

is 10 Å and that between triad images is 17 Å, which correspond to the distances between the projections of the corresponding groups of atoms. The images with the threefold axis of symmetry are obtained when the atoms located at different heights provide essentially different contributions to the scattering. For example, when the thickness of the crystal object is 1.25 times as large as the lattice spacing along $\langle 111 \rangle$, the beam passes twice through the atoms located at heights $\frac{1}{2}$ and $\frac{3}{2}$, and through the others only once.

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An Accurate Reappraisal of the Elemental Form Factors and Charge Density of Copper

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Abstract

The best X-ray atomic scattering factors for copper have been examined carefully to see which are most appropriate for charge density studies. The most consistent values were then used to generate a deformation charge density map, and it would appear that bonding in copper arises from electron charge build

up between nearest-neighbour (n.n.) atoms, next-n.n. atoms *etc.* This is in agreement with conclusions obtained from γ -ray diffraction experiments and the best band-structure calculations, but in marked disagreement with the charge density obtained from earlier band-structure form factors.

Introduction

In most cases the differences between elemental X-ray atomic scattering factors and best free-atom values

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are very small, so it is difficult to carry out charge density studies of these unless very accurate form factors are available. In recent years it has proved possible to measure X-ray form factors far more accurately by X-ray *Pendellösung* methods, γ -ray diffractometry and high-energy electron diffraction (HEED) with errors as low as 0.1% being reported [see, for example, Hansen, Schneider & Larsen (1984) (γ -rays); Aldred & Hart (1973) (X-ray *Pendellösung*); Fox & Fisher (1986) (electron diffraction)]. In addition to these experimental measurements, good form-factor values have also been obtained from improved band-structure calculations for many elements, and some of these were examined by Smart & Humphreys (1980) who then produced some interesting charge density distributions.

As discussed by Schneider, Hansen & Kretschmer (1981), the agreement between experimental and theoretical energy-band dispersions for copper is in general very good. However, it is a well known feature of variational band-structure calculations that a first-order error in the wave function gives rise to only a second-order error in the energy so that good eigenvalues may be obtained with wave functions of somewhat poorer quality. One way to check the accuracy of the appropriate wave functions is to compare the band-structure-calculated form factors with accurately measured values.

Schneider *et al.* (1981) measured a set of 19 form factors for copper up to $(\sin \theta)/\lambda = 0.7 \text{ \AA}^{-1}$ by γ -ray diffractometry and compared them with the values from the following band-structure calculations: Snow (1968), self-consistent augmented plane wave (APW) calculation; Arlinghaus (1967), APW (Chodorow); Wakoh & Yamashita (1971), a self-consistent Green-function method with full Slater exchange; Bagayoko, Laurent, Singhal & Callaway (1980), a self-consistent calculation with a basis of Gaussian orbitals and a local exchange-correlation potential. Unfortunately, Schneider *et al.* could obtain agreement with none of these although they felt that the values of Bagayoko *et al.* should represent the most accurate calculation.

Since Schneider *et al.*'s (1981) paper was published there has been some discussion about the accuracy of their results. The X-ray *Pendellösung* data of Takama & Sato (1982) and the electron diffraction results of Fox & Fisher (1988) both suggest that Schneider *et al.*'s form factors are somewhat low. Mackenzie & Mathieson (1984) suggested that improved extinction corrections were needed for the γ -ray measurements and applied such a correction to the 220 X-ray form factor of Cu and as a result obtained good agreement with the 220 results of Takama & Sato and Fox & Fisher. Schneider (1988, private communication) considers that the problem with the γ -ray values is one of absolute scale and not of extinction; indeed, Schneider *et al.* (1981) cite a possible scaling error of 1%.

The object of the present work is to review the best band-structure-calculated and experimental form factors described above, and to come to a decision as to which are the best. This should then allow an accurate charge density distribution for copper to be produced.

Review of atomic-scattering-factor values for copper

There have been a great number of form-factor measurements for copper and these have been concisely reviewed by Schneider *et al.* (1981). In this work only the 'best' values will be considered. On the experimental side, this means the X-ray *Pendellösung*, γ -ray diffraction and electron diffraction results, and on the theoretical side only those values of Arlinghaus (1967), Wakoh & Yamashita (1971) and Bagayoko *et al.* (1980) will be examined. Later limited theoretical work by MacDonald, Daams, Vosko & Koelling (1982) shows good agreement with the results of Bagayoko *et al.* and so will not be considered separately. More recent calculations by Eckardt, Fritsche & Noffke (1984) give values of form factors for copper which are considerably higher than any of those previously mentioned and have therefore been discounted. Other less-accurate values which have been obtained from X-ray diffraction or from earlier band-structure calculations will not be examined. The results of the work discussed above are summarized in Table 1. In this table the results of Bagayoko *et al.* and Schneider *et al.* were evaluated at low temperatures and so to compare them with other room-temperature measurements an estimate of their room-temperature values is shown in square brackets: These were obtained as described by Schneider *et al.* (1981); the lattice-parameter variation for copper with temperature is well known and so the variation of the free-atom form factors of Doyle & Turner (1968) with temperature could easily be calculated and appropriate corrections made to the low-temperature form factors. Many critical-voltage electron diffraction measurements of the low-angle form factors of Cu have been made (see *e.g.* Lally, Humphreys, Metherell & Fisher, 1972; Rocher & Jouffrey, 1972; Thomas, Shirley, Lally & Fisher, 1974; Fisher & Shirley, 1981; Smart & Humphreys, 1980). These measurements are in excellent agreement for the 111, 200 and 220 reflections. Unfortunately only two measurements of the 311 form factor have been made by this method (Rocher & Jouffrey; Fisher & Shirley) and these are not in good agreement. However, Fox & Fisher (1988) have reviewed carefully all of these measurements and form factors for copper were calculated by them using the best critical-voltage measurements and a Debye-Waller factor of 0.54 \AA^2 ; these are shown in Table 1. It can be seen that the form-factor values of Fox & Fisher (1988) and Takama & Sato (1982) agree closely with one

Table 1. *The best experimental and theoretical form factors for copper*

All values are at 293 K unless otherwise stated.

hkl	Free atom	Experimental				Band theory		
	Doyle & Turner (1968)	Schneider <i>et al.</i> (1981) at 50 K†	Schneider <i>et al.</i> rescaled	Takama & Sato (1982)	Fox & Fisher (1988)	Arlinghaus (1967)	Wakoh & Yamashita (1971)	Bagayoko <i>et al.</i> (1980) at 0 K†
1 1 1	22.08	21.51 (5) [21.54]	21.72	21.80 (6)	21.72 (4)	21.54	21.72	21.68 [21.71]
2 0 0	20.72	20.22 (4) [20.25]	20.42	20.28 (11)	20.45 (4)	20.25	20.46	20.35 [20.38]
2 2 0	16.78	16.45 (5) [16.49]	16.63	16.75 (8)	16.68 (8)	16.39	16.63	16.62 [16.66]
3 1 1	14.78	14.54 (4) [14.58]	14.70	14.74 (4)	14.76 (7)	14.43	14.64	14.70 [14.74]
2 2 2	14.23	14.07 (5) [14.12]	14.23	14.36 (6)		13.90	14.10	14.17 [14.21]
4 0 0	12.46	12.29 (6) [12.33]	12.43	12.46 (6)		12.19	12.34	12.42 [12.46]
3 3 1	11.46	11.30* [11.34]	11.45			11.25	11.35	11.41 [11.45]
4 2 0	11.17	11.02 (6) [11.06]	11.15			10.98	11.07	11.13 [11.17]
4 2 2	10.20	10.08 (6) [10.11]	10.20			10.05		10.16 [10.19]
3 3 3	9.61	9.49 (6) [9.52]	9.60			9.51		9.58 [9.61]
5 1 1	9.61	9.53 (6) [9.56]	9.64			9.51		9.58 [9.61]
4 4 0	8.85	8.84 (8) [8.87]	8.94					
6 0 0	8.37	8.37 (9) [8.39]	8.47					

* No experimental results available. Scattering factor obtained by interpolation.

† Values in square brackets are 293 K estimates - see text.

another and with the theoretical results of Bagayoko *et al.* except for the 200 value of Takama & Sato which seems somewhat low. However, a reappraisal of Takama & Sato's results (Tabbemor, 1989) suggests that this should be nearer 20.39(11) which is much more satisfactory.

There is reasonable agreement between the values of Wakoh & Yamashita (1971), Bagayoko *et al.* (1980), Takama & Sato (1982) and Fox & Fisher (1988) for the 111, 200 and 220 reflections, but at higher angles the Wakoh & Yamashita results seem somewhat low, and in better agreement with the γ -ray diffraction values of Schneider *et al.* (1981). Overall, the results of Schneider *et al.* seem somewhat low and more like the earlier band-structure calculations of Arlinghaus (1967), but even here the agreement is not good.

It is probably difficult to produce defect-free single crystals of Cu for X-ray *Pendellösung* measurements, and for this reason Takama & Sato (1982) used white radiation incident on Cu whiskers; the accuracy of such a technique is not generally as good as for measurements from more conventional wedge-shaped crystals. The possibility of a scaling error in the γ -ray form factors of Schneider *et al.* has previously been mentioned and such an error would not be surprising as these form factors were obtained from intensity measurements. On this basis it would seem that the electron diffraction results are the most accurate. If this is the case then the values of Bagayoko *et al.* (1980) would appear to represent the best theoretical description of the form factors, and, as shown in Table 1, the values of Arlinghaus (1967), Wakoh & Yamashita (1971), and Schneider *et al.* (1981) would seem to be too low. If, however, the values of Schneider *et al.* are rescaled to 293 K using the 111 value of Fox & Fisher (1988) as the reference point then the values marked Schneider *et al.* rescaled

in Table 1 are obtained, and there is striking agreement between these and the 293 K estimates of Bagayoko *et al.*, which suggests that Schneider (1988, private communication) was correct in his opinion about the absolute scale of his results. This also suggests that only the form factors up to $(\sin \theta)/\lambda = 0.39 \text{ \AA}^{-1}$ (220 reflection) are significantly affected by bonding, as at higher angles there is excellent agreement with the free-atom values of Doyle & Turner (1968). These conclusions are shown graphically in Fig. 1 where the differences between the crystal form factors and the Doyle & Turner free-atom values, Δf , are plotted as a function of $(\sin \theta)/\lambda$ up to the 420 reflection for the values of Bagayoko *et al.*, Fox & Fisher, Wakoh & Yamashita and Schneider *et al.* rescaled. It should be mentioned here that Mackenzie & Mathieson's (1984) reinterpretation of Schneider *et al.*'s γ -ray measurements by extrapolation back to the zero-level extinction limit leads to a value of 16.64

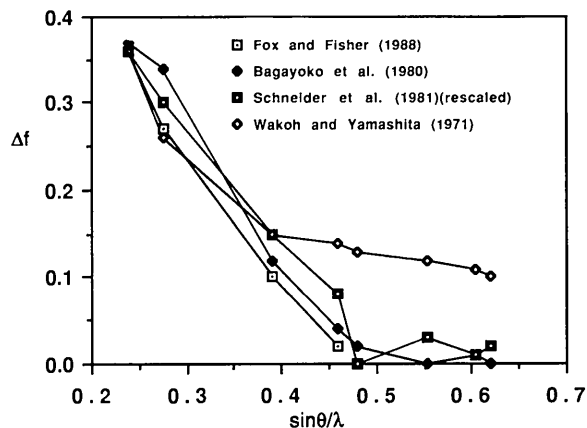


Fig. 1. Graph of difference between crystal and free-atom form factors, Δf , versus $(\sin \theta)/\lambda$ (\AA^{-1}) for copper from various workers. For the sake of clarity error bars are not shown.

for the form factor of the 220 reflection of Cu which is close to the Schneider *et al.* rescaled value. As mentioned previously, Mackenzie & Mathieson considered that Schneider *et al.* consistently underestimated the effects of extinction in their analysis for all reflections, and the possibility therefore exists that if all of Schneider *et al.*'s measurements were recorrected for extinction using the method of Mackenzie & Mathieson (which is not presently possible because Schneider *et al.* only published the γ -ray data for the 220 reflection profile), then all the form factors obtained could agree closely with the Schneider *et al.* rescaled values. Mackenzie & Mathieson's extinction-correction technique should therefore not be rejected out of hand. It is very satisfying that the sophisticated theory of Bagayoko *et al.* (1980) leads to what appear to be the most accurate form factors for Cu. This, however, is not surprising as their band-structure calculations also agree very closely with the highly accurate energy band dispersions $E_n(k)$ of Thiry, Chandresis, Lecante, Guillot, Pinchaux & Petroff (1979) obtained from extended angle-resolved photoemission experiments.

The charge density distribution of copper

Deformation charge density distributions for copper have previously been determined by Smart & Humphreys (1980) and Schneider *et al.* (1981). These workers produced deformation density maps using the crystal form factors and Debye-Waller factors that they considered best, and the free-atom form factors of Doyle & Turner (1968); this approach will also be adopted in the present work.

Smart & Humphreys (1980) used electron diffraction results for the 111, 200 and 220 crystal form factors and the values of Wakoh & Yamashita (1971) for higher angles with a room-temperature Debye-Waller factor B of 0.54 \AA^2 . This value of B agrees with that obtained from the best X-ray measurements and the γ -ray work of Schneider *et al.* (1981). A (011) deformation density map based on this choice is shown in Fig. 2, and it can be seen that there is depletion of electrons from atomic sites and build up at both the tetrahedral and octahedral interstitial sites. Smart & Humphreys felt that the form of this map was evidence for split (100) self-interstitials. However, the absence of charge build up between n.n. atoms indicated by this map does not agree with what would be expected for a 'normal' metallic bonding scheme. It should be noted that the form factors of Wakoh & Yamashita were only calculated up to and including the 420 reflection, and that even at this higher angle convergence to the free-atom values of Doyle & Turner (1968) has not been achieved. This means that there are most likely to be series-truncation errors in this charge density map.

A (011) deformation density map based on the results of Schneider *et al.* (1981) at 50 K with $B = 0.167 \text{ \AA}^2$ is completely different and this is shown in Fig. 3. Again there is depletion of electrons at atomic sites, but this time there is build up of charge between n.n. atoms, and somewhat lower build up between second-nearest neighbours, which is consistent with 'conventional' metallic bonding schemes.

In Fig. 4 a 0 K (011) deformation density map obtained from the crystal form factors of Bagayoko *et al.* (1980) with $B = 0.023 \text{ \AA}^2$ (calculated using a Debye temperature of 320 K) is shown. According to the present authors this should be the best. This map is similar to Fig. 3 in that there is a depletion of electrons from atomic sites and build up of charge between n.n. atoms with a somewhat lower build up between next-nearest neighbours. This can be seen better in the three-dimensional (011) map shown in

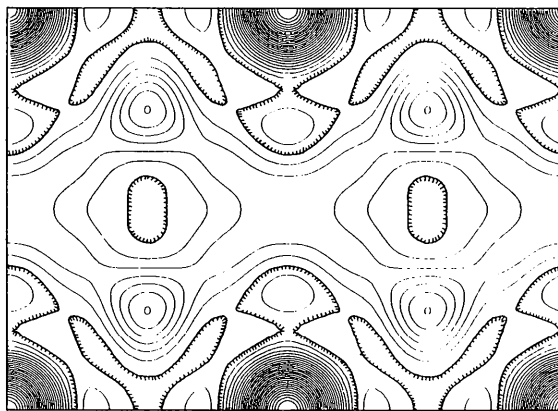


Fig. 2. (011) deformation density map for Cu based on the atomic scattering factors of Smart & Humphreys (1980). The contour spacing is 0.04 e\AA^{-3} with the zero contours ticked on the downhill side. The atom sites are clearly evident where there is a high density of contours.

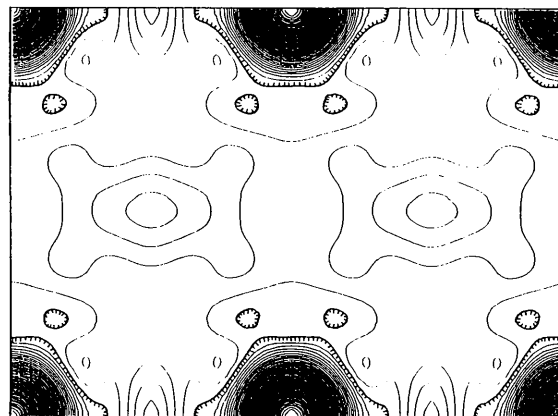


Fig. 3. (011) deformation density map for Cu based on the atomic scattering factors of Schneider *et al.* (1981) with contour spacing of 0.04 e\AA^{-3} .

Fig. 5. However, because the atomic form factors of Bagayoko *et al.* are much nearer to the free-atom values of Doyle & Turner (1968) the amount of depletion at atomic sites is less than that obtained with the form factors of Schneider *et al.* (1981) and the amount of build up between n.n. atoms is correspondingly less.

These results show the importance of having form factors showing the accurate *trend* with $(\sin \theta)/\lambda$ in order to produce good charge density distributions. Although the results of Bagayoko *et al.* (1980) and Schneider *et al.* (1981) are different in absolute scale their variation with $(\sin \theta)/\lambda$ follows the same pattern and so their deformation density maps show essentially the same features. Stevens & Coppens (1976) have previously noticed that small differences in scale between sets of atomic scattering factors make only minor differences to calculated charge density maps. Whether the scale differences between the results of Bagayoko *et al.* and Schneider *et al.* can be considered 'small' is open to discussion, but as noted above the charge densities produced from their set of atomic scattering factors have very similar forms.

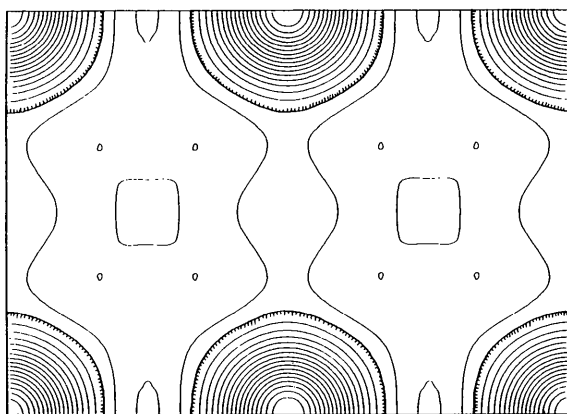


Fig. 4. (011) deformation density map for Cu based on the atomic scattering factors of Bagayoko *et al.* (1980) with contour spacing of $0.04 \text{ e}\text{\AA}^{-3}$.

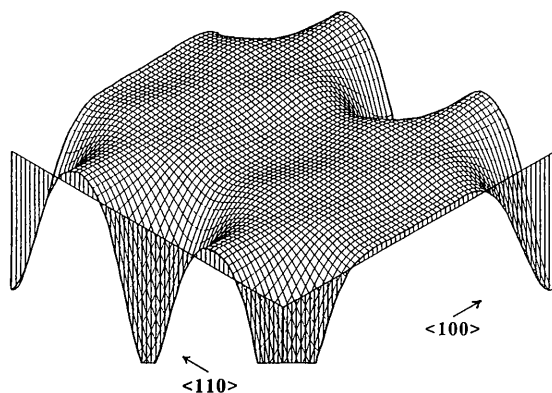


Fig. 5. Three-dimensional representation of Fig. 4.

Summary

The best X-ray atomic scattering factors for copper have been reviewed, and it would appear that the theoretical band-structure calculations of Bagayoko *et al.* (1980) represent the most accurate theoretical values over the complete range of $(\sin \theta)/\lambda$, agreeing very closely with the best experimental values from the low-angle electron diffraction results of Fox & Fisher (1988). The X-ray *Pendellösung* data of Takama & Sato (1982) also show good agreement with these values. The γ -ray values of Schneider *et al.* (1981) seem somewhat low but these can be rescaled to give very close agreement with those of Bagayoko *et al.* and Fox & Fisher.

Deformation density maps for copper based on the form factors of Smart & Humphreys (1980), Schneider *et al.* (1981) and Bagayoko *et al.* (1980) show the importance of having good form factors to plot accurate charge density distributions. The charge density map derived from the form factors of Bagayoko *et al.* (which appear to be best) indicates that bonding in Cu arises from the build up of electronic charge between n.n. atoms, next-n.n. atoms *etc.*, which is consistent with conventional metallic bonding schemes.

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Corrections to Tabulated Anomalous-Scattering Factors

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Abstract

Z-dependent energy-independent corrections to the relativistic anomalous-scattering factors tabulated by a number of workers are given. These corrections are most significant for medium-Z and high-Z atoms, but are experimentally observable even in low-Z elements. Examples of use of the correction factors are provided for the real anomalous-scattering factor f' and for the differential elastic scattering cross section $d\sigma/d\Omega$.

Introduction

We give here a tabulation (Table 1) of the correction factors $\delta f'$ which should be added to the relativistic anomalous-scattering factors f' of Cromer & Liberman (1970*a, b*, 1976, 1981), Cromer (1974, 1983) and Henke, Lee, Tanaka, Shimabukuro & Fujikawa (1981, 1982), as discussed by Parker & Pratt (1984) and more recently, and in greater detail, by Smith (1987). This issue does not arise in a non-relativistic theory, in which f' vanishes in the high-energy limit. The correction, of relativistic origin, is Z dependent but energy independent; it is most significant in heavier elements. It has been observed experimentally, as Parker & Pratt (1984) noted in mentioning the systematic discrepancies which had been reported by Creagh (1975, 1980); more extensive

comparisons and references are given by Smith (1987).

The problem arose from Cromer & Liberman's use of a dipole approximation in estimating relativistic corrections to the high-energy limit of forward scattering. Higher multipoles in fact become important at high energy. Jensen (1979, 1980) identified this as a problem, but did not succeed in calculating the corrections. In fact, $(5/3)(E_{\text{tot}}/mc^2)$, enumerated in Table II of Cromer & Liberman (1970*b*), is better replaced by (E_{tot}/mc^2) , where E_{tot} is the total binding energy of the atomic electrons. The later Cromer (1983) program, incorporating the first Jensen (1979) term, should not be used unless the Jensen term is then explicitly subtracted out. The correct high-energy limit had actually been obtained earlier in other contexts. It appears to be contained, for example, in the relativistic modified form-factor approximation of Franz (1936). The Coulomb K-shell result was given by Levinger & Rustgi (1956), more generally by Goldberger & Low (1968) and Florescu & Gavrila (1976). The general result for a central potential was obtained by Levinger, Rustgi & Okamoto (1957). Beginning with the relativistic dispersion relation, Wang (1986) derived a form of the relation accurate to order $(Z\alpha)^2$ suitable for numerical evaluation.

Numerical multipole calculations based on the second-order S matrix began with the work of Brown,