−1	0.177E+0	0.135E+1	0.430E+1	0.122E+2	0.390E+2	0.011
Cr^{3+}	24	0.393E+0	0.105E+1	0.162E+1	−0.115E+1	0.407E+0	0.359E+0	0.257E+1	0.868E+1	0.110E+2	0.158E+2	0.011
Cr^{4+}	24	0.132E+0	0.292E+0	0.703E+0	0.692E+0	0.959E−1	0.109E+0	0.695E+0	0.239E+1	0.565E+1	0.147E+2	0.013
Mn^{2+}	25	0.576E−1	0.210E+0	0.604E+0	0.132E+1	0.659E+0	0.398E−1	0.284E+0	0.129E+1	0.423E+1	0.145E+2	0.034
Mn^{3+}	25	0.116E+0	0.523E+0	0.881E+0	0.589E+0	0.214E+0	0.117E−1	0.876E+0	0.306E+1	0.644E+1	0.143E+2	0.009
Mn^{4+}	25	0.381E+0	0.183E+1	−0.133E+1	0.995E+0	0.618E−1	0.354E+0	0.272E+1	0.347E+1	0.547E+1	0.161E+2	0.017
Fe^{2+}	26	0.307E+0	0.838E+0	0.111E+1	0.280E+0	0.277E+0	0.230E+0	0.162E+1	0.487E+1	0.107E+2	0.192E+2	0.016
Fe^{3+}	26	0.198E+0	0.387E+0	0.889E+0	0.709E+0	0.117E+0	0.154E+0	0.893E+0	0.262E+1	0.665E+1	0.180E+2	0.012
Co^{2+}	27	0.213E+0	0.488E+0	0.998E+0	0.828E+0	0.230E+0	0.148E+0	0.939E+0	0.278E+1	0.731E+1	0.207E+2	0.016
Co^{3+}	27	0.331E+0	0.487E+0	0.729E+0	0.608E+0	0.131E+0	0.267E+0	0.141E+1	0.289E+1	0.645E+1	0.158E+2	0.010
Ni^{2+}	28	0.338E+0	0.982E+0	0.132E+1	−0.356E+1	0.362E+1	0.237E+0	0.167E+1	0.573E+1	0.114E+2	0.121E+2	0.018
Ni^{3+}	28	0.347E+0	0.877E+0	0.790E+0	0.538E−1	0.192E+0	0.260E+0	0.171E+1	0.475E+1	0.751E+1	0.130E+2	0.011
Cu^{1+}	29	0.312E+0	0.812E+0	0.111E+1	0.794E+0	0.257E+0	0.201E+0	0.131E+1	0.380E+1	0.105E+2	0.282E+2	0.003
Cu^{2+}	29	0.224E+0	0.544E+0	0.970E+0	0.727E+0	0.182E+0	0.145E+0	0.933E+0	0.269E+1	0.711E+1	0.194E+2	0.013
Zn^{2+}	30	0.252E+0	0.600E+0	0.917E+0	0.663E+0	0.161E+0	0.161E+0	0.101E+1	0.276E+1	0.708E+1	0.190E+2	0.013
Ga^{3+}	31	0.391E+0	0.947E+0	0.690E+0	0.709E−1	0.653E−1	0.264E+0	0.165E+1	0.482E+1	0.107E+2	0.152E+2	0.014
Ge^{4+}	32	0.346E+0	0.830E+0	0.599E+0	0.949E−1	−0.217E−1	0.232E+0	0.145E+1	0.408E+1	0.132E+2	0.295E+2	0.016
Br^{1-}	35	0.125E+0	0.563E+0	0.143E+1	0.352E+1	0.322E+1	0.530E−1	0.469E+0	0.215E+1	0.111E+2	0.389E+2	0.057
Br^{1+}	37	0.368E+0	0.884E+0	0.114E+1	0.226E+1	0.881E+0	0.187E+0	0.112E+1	0.398E+1	0.109E+2	0.266E+2	0.012
Sr^{2+}	38	0.346E+0	0.804E+0	0.988E+0	0.189E+1	0.609E+0	0.176E+0	0.104E+1	0.359E+1	0.932E+1	0.214E+2	0.012
Y^{3+}	39	0.465E+0	0.923E+0	0.241E+1	−0.231E+1	0.248E+1	0.240E+0	0.143E+1	0.645E+1	0.997E+1	0.122E+2	0.018
Zr^{4+}	40	0.234E+0	0.642E+0	0.747E+0	0.147E+1	0.377E+0	0.113E+0	0.736E+0	0.254E+1	0.672E+1	0.147E+2	0.014
Nb^{3+}	41	0.377E+0	0.749E+0	0.129E+1	0.161E+1	0.481E+0	0.184E+0	0.102E+1	0.380E+1	0.944E+1	0.257E+2	0.008
Nb^{5+}	41	0.828E−1	0.271E+0	0.654E+0	0.124E+1	0.829E+0	0.369E−1	0.261E+0	0.957E+0	0.394E+1	0.944E+1	0.017
Mo^{3+}	42	0.401E+0	0.756E+0	0.138E+1	0.158E+1	0.497E+0	0.191E+0	0.106E+1	0.384E+1	0.938E+1	0.246E+2	0.007
Mo^{5+}	42	0.479E+0	0.846E+0	0.156E+2	−0.152E+2	0.160E+1	0.241E+0	0.146E+1	0.679E+1	0.713E+1	0.104E+2	0.011
Mo^{6+}	42	0.203E+0	0.567E+0	0.646E+0	0.116E+1	0.171E+0	0.971E−1	0.647E+0	0.228E+1	0.561E+1	0.124E+2	0.013
Ru^{3+}	44	0.428E+0	0.773E+0	0.155E+1	0.146E+1	0.486E+0	0.191E+0	0.109E+1	0.382E+1	0.908E+1	0.217E+2	0.006
Ru^{4+}	44	0.282E+0	0.653E+0	0.114E+1	0.153E+1	0.418E+0	0.125E+0	0.753E+0	0.285E+1	0.701E+1	0.175E+2	0.006
Rh^{3+}	45	0.352E+0	0.723E+0	0.150E+1	0.163E+1	0.499E+0	0.151E+0	0.878E+0	0.328E+1	0.816E+1	0.207E+2	0.006
Rh^{4+}	45	0.397E+0	0.725E+0	0.151E+1	0.119E+1	0.251E+0	0.177E+0	0.101E+1	0.362E+1	0.856E+1	0.189E+2	0.008
Pd^{2+}	46	0.935E+0	0.311E+1	0.246E+2	−0.436E+2	0.211E+2	0.393E+0	0.406E+1	0.431E+2	0.540E+2	0.698E+2	0.263
Pd^{4+}	46	0.348E+0	0.640E+0	0.122E+1	0.145E+1	0.427E+0	0.151E+0	0.832E+0	0.285E+1	0.659E+1	0.156E+2	0.012
Ag^{1+}	47	0.503E+0	0.940E+0	0.217E+1	0.199E+1	0.726E+0	0.199E+0	0.119E+1	0.405E+1	0.113E+2	0.324E+2	0.007
Ag^{2+}	47	0.431E+0	0.756E+0	0.172E+1	0.178E+1	0.526E+0	0.175E+0	0.979E+0	0.330E+1	0.824E+1	0.214E+2	0.014
Cd^{2+}	48	0.425E+0	0.745E+0	0.173E+1	0.174E+1	0.487E+0	0.168E+0	0.944E+0	0.314E+1	0.784E+1	0.204E+2	0.014
In^{3+}	49	0.417E+0	0.755E+0	0.159E+1	0.136E+1	0.451E+0	0.164E+0	0.960E+0	0.308E+1	0.703E+1	0.161E+2	0.007
Sn^{2+}	50	0.797E+0	0.213E+1	0.215E+1	−0.164E+1	0.272E+1	0.317E+0	0.251E+1	0.904E+1	0.242E+2	0.264E+2	0.006
Sn^{4+}	50	0.261E+0	0.642E+0	0.153E+1	0.136E+1	0.177E+0	0.957E−1	0.625E+0	0.251E+1	0.631E+1	0.159E+2	0.009
Sb^{3+}	51	0.552E+0	0.114E+1	0.187E+1	0.136E+1	0.414E+0	0.212E+0	0.142E+1	0.421E+1	0.125E+2	0.290E+2	0.009
Sb^{5+}	51	0.377E+0	0.588E+0	0.122E+1	0.118E+1	0.244E+0	0.151E+0	0.812E+0	0.240E+1	0.527E+1	0.119E+2	0.009
I^{1-}	53	0.901E+0	0.280E+1	0.561E+1	−0.869E+1	0.126E+2	0.312E+0	0.259E+1	0.141E+2	0.344E+2	0.395E+2	0.060
Cs^{1+}	55	0.587E+0	0.140E+1	0.187E+1	0.348E+1	0.167E+1	0.200E+0	0.138E+1	0.412E+1	0.130E+2	0.318E+2	0.011
Ba^{2+}	56	0.733E+0	0.205E+1	0.230E+2	−0.152E+3	0.134E+3	0.258E+0	0.196E+1	0.118E+2	0.144E+2	0.149E+2	0.025
La^{3+}	57	0.493E+0	0.110E+1	0.150E+1	0.270E+1	0.108E+1	0.167E+0	0.111E+1	0.311E+1	0.961E+1	0.212E+2	0.012
Ce^{3+}	58	0.560E+0	0.135E+1	0.159E+1	0.263E+1	0.706E+0	0.190E+0	0.130E+1	0.393E+1	0.107E+2	0.238E+2	0.004

Table 1 (*cont.*)

Ion	Z	a_1	a_2	a_3	a_4	a_5	b_1	b_2	b_3	b_4	b_5	R (%)
Ce^{4+}	58	0.483E+0	0.109E+1	0.134E+1	0.245E+1	0.797E+0	0.165E+0	0.110E+1	0.302E+1	0.885E+1	0.188E+2	0.013
Pr^{3+}	59	0.663E+0	0.173E+1	0.235E+1	0.351E+0	0.159E+1	0.226E+0	0.161E+1	0.633E+1	0.110E+2	0.169E+2	0.017
Pr^{4+}	59	0.521E+0	0.119E+1	0.133E+1	0.236E+1	0.690E+0	0.177E+0	0.117E+1	0.328E+1	0.894E+1	0.193E+2	0.008
Nd^{3+}	60	0.501E+0	0.118E+1	0.145E+1	0.253E+1	0.920E+0	0.162E+0	0.108E+1	0.306E+1	0.880E+1	0.196E+2	0.012
Pm^{3+}	61	0.496E+0	0.120E+1	0.147E+1	0.243E+1	0.943E+0	0.156E+0	0.105E+1	0.307E+1	0.856E+1	0.192E+2	0.004
Sm^{3+}	62	0.518E+0	0.124E+1	0.143E+1	0.240E+1	0.781E+0	0.163E+0	0.108E+1	0.311E+1	0.852E+1	0.191E+2	0.012
Eu^{2+}	63	0.613E+0	0.153E+1	0.184E+1	0.246E+1	0.714E+0	0.190E+0	0.127E+1	0.418E+1	0.107E+2	0.262E+2	0.005
Eu^{3+}	63	0.496E+0	0.121E+1	0.145E+1	0.236E+1	0.774E+0	0.152E+0	0.101E+1	0.295E+1	0.818E+1	0.185E+2	0.013
Gd^{3+}	64	0.490E+0	0.119E+1	0.142E+1	0.230E+1	0.795E+0	0.148E+0	0.974E+0	0.281E+1	0.778E+1	0.177E+2	0.013
Tb^{3+}	65	0.503E+0	0.122E+1	0.142E+1	0.224E+1	0.710E+0	0.150E+0	0.982E+0	0.286E+1	0.777E+1	0.177E+2	0.013
Dy^{3+}	66	0.503E+0	0.124E+1	0.144E+1	0.217E+1	0.643E+0	0.148E+0	0.970E+0	0.288E+1	0.773E+1	0.176E+2	0.013
Ho^{3+}	67	0.456E+0	0.117E+1	0.143E+1	0.215E+1	0.692E+0	0.129E+0	0.869E+0	0.261E+1	0.724E+1	0.167E+2	0.013
Er^{3+}	68	0.522E+0	0.128E+1	0.146E+1	0.205E+1	0.508E+0	0.150E+0	0.964E+0	0.293E+1	0.772E+1	0.178E+2	0.013
Tm^{3+}	69	0.475E+0	0.120E+1	0.142E+1	0.205E+1-	0.584E+0	0.132E+0	0.864E+0	0.260E+1	0.709E+1	0.166E+2	0.014
Yb^{2+}	70	0.508E+0	0.137E+1	0.176E+1	0.223E+1	0.584E+0	0.136E+0	0.922E+0	0.312E+1	0.872E+1	0.237E+2	0.006
Yb^{3+}	70	0.498E+0	0.122E+1	0.139E+1	0.197E+1	0.559E+0	0.138E+0	0.881E+0	0.263E+1	0.699E+1	0.163E+2	0.012
Lu^{3+}	71	0.483E+0	0.121E+1	0.141E+1	0.194E+1	0.522E+0	0.131E+0	0.845E+0	0.257E+1	0.688E+1	0.162E+2	0.013
Hf^{4+}	72	0.522E+0	0.122E+1	0.137E+1	0.168E+1	0.312E+0	0.145E+0	0.896E+0	0.274E+1	0.691E+1	0.161E+2	0.006
Ta^{5+}	73	0.569E+0	0.126E+1	0.979E+0	0.129E+1	0.551E+0	0.161E+0	0.972E+0	0.276E+1	0.540E+1	0.109E+2	0.008
W^{6+}	74	0.181E+0	0.873E+0	0.118E+1	0.148E+1	0.562E+0	0.118E−1	0.442E+0	0.152E+1	0.435E+1	0.942E+1	0.005
Os^{4+}	76	0.586E+0	0.131E+1	0.163E+1	0.171E+1	0.540E+0	0.155E+0	0.938E+0	0.319E+1	0.784E+1	0.193E+2	0.005
Ir^{3+}	77	0.692E+0	0.137E+1	0.180E+1	0.197E+1	0.804E+0	0.182E+0	0.104E+1	0.347E+1	0.851E+1	0.212E+2	0.004
Ir^{4+}	77	0.653E+0	0.129E+1	0.150E+1	0.174E+1	0.683E+0	0.174E+0	0.992E+0	0.314E+1	0.722E+1	0.172E+2	0.006
Pt^{2+}	78	0.872E+0	0.168E+1	0.263E+1	0.193E+1	0.475E+0	0.223E+0	0.135E+1	0.499E+1	0.136E+2	0.330E+2	0.005
Pt^{4+}	78	0.550E+0	0.121E+1	0.162E+1	0.195E+1	0.610E+0	0.142E+0	0.833E+0	0.281E+1	0.721E+1	0.177E+2	0.005
Au^{1+}	79	0.811E+0	0.157E+1	0.263E+1	0.268E+1	0.998E+0	0.201E+0	0.118E+1	0.425E+1	0.121E+2	0.344E+2	0.006
Au^{3+}	79	0.722E+0	0.139E+1	0.194E+1	0.194E+1	0.699E+0	0.184E+0	0.106E+1	0.358E+1	0.856E+1	0.204E+2	0.007
Hg^{1+}	80	0.796E+0	0.156E+1	0.272E+1	0.276E+1	0.118E+1	0.194E+0	0.114E+1	0.421E+1	0.124E+2	0.362E+2	0.005
Hg^{2+}	80	0.773E+0	0.149E+1	0.245E+1	0.223E+1	0.570E+0	0.191E+0	0.112E+1	0.400E+1	0.108E+2	0.276E+2	0.005
Tl^{1+}	81	0.820E+0	0.157E+1	0.278E+1	0.282E+1	0.131E+1	0.197E+0	0.116E+1	0.423E+1	0.127E+2	0.357E+2	0.004
Tl^{3+}	81	0.836E+0	0.143E+1	0.394E+0	0.251E+1	0.150E+1	0.208E+0	0.120E+1	0.257E+1	0.486E+1	0.135E+2	0.015
Pb^{2+}	82	0.755E+0	0.144E+1	0.248E+1	0.245E+1	0.103E+1	0.181E+0	0.105E+1	0.375E+1	0.106E+2	0.279E+2	0.004
Pb^{4+}	82	0.583E+0	0.114E+1	0.160E+1	0.206E+1	0.662E+0	0.144E+0	0.796E+0	0.258E+1	0.622E+1	0.148E+2	0.004
Bi^{3+}	83	0.708E+0	0.135E+1	0.228E+1	0.218E+1	0.797E+0	0.170E+0	0.981E+0	0.344E+1	0.941E+1	0.237E+2	0.007
Bi^{5+}	83	0.654E+0	0.118E+1	0.125E+1	0.166E+1	0.778E+0	0.162E+0	0.905E+0	0.268E+1	0.514E+1	0.112E+2	0.007
Ra^{2+}	88	0.911E+0	0.165E+1	0.253E+1	0.362E+1	0.158E+1	0.204E+0	0.126E+1	0.403E+1	0.126E+2	0.300E+2	0.005
Ac^{3+}	89	0.915E+0	0.164E+1	0.226E+1	0.318E+1	0.125E+1	0.205E+0	0.128E+1	0.392E+1	0.113E+2	0.251E+2	0.005
U^{3+}	92	0.114E+1	0.248E+1	0.361E+1	0.113E+1	0.900E+0	0.250E+0	0.184E+1	0.739E+1	0.180E+2	0.227E+2	0.007
U^{4+}	92	0.109E+1	0.232E+1	0.120E+2	−0.911E+1	0.215E+1	0.243E+0	0.175E+1	0.779E+1	0.831E+1	0.165E+2	0.005
U^{6+}	92	0.687E+0	0.114E+1	0.183E+1	0.253E+1	0.957E+0	0.154E+0	0.861E+0	0.258E+1	0.770E+1	0.159E+2	0.003

In principle, *ab initio* numerical values obtained by the above authors may be fitted using the same analytical form (1) as for neutral atoms. However, since expression (1) *does not* diverge for the zero angle of scattering as it should do for an ion, it is not suitable for accurate fitting of ionic scattering factors [for a discussion of the errors introduced by this procedure, see Peng *et al.* (1998)]. Instead the electron scattering factor of an ion is represented as

$$f^{(e)}(s) = \sum_j a_j \exp(-b_j s^2) + (m_0 e^2/8\pi^2\hbar^2)(\Delta Z/s^2), \quad (5)$$

in which the finite scattering amplitude of the electron by the screened atomic field $f_0^{(e)}(s)$ is represented as a sum of Gaussians. In equation (5), the pre-factor of the second term $(m_0 e^2)/(8\pi^2\hbar^2) = 0.023934$ if s is given in Å^{-1} and $f^{(e)}(s)$ is in Å. The parameterization is made using the method of simulated annealing and the computer program developed by Peng and Ren, for details see Peng *et al.* (1996). This program can be obtained free of charge by contacting Lian-Mao Peng at lmpeng@lmplab.blem.ac.cn. In a general case where a crystal is characterized by an intermediate degree of ionicity α, the electron scattering factor may be expressed as

$$f^{(e)}(s) = (1-\alpha) f^{(e)}_{\text{neutral}}(s) + \alpha f^{(e)}_{\text{ion}}(s), \quad (6)$$

where $f^{(e)}_{\text{neutral}}(s)$ and $f^{(e)}_{\text{ion}}(s)$ are scattering factors of neutral atoms and their ions, respectively. A recent study of RHEED from the (100) surface of NiO shows that this scheme works well in describing experimental electron diffraction data by planes parallel to the surface (Peng *et al.*, 1997). The absorptive scattering factors of ions may be calculated numerically following the procedure of Hall & Hirsch (1965) and parameterized as for the neutral atoms (Peng *et al.*, 1996).

3. Results

Table 1 contains sets of five fitting parameters a_i and b_i tabulated for 106 ions spanning over the entire Periodic Table. In most cases, we used *ab initio* data for X-ray scattering factors of ions calculated by Rez *et al.* (1994). For large angles of scattering, these numerical data were converted into electron scattering factors using the Mott formula (3). For small angles of scattering where X-ray data are less reliable (see for example Peng & Cowley, 1988), we fit $f_0^{(e)}(s)$ at zero angle to the value given in Table 7 of Rez *et al.* (1994). It needs to be pointed out that in this table the number of electrons associated with Pd^{2+} should have been equal to 44 rather than to 45, and in our Table 1 this misprint has now been corrected. For ions where no recent *ab initio* data are available, we used the comprehensive tabulation of Cowley (1992). Numerical electron scattering factors of 59 ions were taken from his Table 4.3.1.2 (Cowley, 1992). Values of $f_0^{(e)}(s)$ were first separated from the values given by Cowley (1992) and then they were fitted to a linear combination of five Gaussians by using equation (5). In doing this, we found several data points that displayed anomalous deviation from the rest of the data, and Fig. 1 shows three fitted curves of electron scattering factors of $f_0^{(e)}(s)$ for Ge^{4+}, Pt^{4+} and Hg^{1+} ions together with numerical data taken from Cowley's (1992) table. These curves suggest that in Cowley (1992) several data points have been misprinted, and these include data for Ge^{4+} at $s = 0.15$, Pt^{4+} at $s = 0.32$ and Hg^{1+} at $s = 0.11$. These data points have been identified and subsequently neglected in our fitting. To illustrate the goodness of the fit, Table 1 also shows values of the R factor defined as

$$R = \sum_i \left| f_0^{(e)}(s_i) - \sum_j a_j \exp(-b_j s_i^2) \right| \Big/ \sum_i |f_0^{(e)}(s_i)|, \quad (7)$$

where i indexes the data points. Table 1 shows that for all the ions the R factors are smaller than 1.0×10^{-3}, the only exception being the case of Pd^{2+}. Further analysis revealed that the values of X-ray scattering factors given in Table 2 of Rez *et al.* (1994) for small s are too large to be interpolated smoothly to the value of $f_0^{(e)}(0)$ given in Table 7 from the same source. We have therefore disregarded numerical data at $s = 0.05$ and fitted the rest by expression (5). Although visually one cannot distinguish *ab initio* numerical data from fitted data, the R factor shows that the accuracy of fitting in this case is an order of magnitude worse than for other ions. This suggests that for this particular ion the numerical data given in Rez *et al.* (1994) may not be sufficiently accurate.

Fig. 2 shows the absorptive scattering factors for neutral atoms Mg and O and their ions Mg^{2+} and O^{2-}. The calculations were made for a primary-beam energy of 100 keV and room-temperature Debye–Waller factors of $B_{Mg} = 0.305$ and $B_O = 0.340$ (Zuo *et al.*, 1997). For neutral atoms, the results were obtained both by direct intergration and by Bird & King's (1990) *ATOM* routine. It is seen that for the whole range of scattering angles our results agree well with those of Bird & King. The absorptive scattering factors of Mg^{2+} and O^{2-} ions are seen to deviate from those of neutral atoms Mg and O only for small values of s. Numerical calculations have also been carried out for other ions and Debye–Waller factors. In general, the absorptive scattering factors of ions differ from those of neutral atoms appreciably only for $s < 0.3$ Å^{-1}. Since for most materials the lattice spacings are smaller than 1.5 Å, we expect therefore that for most transmission electron diffraction (TED) applications the effects of crystal ionicity on the absorptive scattering factors are negligible, and this is consistent with the accurate measure-

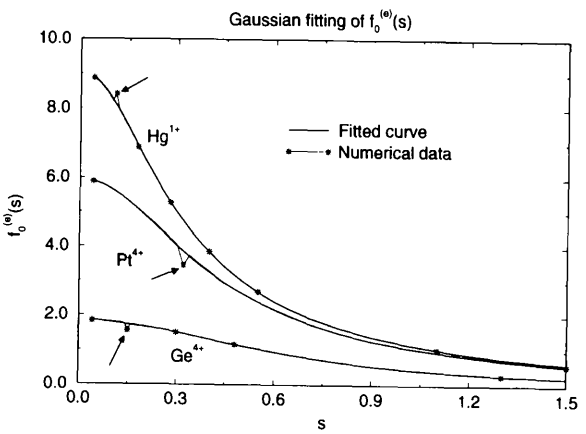

Fig. 1. Numerical and analytically fitted electron atomic scattering factors $f_0^{(e)}(s)$ for Ge^{4+}, Pt^{4+} and Hg^{1+} ions. These curves show that there exist three numerical data points that are well off the rest of the data, suggesting that these are misprints in *International Tables for X-ray Crystallography*.

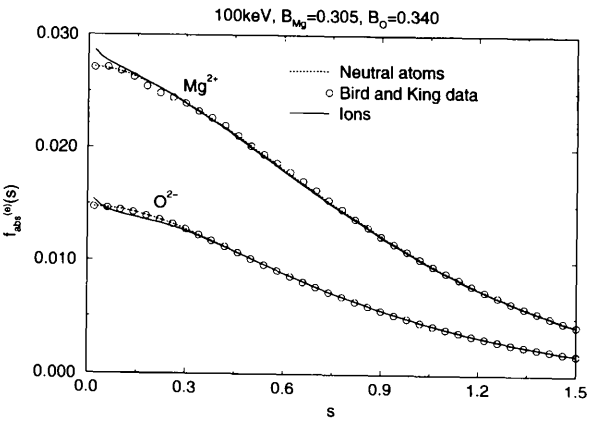

Fig. 2. Numerical absorptive electron atomic scattering factors $f_{abs}^{(e)}(s)$ for neutral atoms Mg and O and their ions Mg^{2+} and O^{2-}. The solid lines in the figure were calculated for ions and dotted curves were calculated for neutral atoms by direct numerical integration. The Bird & King data were obtained using the computer program *ATOM* (Bird & King, 1990).

ment of crystal structure factors of MgO (Zuo *et al.*, 1997).

4. Conclusions

In summary, elastic electron scattering factors of 106 ions have been represented in a parameterized form suitable for many-beam analysis of high-energy electron diffraction. The analytical representation of electron scattering factors of ions provides a more convenient and numerically more accurate way of interpolating these factors in the region of small angles of scattering than conventional cubic splines or linear interpolation. In particular, the new parameterization is shown to be capable of identifying values of the scattering factors misprinted in previous publications.

The absorptive electron scattering factors have been calculated for a wide range of ions and Debye–Waller factors. It is found that the absorptive scattering factors of ions differ appreciably from that of corresponding neutral atoms only for $s < 0.3$ Å^{-1}, and for most TED applications the effects of crystal ionicity on the absorptive crystal structure factors are negligible.

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References

Bird, D. & King, Q. (1990). *Acta Cryst.* A**46**, 202–208.
Cowley, J. M. (1992). In *International Tables for Crystallography*, Vol. C, edited by A. J. C. Wilson. Dordrecht/Boston/London: Kluwer Academic Publishers.
Doyle, P. & Turner, P. (1968). *Acta Cryst.* A**24**, 390–397.
Hall, C. & Hirsch, P. (1965). *Proc. R. Soc. London Ser. A*, **286**, 158–177.
James, R. (1965). *The Optical Principles of the Diffraction of X-rays*. London: Bell.
Mott, N. & Massey, H. (1965). *The Theory of Atomic Collisions*. Oxford: Clarendon Press.
Peng, L.-M. & Cowley, J. (1988). *Acta Cryst.* A**44**, 1–5.
Peng, L.-M., Dudarev, S. & Whelan, M. (1997). *Phys. Rev. B*, **56**, 15314–15319.
Peng, L.-M., Dudarev, S. & Whelan, M. (1998). *Phys. Rev. B*, **57**, 7259–7265.
Peng, L.-M., Ren, G., Dudarev, S. & Whelan, M. (1996). *Acta Cryst.* A**52**, 257–276.
Rez, D., Rez, P. & Grant, I. (1994). *Acta Cryst.* A**50**, 481–497.
Spence, J. (1993). *Acta Cryst.* A**49**, 231–260.
Zuo, J., O'Keeffe, M., Rez, P. & Spence, J. (1997). *Phys. Rev. Lett.* **78**, 4777–4780.