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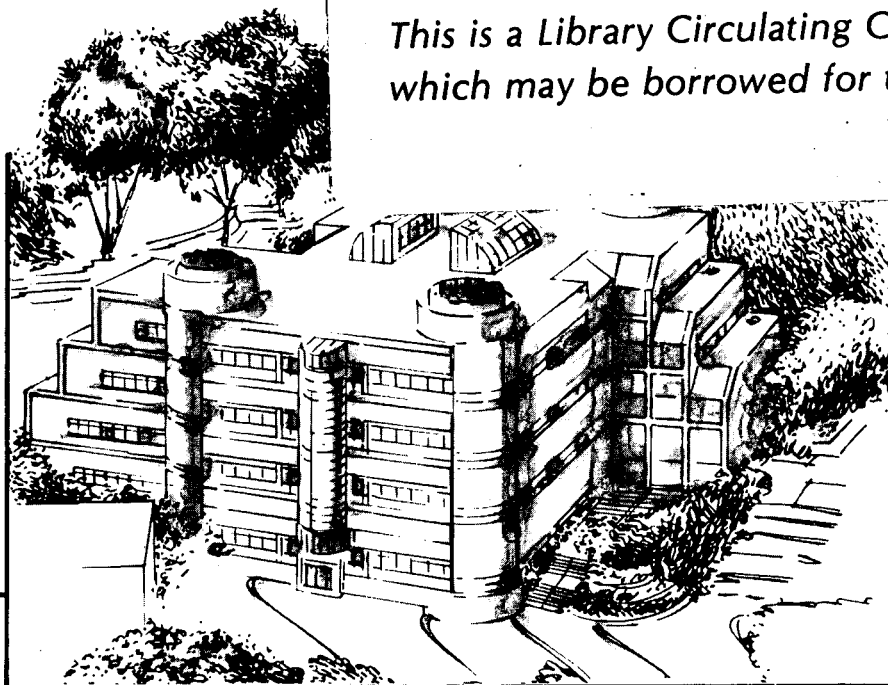
## A Summary of the Low Angle X-Ray Atomic Scattering Factors Which Have Been Measured by the Critical Voltage Effect in High Energy Electron Diffraction (HEED)

A.G. Fox and R.M. Fisher

August 1987

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**A Summary of the Low Angle X-Ray Atomic Scattering  
Factors Which Have Been Measured by the Critical Voltage  
Effect in High Energy Electron Diffraction (HEED)\***

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Abstract

A tabulated summary of all the accurate ( $\sim 0.1\%$ ) low-angle X-ray atomic scattering (form) factors which have been determined by the systematic critical voltage technique in HEED is presented. For low atomic number elements ( $Z \leq 40$ ) the low angle form factors can be significantly different to best free atom values, and so the best band structure calculated and/or X-ray measured form factors consistent with the critical voltage measurements are also indicated. At intermediate atomic numbers ( $Z = 40 \rightarrow 50$ ) only the very low-angle form factors appear to be different to the best free atom values, and even then only by a small amount. For heavy elements ( $Z \geq 70$ ) the best free atom form factors appear to agree very closely with the critical voltage measured values and so, in this case, critical voltage measurements give very accurate measurements of Debye-Waller factors.

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A summary of the low angle X-ray atomic scattering factors which have been measured by the Critical Voltage Effect in High Energy Electron Diffraction. (HEED)

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Abstract

A tabulated summary of all the accurate ( $\sim 0.1\%$ ) low-angle X-ray atomic scattering (form) factors which have been determined by the systematic critical voltage technique in HEED is presented. For low atomic number elements ( $Z \leq 40$ ) the low angle form factors can be significantly different to best free atom values, and so the best band structure calculated and/or X-ray measured form factors consistent with the critical voltage measurements are also indicated. At intermediate atomic numbers  $Z=40-50$  only the very low-angle form factors appear to be different to the best free atom values, and even then only by a small amount. For heavy elements  $Z(\geq 70)$  the best free atom form factors appear to agree very closely with the critical voltage measured values and so, in this case, critical voltage measurements give very accurate measurements of Debye-Waller factors.

1. Introduction

When a crystal is set at the Bragg reflecting position in HEED, the intensity of the diffracted beam is usually strong owing to the constructive interference of waves scattered in the diffracted beam direction. However, for

reflections higher than first order in a systematic row, at a particular electron accelerating voltage known as the critical voltage,  $V_c$ , the diffracted beam intensity can be very small owing to destructive rather than constructive interference (see for example, Lally, Humphreys, Metherell and Fisher 1972). The critical voltage is very sensitive to the low-order Fourier coefficients of the crystal potential for the systematic row concerned, and hence can be used to determine these and related quantities with high accuracy. In particular, low-angle X-ray structure factors can be measured with an accuracy which far exceeds conventional X-ray measurements, and is similar to those achieved by Pendellösung methods. This high accuracy has allowed Smart and Humphreys (1980) to produce accurate sets of atomic scattering (form) factors and thus deformation electron density distributions for several cubic elements. The object of this work is to review all the critical voltage measurements that have been made on both cubic and close-packed hexagonal elements, and to present the best values of the low angle form factors deduced from them.

## 2. Measurement of Systematic Critical Voltages

Sample preparation for critical voltage measurements is very straightforward; all that is required is a conventional electropolished transmission electron microscope specimen. To make the greatest range of  $V_c$  measurements, it is necessary to have a high (as possible) voltage electron microscope (HVEM). Most HVEM's operate

at 1MeV, but 1.5MeV and 3MeV machines are also available, and these can improve the amount of information available by this technique.

As mentioned in section 1, a critical voltage is associated with the minimisation of a Bragg excited reflection of second or higher order in a systematic row. These minimisations can be observed by three methods:-

(1) The disappearance of the Kikuchi lines associated with the Bragg reflection (see for example, Thomas, Shirley, Lally and Fisher 1974). (2) The disappearance of the central maximum of the dark field bend contour associated with the minimising reflection (Lally et al 1972). (3) The disappearance of the central maximum of the rocking curve profile in the Bragg excited convergent beam disc (Sellar, Imeson and Humphreys 1980). Also associated with these minimisations are changes in the asymmetry of Kikuchi lines in the diffraction patterns (for methods (1) and (3)) which allow accuracies of  $\pm 1\text{kV}$  to be obtained in  $V_c$ , although  $\pm 10\text{kV}$  is the routine error for measurements on second order reflections. Higher order minimisations are often less distinct (see for example, Jones 1978 and Fox 1985), but can still give accurate information about low angle X-ray structure factors.

### 3. Analysis of $V_c$ Measurements

As stated in section 1,  $V_c$  depends on the low-angle Fourier coefficients of the systematic row concerned and Lally et al (1972) and Sellar et al (1980) have pointed out that the major contribution to  $V_c$  comes from the first

order low-angle form factor. The second order low-angle form factor and the Debye-Waller factor also make important contributions and, where higher-angle form factors are very different to relativistic Hartree-Fock (RHF) free atom values (which are usually used in  $V_C$  analyses), it is important to use the best higher-angle data available in the analysis of critical voltage measurements. With best values of higher-angle form factors and Debye-Waller factor, then, low-angle X-ray form factors can be measured to within 0.1% or better using the  $V_C$  method (see for example, Hewat and Humphreys 1974). This technique forms the basis for the results presented in the next section.

#### 4. Results

In this section the critical voltage results,  $V_C$  (with appropriate superscript showing the reflection minimising), for many hexagonal and cubic elements are presented together with the best Debye-Waller factors,  $B$ , and higher-angle form factors available (consistent with the  $V_C$  measurements). The low-angle X-ray form factors,  $f$  (with appropriate superscript), determined from the  $V_C$  results, are also shown together with the equivalent RHF form factors in parentheses.

##### 4.1 Hexagonal Elements

Apart from beryllium very few form factor measurements have been made on these materials, and in general free atom RHF form factors are used for the higher-angle reflections, together with the best available anisotropic Debye-Waller factors  $B_C$  and  $B_A$ . This seems to be quite



reasonable for c.p.h. elements, as only the low angle form factors appear to be significantly different from free atom values.

4.1.1 Beryllium.  $B_C = 0.395\overset{0}{\text{\AA}}^2$ ,  $B_a = 0.435\overset{0}{\text{\AA}}^2$  (Larsen, Lehmann and Merisalo 1980). Best higher-angle form factors are  $\gamma$ -ray values of Hansen, Schneider and Larsen (1984) or X-ray values of Larsen and Hansen (1984).

$$V_C^{0004} = 1230(30)\text{kV (Fox and Fisher 1987)} \quad f^{0002} = 1.679 \\ (1.730)$$

$$V_C^{20\bar{2}2} = 718(10)\text{kV (Thomas et al 1974)} \quad f^{10\bar{1}1} = 1.704 \\ (1.707)$$

There is excellent agreement between these results and the values of Hansen et al (1984) and Larsen and Hansen (1984).

4.1.2 Magnesium.  $B_C = 1.23\overset{0}{\text{\AA}}^2$ ,  $B_a = 1.34\overset{0}{\text{\AA}}^2$  (Brindley and Ridley 1938). For higher-angle form factors the RHF free atom values of Doyle and Turner (1968) are used.

$$V_C^{0004} = 678(6)\text{kV (Thomas et al 1974)} \quad f^{0002} = 8.774 \\ (8.855)$$

$$V_C^{20\bar{2}2} = 310(5)\text{kV (Thomas et al 1974)} \quad f^{10\bar{1}1} = 8.624 \\ (8.683)$$

4.1.3 Titanium.  $B_C = 0.55\overset{0}{\text{\AA}}^2$  (Schoening and Witt 1965).

Higher-angle form factors from Doyle and Turner (1968).

$$V_C^{0004} = 236(10)\text{kV (Arii, Uyeda, Terasaki and Watanabe 1973)} \\ f^{0002} = 15.47 \\ (15.621)$$

4.1.4 Cobalt.  $B_C = B_a = 0.39\overset{0}{\text{\AA}}^2$  (Barron, Berg and Morrison 1957). Higher angle form factors from Doyle and Turner (1968).

$$V_C^{0004} = 278(2)\text{kV (Thomas et al 1974)} \quad f^{0002} = 19.461 \\ (19.496)$$

$$V_C^{22\bar{4}0} = 1850(50)\text{kV (Present Work)} \quad f^{11\bar{2}0} = 14.903 \\ (14.772)$$

$$V_C^{20\bar{2}6} = 1210(40)\text{kV (Present Work)} \quad f^{10\bar{1}3} = 13.879 \\ (13.848)$$

4.1.5 Zinc.  $B_c = 2.045\text{\AA}^2$ ,  $B_a = 0.884\text{\AA}^2$  (Skelton and Katz 1968). Higher-angle form factors from Doyle and Turner (1968).

$V_c^{0004} = 112.5(12.5)\text{kV}$ (Jones 1978)	$f^{0002} = 24.19$ (24.22)
$V_c^{20\bar{2}2} = 40\text{kV}$ (Present Work)	$f^{10\bar{1}1} = 22.714$ (22.872)
$V_c^{20\bar{2}6} = 730(30)\text{kV}$ (Jones 1978)	$f^{10\bar{1}3} = 17.75$ (18.275)

These results are in reasonably good agreement with the low-angle X-ray Pendellösung results of Takama, Kobayashi, Hyuagaji, Nittono and Sato (1984).

4.1.6 Cadmium.  $B_c = 2.61\text{\AA}^2$ ,  $B_a = 1.11\text{\AA}^2$  (Brindley and Ridley 1939). Higher-angle form factors from Doyle and Turner (1968).

$V_c^{30\bar{3}0} = 900(30)\text{kV}$ (Jones 1978)	$f^{10\bar{1}0} = 39.30$ (39.299)
$V_c^{0006} = 530(30)\text{kV}$ (Jones 1978)	$f^{0002} = 40.126$ (40.243)
$V_c^{22\bar{4}0} = 1030(30)\text{kV}$ (Jones 1978)	$f^{11\bar{2}0} = 31.516$ (31.335)
$V_c^{20\bar{2}6} = 215(15)\text{kV}$ (Present Work)	$f^{10\bar{1}3} = 31.617$ (31.617)

## 4.2 Diamond Cubic Elements.

These elements have been the subject of considerable study by many workers, in particular silicon, and the current results agree very well with the best X-ray data.

4.2.1 Silicon.  $B = 0.4613\text{\AA}^2$  (Aldred and Hart 1973)

Higher-angle form factors were taken from the X-ray work of Aldred and Hart (1973) with Cromer (1965) anomalous dispersion values.

$$V_C^{333} = 1104(6)\text{kV (Hewat and Humphreys 1974)}$$

$$f^{111} = 10.730 \\ (10.546)$$

$$V_C^{333} = 1101(7)\text{kV (Shishido and Tanaka 1975)}$$

$$f^{222} = -0.185^*$$

\* The  $V_C^{333}$  measurement allows a simple relationship between  $f^{111}$  and  $f^{222}$  to be developed, and by a best choice of  $f^{111}$  (by considering all the values available)  $f^{222}$  was calculated.

$$V_C^{440} = 1101(6) @ 515^\circ\text{C}^\dagger \text{ (Thomas et al 1974)}$$

$$f^{220} = 8.688 \\ (8.698)$$

† Analysed using appropriate high temperature Debye-Waller factor.

4.2.2 Germanium.  $B = 0.543\text{\AA}^2$  (Mair and Barnea 1975)

Higher-angle form factors were taken from the X-ray work of Matsushita and Kohra (1974) with Cromer (1965) anomalous dispersion values.

$$V_C^{333} = 922(5)\text{kV (Hewat and Humphreys 1974)}$$

$$f^{111} = 27.53 \\ (27.389)$$

$$V_C^{333} = 908.5(6.4)\text{kV (Shishido and Tanaka 1976)}$$

$$f^{222} = -0.16^\Delta$$

$$V_C^{440} = 994(5)\text{kV (Hewat and Humphreys 1974)}$$

$$f^{220} = 23.75 \\ (23.78)$$

$\Delta$  Estimated from a combination of  $V_C$  and convergent beam diffraction measurements.

### 4.3 Body-centred Cubic Elements

Surveys of the best Debye-Waller factors for many cubic elements have been carried out by Thomas et al (1974),

Smart and Humphreys (1980) and Fox and Fisher (1986), and the best values of B from these workers are adopted in this section and the next.

4.3.1 Vanadium.  $B = 0.66\text{\AA}^2$ .

Higher-angle form factors were taken from the band structure calculations of Laurent, Wang and Callaway (1978), which have recently been re-evaluated by Fox (1987).

$$V_C^{220} = 230.0(2.5)\text{kV} \text{ (Thomas et al 1974)} \quad f^{110} = 15.90 \\ (15.935)$$

$$V_C^{400} = 1141(37)\text{kV} \text{ (Terasaki, Uchida and Watanabe 1975)} \\ f^{200} = 13.22 \\ (13.218)$$

4.3.2 Chromium.  $B = 0.24\text{\AA}^2$ .

Higher-angle form factors were taken from the band structure calculations of Wakoh and Yamashita (1971).

$$V_C^{220} = 265(3)\text{kV} \text{ (Thomas et al 1974)} \quad f^{110} = 16.259 \\ (16.677)$$

$$V_C^{400} = 1285(31)\text{kV} \text{ (Terasaki et al 1975)} \quad f^{200} = 13.47 \\ (13.606)$$

4.3.3 Iron.  $B = 0.35\text{\AA}^2$ .

Higher-angle form factors were taken from the band structure calculations of Wakoh and Yamashita (1971) or De Cicco and Kitz (1967), both of which are in good agreement with one another.

$$V_C^{220} = 305(3)\text{kV} \text{ (Thomas et al 1974)} \quad f^{110} = 18.278 \\ (18.420)$$

$$V_C^{400} = 1278(4)\text{kV} \text{ (Terasaki et al 1975)} \quad f^{200} = 15.143 \\ (15.232)$$

4.3.4 Niobium.  $B = 0.47\text{\AA}^2$ .

Higher-angle form factors were taken from the RHF values of Cromer and Weber (1974).

$$V_C^{220} = 35(3)\text{kV (Thomas et al 1974)} \quad f^{110} = 31.350 \\ (31.586)$$

$$V_C^{400} = 749(3)\text{kV (Thomas et al 1974)} \quad f^{200} = 27.470 \\ (27.602)$$

#### 4.3.5 Molybdenum. $B = 0.254\text{\AA}^2$ .

Higher-angle form factors were taken from Cromer and Weber (1974).

$$V_C^{220} = 35(3)\text{kV (Thomas et al 1974)} \quad f^{110} = 31.637 \\ (31.904)$$

$$V_C^{400} = 789(2)\text{kV (Thomas et al 1974)} \quad f^{200} = 27.579 \\ (27.591)$$

#### 4.3.6 Tantalum. $B = 0.358\text{\AA}^2$ .

Higher-angle form factors were taken from Cromer and Weber (1974).

$$V_C^{400} = 651(2)\text{kV (Thomas et al 1974)} \quad f^{400} = 54.595 \\ (54.624)$$

#### 4.3.7 Tungsten. $B = 0.19\text{\AA}^2$ .

Higher-angle form factors were taken from Cromer and Weber (1974).

$$V_C^{400} = 660(3)\text{kV (Thomas et al 1974)} \quad f^{400} = 54.479 \\ (54.517)$$

### 4.4 Face-centred Cubic Elements

#### 4.4.1 Aluminium. $B = 0.85\text{\AA}^2$ .

The best higher-angle form factors are the X-ray values of Inkinen, Pesonen and Paakarri (1970), which appear to be better than the band structure calculations of Tawil (1975).

$$V_C^{222} = 425(10)\text{kV (Lally et al 1972)} \quad f^{111} = 8.843 \\ (8.945)$$

$$V_C^{400} = 918(5)\text{kV (Thomas et al 1974)} \quad f^{200} = 8.386 \\ (8.478)$$

#### 4.4.2 Cobalt. $B = 0.39\text{\AA}^2$ .

The higher angle form factors were taken to be the free

atom RHF values of Doyle and Turner (1968) which seem reasonable for cobalt as its electron charge distribution does not appear to be much different from the free atom case.

$$V_C^{222} = 276(2)\text{kV (Thomas et al 1974)} \quad f^{111} = 19.526 \\ (19.543)$$

$$V_C^{400} = 555(3)\text{kV (Thomas et al 1974)} \quad f^{200} = 18.182 \\ (18.252)$$

$$V_C^{440} = 1850(50)\text{kV (Present Work)} \quad f^{220} = 14.872 \\ (14.768)$$

#### 4.4.3 Nickel. $B = 0.4\text{\AA}^2$ .

Higher-angle form factors were taken from the band structure calculations of Wang and Callaway (1977) [vBH calculation].

$$V_C^{222} = 298(2)\text{kV (Thomas et al 1974)} \quad f^{111} = 20.482 \\ (20.530)$$

$$V_C^{400} = 588(3)\text{kV (Thomas et al 1974)} \quad f^{200} = 19.181 \\ (19.205)$$

#### 4.4.4 Copper. $B = 0.54\text{\AA}^2$ .

There are many band structure calculated and experimental form factor values for this element (see for example, Wakoh and Yamashita (1971), Bagayoko, Laurent, Singhal and Callaway (1980), McDonald, Daams, Vosko and Kelling (1982) [Band structure calculations], Takama and Sato (1982) [X-ray experimental] and Schneider, Hansen and Kretschmer (1981) [gamma ray experimental]). Of these, those of Wakoh and Yamashita appear to be the most consistent with the critical voltage measurements, and were therefore, adopted in the calculations.

$$V_C^{222} = 310(3)\text{kV (Thomas et al 1974)} \quad f^{111} = 21.702 \\ (22.066)$$

$$V_C^{400} = 605(3)\text{kV (Thomas et al 1974)} \quad f^{200} = 20.421 \\ (20.682)$$

$$V_C^{440} = 1750(50)\text{kV (Rocher and Jouffrey 1972)}$$

$$f^{220} = 16.675 \\ (16.810)$$

Of the experimental results, the X-ray Pendellösung values of Takama and Sato (1982) show the best agreement with the critical voltage measurements; the gamma ray values of Schneider et al (1981) seem somewhat low.

#### 4.4.5 Silver. $B = 0.655\text{\AA}^2$ .

Higher-angle form factors from Doyle and Turner (1968).

$$V_C^{222} = 55(3)\text{kV (Fukuhara and Yanigasawa 1969)}$$

$$f^{111} = 37.331 \\ (37.454)$$

$$V_C^{400} = 225(10)\text{kV (Lally et al 1972)}$$

$$f^{200} = 35.418 \\ (35.487)$$

$$V_C^{440} = 919(5)\text{kV (Thomas et al 1974)}$$

$$f^{220} = 29.873 \\ (30.057)$$

#### 4.4.6 Platinum. $B = 0.323(10)\text{\AA}^2*$

Higher-angle form factors from Cromer and Weber (1974).

$$V_C^{440} = 800(10)\text{kV (Present Work)}$$

$$f^{220} = 54.262 \\ (54.439)$$

$$V_C^{622} = 1420(20)\text{kV (Present Work)}$$

$$f^{311} = 50.553 \\ (50.553)$$

\* Debye-Waller factor calculated from  $V_C^{622}$  measurement (see section 5).

#### 4.4.7 Gold. $B = 0.655\text{\AA}^2$ .

Higher-angle form factors from Doyle and Turner (1968).

$$V_C^{400} = 108(2)\text{kV (Thomas et al 1974)}$$

$$f^{200} = 63.580 \\ (63.647)$$

$$V_C^{440} = 726(5)\text{kV (Thomas et al 1974)}$$

$$f^{220} = 55.845 \\ (55.988)$$

## 5. Discussion.

It is clear that for heavy elements ( $Z \geq 70$ ) the experimental (crystal) form factors are very close to the best RHF free atom values, and so critical voltage measurements on these can be used to obtain accurate Debye-Waller factors.  $V_c^{622}$  for platinum was used in this way to produce  $B = 0.323(10) \text{ \AA}^2$  for Pt.

For elements with intermediate atomic number ( $Z \approx 40-50$ ), only the very low-angle form factors are different from the best free atom values and so for niobium and molybdenum, the results presented here should be sufficient to plot the charge density (in fact, Smart and Humphreys 1980 have produced a deformation electron density map for Nb). For cadmium, accurate values of  $f^{10T1}$  and  $f^{10T2}$  are needed to complete a charge density analysis.

For light elements ( $Z \leq 35$ ), the crystal form factors may deviate considerably from best free atom values, although these differences seem more severe for cubic elements than they are for close-packed hexagonals. This means that free atom form factor values at higher angles are useable in  $V_c$  analyses on low  $Z$  c.p.h. elements, which is important because, apart from beryllium, very few good theoretical or experimental crystal form factors are available for these. For cubic elements there are plenty of theoretical and experimental crystal form factors for higher angles to choose from, and those which appear to be best are shown in section 4. It should be noted that nearly all the crystal form factors shown in the present



work are less than their equivalent free atom value and, as discussed by Smart and Humphreys (1980), this means that electron charge is being depleted from the outside of atomic sites (in the free atom case) to positions between the atoms.

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