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COMMENTS AND ADDENDA

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Analysis and Interpretation of X-Ray Compton Profiles in Diamond

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Recent measurements by Weiss and Phillips of the Compton profile in a diamond single crystal have been reanalyzed, using an inversion method. The resulting electron momentum density does not show a deficiency of density along the ⟨211⟩ directions, as was concluded by Weiss and Phillips, but rather along the ⟨110⟩ directions. Maxima are found along the ⟨100⟩ and ⟨111⟩ directions. The results are interpreted in terms of filled valence electron states inside the Jones zone, formed by the set of {220} planes, and empty states outside this zone.

Recently, Weiss and Phillips[1] (WP) have studied the electron momentum density in diamond by measuring the x-ray Compton profile in diamond powder and in a single crystal with the scattering vector along five selected crystallographic directions, viz., $[1\bar{1}0]$, $[001]$, $[1\bar{1}1]$, $[1\bar{1}2]$, and $[2\bar{2}1]$. They analyzed their results by a trial-and-error method and concluded that the profiles could be reproduced by transferring some momentum density in the vicinity of 1.3–2.3 a.u. along the ⟨211⟩ directions to similar regions along the ⟨100⟩ directions. However, an attempt to explain these results using an empirical wave function of the form $\psi = A[R_1 + (\alpha xyz/r^3)R_2]$, where R_1 and R_2 are radial wave functions, α an adjustable parameter, and A a normalizing constant, failed to reproduce the observed anisotropy in the Compton profiles. Moreover, it did not explain why the ⟨211⟩ directions would be singled out in this respect.

The Compton profile $J(p_z)$ is related to the momentum density $|\chi(\vec{p})|^2$ by

$$J(p_z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\chi(\vec{p})|^2 \, dp_x \, dp_y ; \qquad (1)$$

i.e., it equals the weighted area of a set of slices through momentum space. In this respect the experiment closely resembles positron annihilation, where an identical relation exists between the angular correlation $N(p_z)$ and the momentum density $\rho(\vec{p})$ of the pair of annihilation quanta[2]:

$$N(p_z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \rho(\vec{p}) \, dp_x \, dp_y . \qquad (2)$$

A few years ago a method of analysis was devised to reconstruct this momentum density by inversion of a number of angular correlations, measured along different directions in a single crystal.[3,4] Because of the equivalence of Eqs. (1) and (2) it follows that this method may also be applied to the analysis of Compton profiles.

To check the analysis of WP the present author has inverted their single-crystal data on diamond.[1] The five profiles were least-squares fitted by an expansion in cubic harmonics[5] containing the terms $l = 0$, 4, 6, and 8. These terms were then used to compute the coefficients in a similar expansion of the momentum density $4\pi|\chi(\vec{p})|^2$. By summing the terms in the latter expansion and normalizing the result according to the condition given by Phillips and Weiss[6] the momentum density was reconstructed. The result is shown in Fig. 1. The left-hand side shows a contour diagram of $4\pi|\chi|^2$ in the (110) plane, while on the right the anisotropy in this plane is shown separately. Contours inside a radius of ~0.9 a.u. have not been drawn because of the violent oscillations caused by the structure in the profiles at low values of momentum.

From Fig. 1(b) it becomes immediately clear that the transferred momentum density originates mainly from the region 1.1–1.8 a.u. along the ⟨110⟩ directions, and not from the ⟨211⟩ directions as

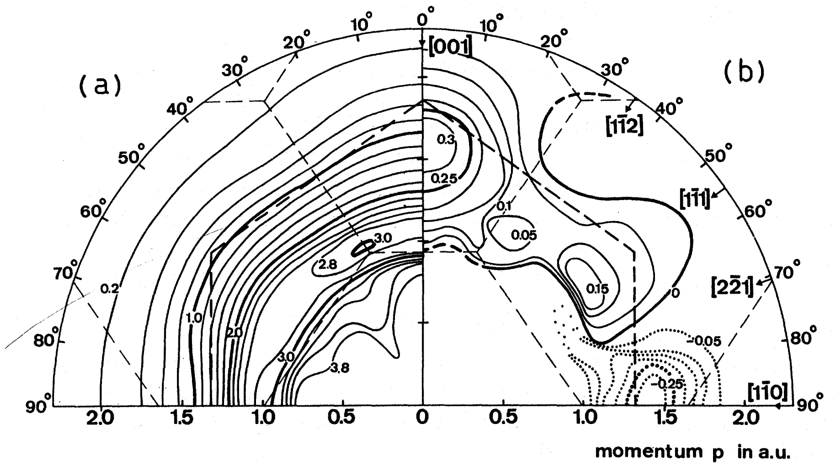

FIG. 1. Electron momentum density in the (110) plane in diamond. (a) Total momentum density $4\pi|\chi|^2$; (b) anisotropic part only. The heavy dashed lines show the intersection of the Jones zone with the (110) plane; the thin dashed lines represent the Brillouin-zone boundaries. Note the difference in contour interval between (a) and (b).

concluded by WP from their trial-and-error method of analysis. A secondary maximum about half as high as the principal maximum is found along the ⟨111⟩ directions. Repetition of the inversion with only three terms in the expansion produced essentially the same result.

An error analysis to assess the significance of the result is complicated by the fact that the relative error of ± 0.01 (a. u.)$^{-1}$ quoted by WP is not solely of statistical origin. If it is assumed, on basis of the scatter displayed by the data, that about half of this value comes from statistics, the uncertainty in the height of the maxima along ⟨100⟩ and ⟨111⟩ and in the depth of the minimum along ⟨110⟩ can be estimated to be ± 0.11, ± 0.08, and ± 0.08, respectively. In this error analysis, track has been kept of the various ways in which the original data become statistically correlated by the unfolding process. It is hard to assess the influence of systematic errors.

The explanation of the present result is similar to the interpretation of Erskine and McGervey[7] of their positron-annihilation experiments on Si and Ge, which are semiconductors having the diamond structure. Mott and Jones[8] have shown that in the extended-zone scheme no energy gap occurs at those Bragg reflections for which the structure factor is zero. Table I shows the structure factor of the first few reflections for the diamond structure. The largest value corresponds to the set of {220} planes. Moreover, the volume of the Jones zone bounded by these planes corresponds to four electrons per C atom; i. e., when this zone is filled, it can just accommodate all valence electrons. Figure 2 shows the shape of the Jones zone, while Fig. 3 shows the intersection of this zone and of the Brillouin zones with the (110) plane. The intersection of the Jones zone with the (001) plane is a square spanned by the reciprocal lattice vectors $(2\pi/a)(0, \pm 2, 0)$ and $(2\pi/a)(\pm 2, 0, 0)$, where $a = 3.56 A = 6.73$ a. u. is the lattice constant of diamond. Although owing to the large value of the energy gap (~5.3 eV) no states outside the Jones zone will be occupied by valence electrons, in accordance with the fact that diamond is an insulator, umklapp processes will give some contribution outside the zone.[9] This contribution will not be large, however, owing to the relatively spread-out character of the valence-electron wave functions. Thus the

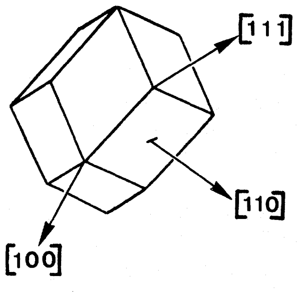

FIG. 2. Jones zone for diamond.

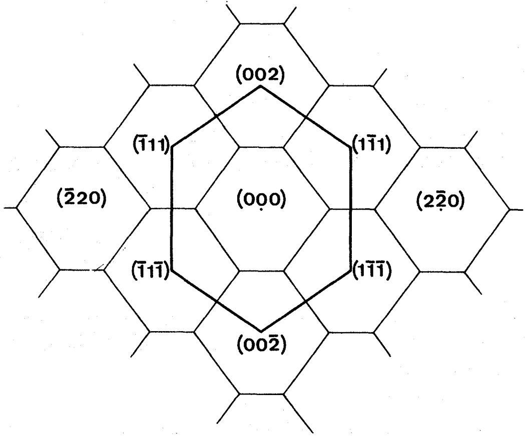

FIG. 3. Intersection of the Jones zone and the Brillouin zones with the (110) plane.

TABLE I. Structure factor for the diamond structure.

hkl	$\|S_{hkl}\|$
111	$4\sqrt{2}$
200	0
220	8
222	0
311	$4\sqrt{2}$

experiment of WP measures the shape of the Jones zone, modified by the fact that the contribution of each quantum state is weighted by its respective Fourier amplitude. This interpretation is supported by Fig. 1(a), in which it is seen that the region of high contour density roughly follows the boundary of the Jones zone. The deviation along the ⟨100⟩ directions will be due to the above-mentioned weighting, and to the fact that the truncation at $l = 8$ of the expansion in cubic harmonics will cause some smearing of the angular variations in the momentum density. Figure 1(b) shows that the maxima in the ⟨100⟩ and ⟨111⟩ directions are necessary to fill up the corners of the Jones zone, while the negative areas along the ⟨110⟩ directions serve to compress the distribution in these directions. For a more quantitative comparison of experiment and theory a band computation of the wave functions would be needed, which is outside the scope of this note.

One final question may be asked, namely, why the reconstructed momentum density exhibits anisotropy for momenta larger than 1.6 a.u., while the observed profiles are isotropic from $p_z = 1.6$ a.u. upwards (cf. Table II of Ref. 1). The answer must be sought in the limited accuracy of the profiles. It is possible to show on general grounds that, if the measured Compton profiles are expanded[3] in a series of lattice harmonics F_l according to

$$J_{\beta,\alpha}(p_z) = \sum_l F_l\,(\beta,\alpha)\,g_l(p_z), \tag{3}$$

where (β, α) denote, respectively, the polar and azimuthal angles of the x-ray scattering vector with respect to the crystal axes, the $g_l(p_z)$ *must* satisfy

$$\int_0^\infty g_l(z)\,P_l''(z/p)\,dz = 0\ . \tag{4}$$

Here p is an arbitrary quantity and $P_l''(x)$ denotes the second derivative of the lth-order Legendre polynomial. Equation (4) forms a rather stringent requirement on the experimental data, which is not quite met by the profiles of WP. Consequently, although at $p_z > 1.6$ a.u. the $g_l(p_z)$ $(l \neq 0)$ have vanished, this is not true of the expansion coefficients in the expansion of the momentum density, which results in the anisotropy extending beyond $p = 1.6$ a.u.

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Deformation-Potential Constants in the Acceptor-Hole–Phonon Interaction in Germanium

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It is shown that the values of the deformation-potential constants D_u^a and $D_{u'}^a$ in the interaction of acceptor holes with thermal phonons in Ge are larger than those in the interaction with static strains.

In a recent paper[1] we have calculated the low-temperature thermal conductivity of In-doped Ge and obtained good agreement with experiment. However, the values of the deformation-potential constants, $D_u^a = 4.2$ eV and $D_{u'}^a = 4.9$ eV, employed in our numerical calculations are considerably