Aspherical Charge Distribution in Chromium Metal

By S. Ohba,* Y. Saito* and S. Wakoh†

The Institute for Solid State Physics, The University of Tokyo, Roppongi-7, Minato-ku, Tokyo 106, Japan

Abstract

The charge distribution in crystals of metallic chromium has been determined based on the reflection data measured up to $\sin \theta/\lambda = 1\cdot72$ Å^{-1} with Ag $K\alpha$ radiation with a spherical specimen of $0\cdot215$ (7) mm in diameter. In the difference synthesis a positive peak of $1\cdot4$ (1) e Å^{-3} was found in the direction toward the nearest neighbors at $0\cdot25$ Å from the Cr nucleus. This is presumably due to the asphericity arising from $3d$ electrons in t_{2g} orbitals. The ratios of the integrated intensity of paired reflections agreed well with those obtained from plate-like crystal [Diana & Mazzone (1972). *Phys. Rev. B*, **5**, 3832–3836], but the theoretical values calculated by means of the APW method with orbital-dependent potentials showed larger asphericity than the experimental values. Influence of anharmonic vibration on the structure factor was found for vanadium metal.

Introduction

For vanadium metal, the ratios of the X-ray integrated intensity of paired reflections, *i.e.* reflections occurring at the same Bragg angle, measured with a spherical crystal (Ohba, Sato & Saito, 1981) were significantly smaller than those obtained from plate-like crystals (Weiss & DeMarco, 1965; Diana & Mazzone, 1975). In order to examine whether the disagreement is caused essentially from the difference in experimental techniques, another b.c.c. metal, chromium, has been studied for a spherical specimen and intensity ratios have been compared with those obtained from the plate-like crystal of the same substance (Diana & Mazzone, 1972) as well as with the theoretical values calculated by the augmented plane wave (APW) method.

Since Iwata & Saito (1973) detected the aspherical *d*-electron distribution in crystals of [Co(NH₃)₆] [Co(CN)₆], several types of transition-metal complexes and spinels have been investigated by accurate

---

* Present address: Department of Chemistry, Faculty of Science and Technology, Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama 223, Japan.

† Present address: University of Library and Information Science, Yatabe-machi, Tsukuba-gun, Ibaraki 305, Japan.

X-ray diffraction data (Saito, 1979; Stevens & Coppens, 1979). Asphericity of charge distribution in b.c.c. metals V, Cr and Fe has been studied only through the integrated intensity ratios of paired reflections (for example see Table 1 of Wakoh & Kubo, 1980). It is instructive to show the charge asphericity in real space. However, asphericity around the V atom could not be seen. This seems to be due to the smearing of charge distribution by thermal vibration of the atoms. The thermal parameter of Cr is expected to be about a half of that for V in view of their Debye characteristic temperatures. Thus the aspherical *d*-electron distribution around the Cr atom is expected to be clearly observed in the difference synthesis.

Experimental

The chromium single crystals were grown by a sublimation method at Materials Research Corp. The experimental procedure of the X-ray intensity measurements was broadly similar to that reported previously (Ohba, Sato & Saito, 1981). Unit-cell dimensions were obtained by least-squares refinement with 69 2θ values in the range $71 < 2\theta < 81°$, measured on a diffractometer with Ag $K\alpha_1$ radiation ($\lambda = 0\cdot55941$ Å). Crystal data are listed in Table 1 together with the

Table 1. *Crystal data and experimental conditions*

Cr (at 297 K)
Cubic, $a = 2\cdot8841$ (1) Å, $V = 23\cdot989$ (2) Å³
Space group $Im3m$, $Z = 2$, μ(Ag $K\alpha$) = $11\cdot42$ mm^{-1}
$C_{11} = 0\cdot3500$, $C_{12} = 0\cdot0678$, $C_{44} = 0\cdot1008$ N μm^{-2} (Bolef & de Klerk, 1963)

Diameter of crystal specimen	$0\cdot215$ (7) mm
Radiation	Ag $K\alpha$ ($\lambda = 0\cdot5608$ Å)
Monochromator	Graphite plate
Collimator	$0\cdot5$ mm $\varnothing$
Detector aperture	$8\cdot6$ mm $\varnothing$ ($2\cdot1°$)
$(\sin \theta/\lambda)_{max}$ of the observed reflection	$1\cdot72$ Å^{-1}
Scan mode	θ–2θ scan
Scan speed	$2°$ min^{-1} in θ
Scan width	$(2\cdot2 + \tan \theta)°$
Maximum number of repetitions	4
Criterion to terminate repetition	$\sigma(|F|)/|F| \leq 0\cdot002$
Number of reflections measured	1110
Number of non-zero reflections	1110
Number of independent reflections	70

experimental conditions. Integrated intensities were measured at room temperature (297 K) by the θ–2θ scan technique in the hemisphere ($l \geq 0$) up to $\sin \theta/\lambda$ = $1\cdot72$ Å^{-1}. The intensities of standard reflections decreased by $1\cdot5\%$ in a month. In order to reduce the statistical error, collection of reflection data ($\sin \theta/\lambda \leq 1\cdot25$ Å^{-1}) was repeated three times and, furthermore, the paired reflections ($\sin \theta/\lambda \leq 1\cdot60$ Å^{-1}) were remeasured several times. In all, 3442 intensities were obtained. By taking averages of identical data, the number of reflection data was reduced to 1110. Of these, 70 were independent.

After corrections for thermal diffuse scattering, by the program $TDS2$ (Stevens, 1974) using the elastic constant data listed in Table 1 (Bolef & de Klerk, 1963), and absorption as a sphere with $\mu r = 1\cdot23$ (Dwiggins, 1975), the scale factor, the isotropic thermal parameter and the isotropic secondary extinction parameter were refined with the full-matrix least-squares program $RADIEL$ (Coppens, Guru Row, Leung, Stevens, Becker & Yang, 1979); the R factor ($= \sum \|F_o\| - |F_c\|/\sum |F_o|$) obtained was 0·015. The smallest extinction factor y ($= F_o^2/F_c^2$) was 0·50 for 110. The variations of the integrated intensities with the angle Ψ around the scattering vector were measured for some low-angle reflections, the maximum intensity variation being as large as 9% in $|F_o|$ for the 002 reflection. Anisotropic secondary extinction corrections of type I (Coppens & Hamilton, 1970) were applied. The final R became 0·014 and R_w ($= [\sum w(|F_o| - |F_c|)^2/\sum w|F_o|^2]^{1/2}$) = 0·024 for 1184 observed reflections, where w is the weight of reflection in the refinement: $w = [\sigma_F^2 \text{ (count)} + (0\cdot015 |F_o|)^2]^{-1}$. After averaging equivalent reflections, R and R_w were 0·012 and 0·011 for 70 unique reflections, respectively.* The internal agreement factor of each independent reflection ($= \sum \|F_o\| - \langle|F_o|\rangle|/\sum |F_o|$) was in the range from 0·003 to 0·014. The atomic form factor and anomalous dispersion correction factors for Cr were taken from *International Tables for X-ray Crystallography* (1974).

The thermal parameter U was determined to be 0·00407 (2) Å^2, the corresponding Debye characteristic temperature being 470 K. This value is close to the 485 K derived from specific-heat data (Lonsdale, 1948). The thermal parameter of Cr was confirmed to be about half of that for V, 0·00758 (1) Å^2 (Ohba, Sato & Saito, 1981).

Theoretical calculation

The electronic structure of chromium metal has been investigated by one of the authors (SW) by means of

the APW method with orbital-dependent potentials (Wakoh & Yamashita, 1973). The orbital-dependent potential for the e_g orbital was shifted upwards by 0·04 Ryd (0·44 μm^{-1}) with respect to that for the t_{2g} orbital to give a good reproduction of the dimensions and shape of the Fermi hole pocket at N points in the Brillouin zone determined by the de Haas–van Alphen experiments. The computational procedure is broadly similar to that reported in the previous paper (Wakoh & Kubo, 1980). The theoretical X-ray form factors of the first 23 non-equivalent scattering vectors are tabulated in Table 2, together with contributions from the core electrons.

Results and discussion

Ratios of the integrated intensity of paired reflections obtained from mean values of the observed structure factors are listed in Table 3. The present experimental results agree with those of the experiment using a plate-like crystal of chromium (Diana & Mazzone, 1972). For vanadium metal, the results obtained from a plate-like or spherical specimen did not agree well. Accordingly, the disagreement in the experimental studies of vanadium metal cannot necessarily be attributed to the difference in experimental techniques. For the lowest-angle reflection pair, 330–411, the experimental and theoretical values are almost the same. But the theoretical values of the present study are generally larger than the experimental values. Further experimental and theoretical investigations are neces-

Table 2. *Theoretical form factors of metallic chromium*

The third column gives the form factors due to the core electrons; the fourth column gives those due to the band electrons; the fifth column gives the total of those in the third and fourth columns.

$h\,k\,l$	$\sin \theta/\lambda$	f_{core}	f_{band}	f_{total}
1 1 0	0·2455	14·645	1·613	16·258
2 0 0	0·3473	12·445	0·951	13·396
2 1 1	0·4253	10·951	0·672	11·623
2 2 0	0·4911	9·899	0·440	10·339
3 1 0	0·5491	9·136	0·208	9·344
2 2 2	0·6015	8·566	0·244	8·810
3 2 1	0·6497	8·127	0·124	8·251
4 0 0	0·6945	7·779	−0·063	7·716
3 3 0	0·7366	7·494	0·043	7·537
4 1 1	0·7366	7·494	−0·037	7·457
4 2 0	0·7765	7·255	−0·027	7·228
3 3 2	0·8144	7·048	0·034	7·082
4 2 2	0·8506	6·866	−0·010	6·856
4 3 1	0·8853	6·701	−0·018	6·683
5 1 0	0·8853	6·701	−0·115	6·586
5 2 1	0·9510	6·408	−0·070	6·338
4 4 0	0·9822	6·274	−0·027	6·247
4 3 3	1·0125	6·147	0·000	6·147
5 3 0	1·0125	6·147	−0·049	6·098
4 4 2	1·0418	6·025	−0·008	6·017
6 0 0	1·0418	6·025	−0·120	5·905
5 3 2	1·0703	5·908	−0·024	5·884
6 1 1	1·0703	5·908	−0·097	5·811

sary for quantitative discussion on the charge aspheri-city in b.c.c. metals.

The asphericity in charge distribution is obtained from the difference synthesis

$$D(xyz) = (1/V)\sum_h \sum_k \sum_l \Delta F(hkl) \cos 2\pi (hx + ky + lz),$$

where x, y and z are the fractional coordinates of a point in the unit cell, V is the cell volume, and ΔF ($=F_o - F_c$) is calculated based on Hartree–Fock free-atom scattering factors.* A three-dimensional difference synthesis was calculated based on the 70 independent reflections with $(\sin \theta/\lambda)_{max} = 1\cdot 72$ Å^{-1}. Fig. 1 shows a section through the Cr nucleus and parallel to the (100) plane. There is a positive peak in the [110] direction around the Cr atom. This electron-excess region has a maximum peak in the [111] direction as shown in Fig. 2. This is a section through the Cr nucleus and two-body diagonal axes. A positive peak of $1\cdot 4$ (1) e Å^{-3} is observed on the body diagonal axis at $0\cdot 25$ Å from the Cr nucleus.†

In all, eight equivalent peaks are arranged at apices of a cube around the Cr atom and they are linked together with a high electron density region. A theoretical valence electron density map of the (110) plane computed from the present band calculation is shown in Fig. 3. Peaks of $5\cdot 8$ e Å^{-3} are found on the [111] axes at $0\cdot 23$ Å from the Cr nucleus. The $3d$ radial wavefunctions of V and Cr have a peak around

---

* The charge distribution in a metallic state is much different from that in a free atomic state and X-ray form factors are known to be a few percent smaller than those for free atoms. These solid-state effects were ignored in the present experimental study and a scale for the $|F_o|$ was determined by least-squares fit with the free-atom values. The valence form factor (κ) was not introduced.

† The standard deviation assigned to the deformation density was estimated from the errors in the observed structure factors and an error in the scale factor (Toriumi & Saito, 1978).

Table 3. *Experimental and theoretical ratios of the integrated intensities of the reflection pairs for chromium metal*

Standard deviations of the experimental values are shown in parentheses.

	Experimental		Theoretical	
$F^2/F^2\ddagger$	Present study	Diana & Mazzone (1972)	Present study	Rath & Callaway (1973)
330/411	1·018 (14)	1·026 (14)	1·022	1·016
413/510	1·017 (10)		1·030	
433/530	1·013 (12)		1·016	
442/600	1·025 (16)	1·028 (14)	1·038	
532/611	1·013 (11)		1·025	

‡ The ratio of the paired reflections $h_1 k_1 l_1$ and $h_2 k_2 l_2$ is defined as $F^2(h_1 k_1 l_1)/F^2(h_2 k_2 l_2)$, where the value of $h_1^4 + k_1^4 + l_1^4$ is always selected to be less than that of $h_2^4 + k_2^4 + l_2^4$.
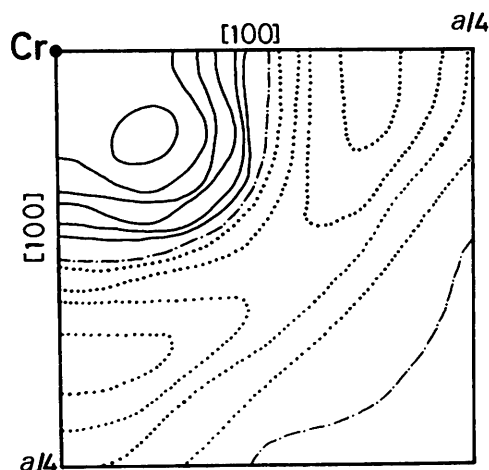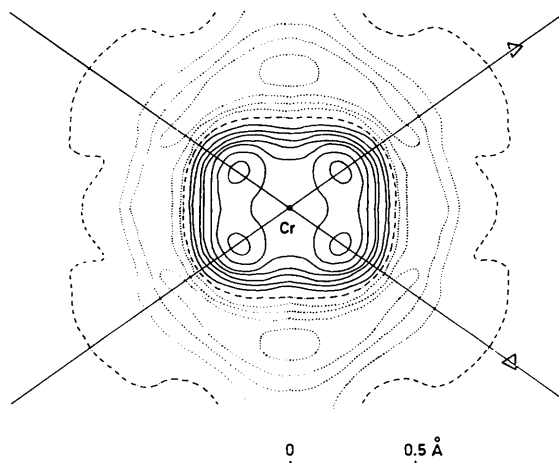

Fig. 1. A section of the difference synthesis through the Cr nucleus and parallel to the (100) plane. Contours are drawn at intervals of $0\cdot 2$ e Å^{-3}. Negative contours are dotted, zero contours are chain-dotted.

Fig. 2. A section of the difference synthesis through the Cr nucleus and parallel to the (110) plane. Contours are drawn at intervals of $0\cdot 2$ e Å^{-3}.
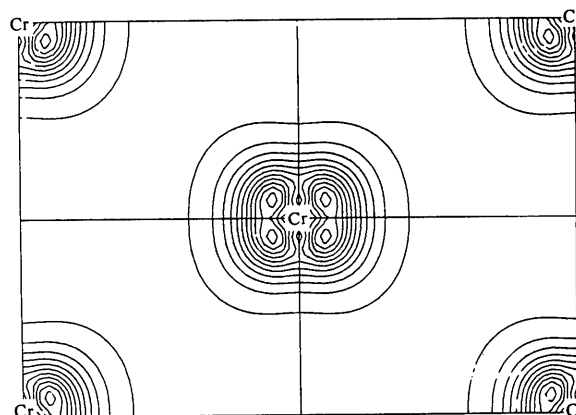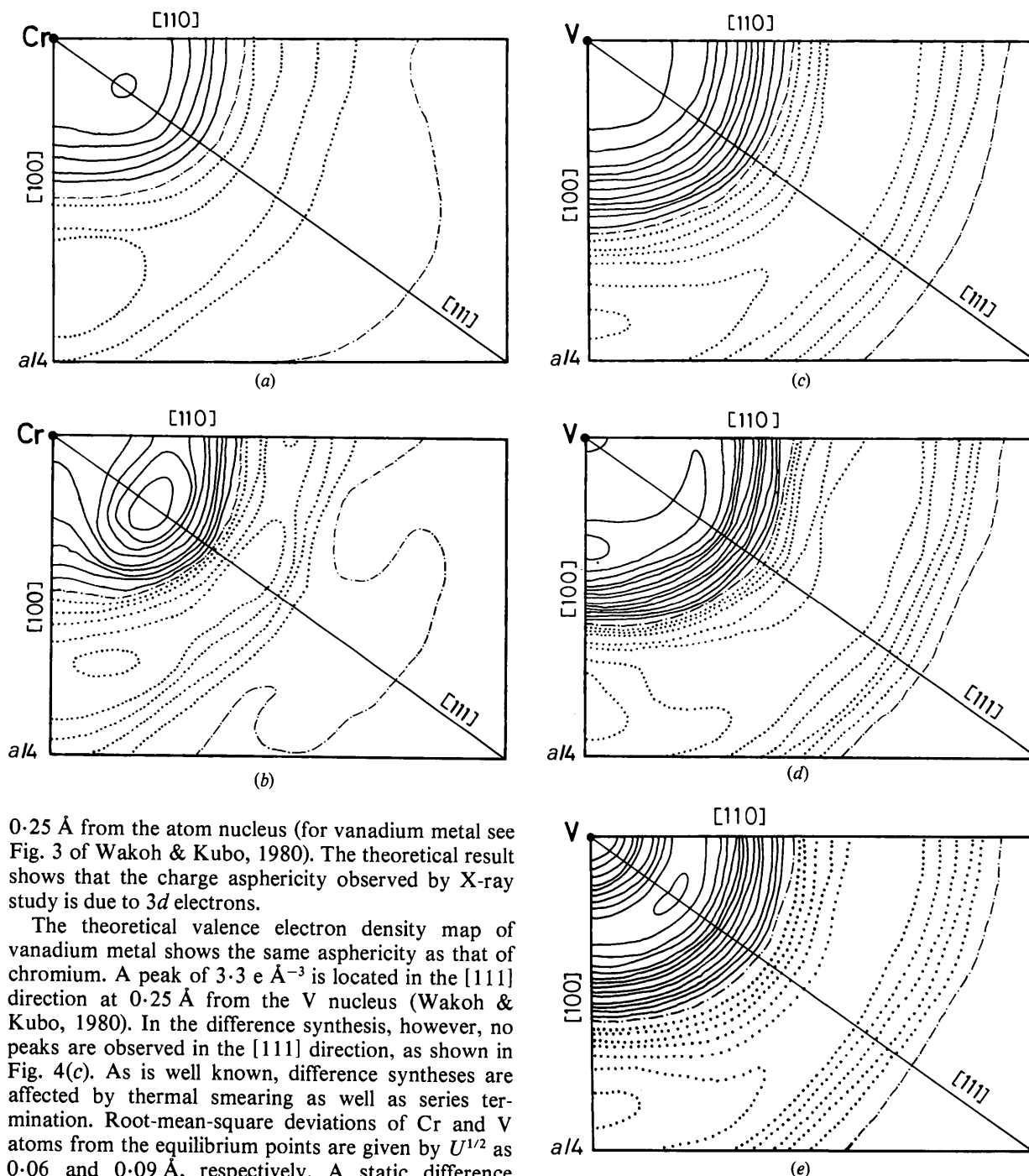

Fig. 3. Theoretical contour map of valence electron distribution on the (110) plane for chromium metal. Contours are drawn at intervals of $0\cdot 5$ e Å^{-3}.

0·25 Å from the atom nucleus (for vanadium metal see Fig. 3 of Wakoh & Kubo, 1980). The theoretical result shows that the charge asphericity observed by X-ray study is due to $3d$ electrons.

The theoretical valence electron density map of vanadium metal shows the same asphericity as that of chromium. A peak of $3\cdot3$ e Å^{-3} is located in the [111] direction at $0\cdot25$ Å from the V nucleus (Wakoh & Kubo, 1980). In the difference synthesis, however, no peaks are observed in the [111] direction, as shown in Fig. 4(c). As is well known, difference syntheses are affected by thermal smearing as well as series termination. Root-mean-square deviations of Cr and V atoms from the equilibrium points are given by $U^{1/2}$ as $0\cdot06$ and $0\cdot09$ Å, respectively. A static difference synthesis, i.e. $U^{1/2} = 0$ Å, can be calculated easily by means of the modified structure factors $\Delta F(hkl)$ $\times \exp[8\pi^2 U(\sin \theta/\lambda)^2]$. For chromium, such a section through the (110) plane is shown in Fig. 4(b). Fig. 4(a) shows a section of difference synthesis affected by thermal smearing with the same vibrational amplitude as that of vanadium metal. The sharp peak that appears in the [111] direction in Fig. 4(b) is smeared out in Fig. 4(a). On the other hand, the static difference synthesis

Fig. 4. Sections of difference syntheses parallel to (110) for Cr and V. (a) Cr, hypothetical difference synthesis calculated on the basis of observed structure amplitudes with the same U values as observed for V; (b) Cr, hypothetical static difference synthesis on the basis of observed structure amplitudes with $U = 0$ Å^2; (c) V, observed difference synthesis; (d) V, hypothetical static difference synthesis, the cut-off value of $(\sin \theta/\lambda)_{max}$ being $1\cdot72$ Å^{-1}; (e) V, the same as (d) but the series was terminated at a $\sin \theta/\lambda$ value of $1\cdot50$ Å^{-1}. Contours are drawn at intervals of $0\cdot2$ e Å^{-3}.

for vanadium metal shows a positive peak in the [100] direction at 0·27 Å from the V nucleus (see Fig. 4d). This suggests anharmonic vibration of the V atoms. In Fig. 5, integrated intensity ratios of all the reflection pairs are plotted against $\sin \theta/\lambda$. For three-paired reflections the ratios are defined as

$$F^2(h_1k_1l_1)/F^2(h_2k_2l_2), \quad F^2(h_1k_1l_1)/F^2(h_3k_3l_3)$$

$$\text{and } F^2(h_2k_2l_2)/F^2(h_3k_3l_3),$$

where $h_1^4 + k_1^4 + l_1^4 < h_2^4 + k_2^4 + l_2^4 < h_3^4 + k_3^4 + l_3^4$,

and their points in the figure are linked together with a vertical line. For chromium metal, ratios are generally greater than unity, but for vanadium metal some values in the high-angle region are less than unity, indicating anisotropic vibration of the V atoms as expected in Fig. 4(d).

The effect of the anharmonic vibration on the structure factors can be estimated as follows: the structure factor $F(\mathbf{Q})$ is represented as $F(\mathbf{Q}) = 2f(\mathbf{Q}) \times T(\mathbf{Q})$, where $f(\mathbf{Q})$ is the atomic form factor, $T(\mathbf{Q})$ is the temperature factor depending on the scattering vector $\mathbf{Q}$. By terminating the potential expansion at the fourth-order terms, an effective one-particle-potential of the atom in a cubic centrosymmetric field can be expressed as

$$V(u_1u_2u_3) = V_0 + \alpha/2(u_1^2 + u_2^2 + u_3^2) + \gamma(u_1^2 + u_2^2 + u_3^2)^2$$
$$+ \delta[(u_1^4 + u_2^4 + u_3^4) - 3/5(u_1^2 + u_2^2 + u_3^2)^2],$$

where u_1, u_2 and u_3 are the components of the displacement of an atom from its equilibrium position (Willis, 1969). Then the temperature factor is given by the following expression:

$$T(\mathbf{Q}) = [1 - 15 (k_BT/\alpha) (\gamma/\alpha)]^{-1} \exp[-Q^2k_BT/2\alpha]$$

$$\times \{1 - 15(k_BT/\alpha) (\gamma/\alpha)$$
$$+ 10(k_BT/\alpha)^2(2\pi/a)^2(\gamma/\alpha) (h^2 + k^2 + l^2)$$
$$- (k_BT/\alpha)^3(2\pi/a)^4(\gamma/\alpha)(h^2 + k^2 + l^2)^2$$
$$- (k_BT/\alpha)^3(2\pi/a)^4(\delta/\alpha) [(h^4 + k^4 + l^4)$$
$$- 3/5(h^2 + k^2 + l^2)^2]\},$$

where k_B is Boltzman's constant and T is the temperature, a is the lattice constant and hkl is the index of the reflection corresponding to the scattering vector $\mathbf{Q}$. The ratio of the structure factors of the paired reflections $h_1k_1l_1$ and $h_2k_2l_2$ becomes

$$F(\mathbf{Q}_1)/F(\mathbf{Q}_2) = f(\mathbf{Q}_1)/f(\mathbf{Q}_2) \times T(\mathbf{Q}_1)/T(\mathbf{Q}_2).$$

In harmonic approximation ($\gamma = \delta = 0$), k_BT/α is equal to the isotropic thermal parameter U, and $T(\mathbf{Q}_1)/T(\mathbf{Q}_2)$ is always unity. Anharmonic terms in the temperature factor will be small compared to the harmonic one so that the ratio can be reduced to

$$T(\mathbf{Q}_1)/T(\mathbf{Q}_2) = 1 + (k_BT/\alpha)^3(\delta/\alpha) (2\pi/a)^4$$
$$\times [(h_2^4 + k_2^4 + l_2^4) - (h_1^4 + k_1^4 + l_1^4)].$$

Thus we obtain for vanadium metal:

$$F(\mathbf{Q}_1)/F(\mathbf{Q}_2) = [f(\mathbf{Q}_1)/f(\mathbf{Q}_2)]$$
$$\times \{1 + 8·1 \times 10^{-6}(\delta/\alpha)[(h_2^4 + k_2^4 + l_2^4)$$
$$- (h_1^4 + k_1^4 + l_1^4)]\}.$$

As Willis (1969) pointed out, 'the potential is expected to increase along nearest-neighbor directions' so that δ is negative. When the value of $h_1^4 + k_1^4 + l_1^4$ is less than that of $h_2^4 + k_2^4 + l_2^4$, the ratio $f(\mathbf{Q}_1)/f(\mathbf{Q}_2)$ is greater than unity because of charge asphericity. On the other hand, $T(\mathbf{Q}_1)/T(\mathbf{Q}_2)$ is less than unity. Accordingly the difference in the structure factor between paired reflections will tend to cancel. For example, ratios of the temperature factors for some paired reflections are estimated with $\delta/\alpha = -1/2$ and tabulated in Table 4. If
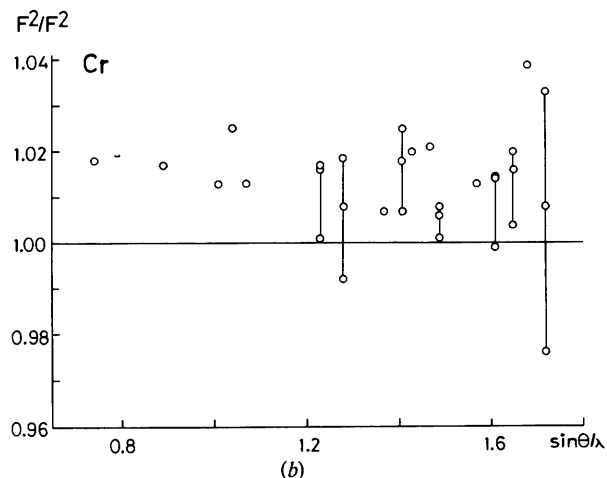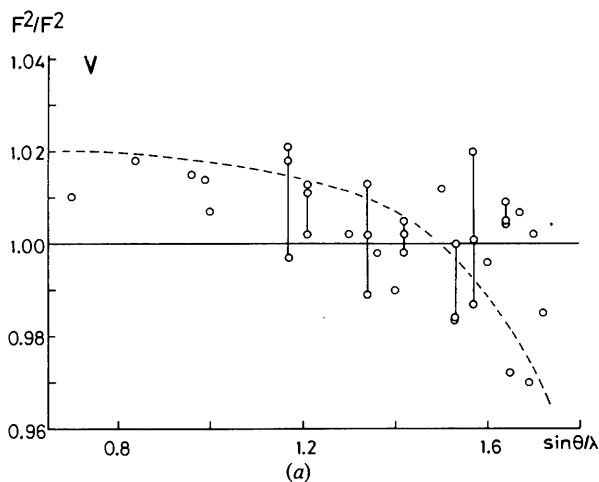

Fig. 5. Plot of the integrated intensity ratios of paired reflections against $\sin \theta/\lambda$ for (a) vanadium and (b) chromium metals. The ratios of the three-paired reflections are linked together with a vertical line. The broken line in (a) shows the effect of anharmonic vibration assuming that $f(\mathbf{Q}_1)/f(\mathbf{Q}_2) = 1·01$ and $\delta/\alpha = -1/2$.

Table 4. *Estimated ratios of the temperature factor of paired reflections for vanadium metal affected by the anharmonic vibration,* $\delta/a = -1/2$

$\dfrac{h_1k_1l_1}{h_2k_2l_2}$	$\sin \theta/\lambda$	$\dfrac{(h_2^4 + k_2^4 + l_2^4)}{-(h_1^4 + k_1^4 + l_1^4)}$	$\dfrac{T(Q_1)}{T(Q_2)}$	$\dfrac{1 \cdot 01\,T(Q_1)}{T(Q_2)^2}$
330/411	0·701	96	1·000	1·019
442/600	0·992	768	0·997	1·014
615/732	1·301	576	0·998	1·015
660/822	1·402	1536	0·994	1·007
833/910	1·496	2304	0·991	1·001
763/932	1·602	2880	0·988	0·996
666/1022	1·717	6144	0·975	0·970

we assume that $f(Q_1)/f(Q_2)$ is always equal to 1·01, the variation of the ratio $F^2(Q_1)/F^2(Q_2)$ is illustrated by the broken line in Fig. 5(*a*). For the low-angle reflection pairs the effect of anharmonic vibration is negligible as Weiss & DeMarco (1965) estimated. But for high-angle reflection pairs, the effect rapidly increases. In difference synthesis, the peaks of charge asphericity and those caused by the anisotropic vibration can be distinguished by their different $\sin \theta/\lambda$ dependence. The static difference synthesis of vanadium metal calculated for cut-off value $(\sin \theta/\lambda)_{max}$ equal to 1·50 Å^{-1} shows a positive peak in the [111] direction at 0·26 Å from the V nucleus, as shown in Fig. 4(*e*). On the other hand, the positive peak shown in Fig. 4(*d*) in the [100] direction disappeared. Accordingly, we can conclude that the aspherical charge distribution in vanadium metal is identical to that in chromium metal.

References

BOLEF, D. I. & DE KLERK, J. (1963). *Phys. Rev.* **129**, 1063–1067.
COPPENS, P., GURU-ROW, T. N., LEUNG, P., STEVENS, E. D., BECKER, P. J. & YANG, Y. W. (1979). *Acta Cryst.* A**35**, 63–72.
COPPENS, P. & HAMILTON, W. C. (1970). *Acta Cryst.* A**26**, 71–83.
DIANA, M. & MAZZONE, G. (1972). *Phys. Rev. B*, **5**, 3832–3836.
DIANA, M. & MAZZONE, G. (1975). *Philos. Mag.* **32**, 1227–1230.
DWIGGINS, C. W. JR (1975). *Acta Cryst.* A**31**, 395–396.
International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press.
IWATA, M. & SAITO, Y. (1973). *Acta Cryst.* B**29**, 822–832.
LONSDALE, K. (1948). *Acta Cryst.* **1**, 142–149.
OHBA, S., SATO, S. & SAITO, Y. (1981). *Acta Cryst.* A**37**, 697–701.
RATH, J. & CALLAWAY, J. (1973). *Phys. Rev. B*, **8**, 5398–5403.
SAITO, Y. (1979). *Inorganic Molecular Dissymmetry*, pp. 89–115. Berlin: Springer-Verlag.
STEVENS, E. D. (1974). *Acta Cryst.* A**30**, 184–189.
STEVENS, E. D. & COPPENS, P. (1979). *Acta Cryst.* A**35**, 536–539.
TORIUMI, K. & SAITO, Y. (1978). *Acta Cryst.* B**34**, 3149–3156.
WAKOH, S. & KUBO, Y. (1980). *J. Phys. F,* **10**, 2707–2715.
WAKOH, S. & YAMASHITA, J. (1973). *J. Phys. Soc. Jpn*, **35**, 1394–1401.
WEISS, R. J. & DEMARCO, J. J. (1965). *Phys. Rev.* **140**, A1223–1225.
WILLIS, B. T. M. (1969). *Acta Cryst.* A**25**, 277–300.

Le Groupe *P*1 et ses Sous-Groupes.
IV. Traitement Systématique de la Conservation Réticulaire*

PAR MONIQUE ROLLEY-LE COZ

Laboratoire MR3 (Algèbre de Von Neumann et Algèbres Commutatives), Université de Bretagne Occidentale, 6, avenue Le Gorgeu, 29283 Brest, France

Abstract

The present paper is the continuation of another devoted to the theoretical aspects of lattice-row and lattice-plane preservation in the isomorphic subgroups of space group *P*1. In the present paper the lattice preservation is studied as a function of the values of row indices [*U*,*V*,*W*] and plane indices (*H*,*K*,*L*) via the diagonalization of the change matrix defining the subgroup. The diagonalization is carried out by means of the program *MONIC* (Fortran IV, 220 instructions).

---

* English translations, not 'refereed', may be obtained from the author upon request.