where f is the normal atomic scattering factor, $\Delta f'$ and $\Delta f''$ are the real and imaginary parts of the anomalous scattering, $(A_j \pm iB_j)$, the geometric part of the structure factor for the jth atom for hkl and $\bar{h}\bar{k}\bar{l}$ respectively and (temperature factor)$_j$ is of the anisotropic form for the jth atom in the unit cell. The temperature factors for this pair are usually assumed to be the same since the thermal ellipsoid is centrosymmetric. The intensities of these two inverse reflexions would therefore be equal and 'Bijvoet differences', i.e. intensity differences due to anomalous scattering and deviation from Friedel's law, cannot arise in principle in such non-centrosymmetric structures of the elements, even if the anomalous scattering is appreciable. These ideas can also be elegantly visualized on the Argand diagram construction.

However, if it is postulated that (i) the temperature factors can be different for the different atoms in the unit cell and also that (ii) the temperature factors for the normal and anomalous components of the scattering can be appreciably different, then a simple algebraic exercise with the complex quantities in the structure factor expressions in equation (1) would show that Bijvoet differences can occur even in such structures. Physically the assumptions would mean that the ratios between the imaginary and real part of the scattering powers of the atoms become different, which is the condition required for the observation of Bijvoet differences.

The plausibility of these assumptions is difficult to consider theoretically. One could state that in a case like α-manganese ($I\bar{4}3m$), with 58 atoms in the unit cell, the former of the two assumptions is not unrealistic. Regarding (ii), it is well known that the anomalous scattering components depend mainly on the inner electrons only, in contrast to the normal scattering, and for this reason the angular dependences of these scattering factors are markedly different. Their temperature factors are, however, usually assumed to be the same.

It appears to the present author that a direct check is possible and would be desirable, by looking for Bijvoet differences in single crystals of α-manganese and the hexagonal isomorphous selenium and tellurium (enantiomorphous, $P3_121$ or $P3_221$). If appreciable Bijvoet differences are observed for a good number of reflexions, over and above what can be attributed reasonably to errors of measurement due to absorption and shape effects, then it would be a definite indication that the physical factors in the two above assumptions are operative and detailed work would be of interest in understanding the behaviour of temperature factors in X-ray diffraction, in addition to settling the absolute configuration of the structures. For a control on the experimental measurements, one would of course utilize the fact that the intensities of the pair would still be equal, despite these assumptions, for reflexions where the geometric parts in equation (1) are real – for example, reflexions with h or k or l, zero in α-manganese.

These proposals seem opportune now, since accurate refinements of such structures have recently been carried out: α-manganese (Gazzara, Middleton, Weiss & Hall, 1967) and hexagonal selenium (Cherin & Unger, 1966). It should also be mentioned that Bijvoet differences in such structures had been suggested for electron diffraction (Parthasarathy, 1961), through arguments based on the dynamical theory.

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An apparent variation of structure factors for electrons with the accelerating voltage. An observation through Kikuchi patterns.

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It is shown that the intensity of the Kikuchi line of the second order reflexion 220 in electron diffraction patterns from a thin single crystal of Fe–20 at.% Al alloy gradually changes with the accelerating voltage for incident electrons and vanishes at about 340 kV owing to the systematic dynamical interactions combined with the relativistic change of electron mass.

The structure factor for electrons $U_h = (2me/h^2)V_h$ changes with the accelerating voltage because of the relativistic change of electron mass (Fujiwara, 1961):

$$m = m_0/(1-\beta^2)^{\frac{1}{2}} = m_0\{1 + eE/(m_0c^2)\} \qquad (1),$$

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where V_h is the Fourier coefficient of the crystal potential, E the accelerating voltage, and β, e, h, m_0 and c have their usual meanings. The apparent value of structure factor U'_h, which is determined, for example, directly from the ring intensity on the basis of the current formula, changes more with the accelerating voltage owing to the dynamical many-beam interactions. Under certain conditions, approximate values of U'_h can be calculated by Bethe's second approximation (Bethe, 1928; Miyake, Fujiwara & Suzuki, 1963),
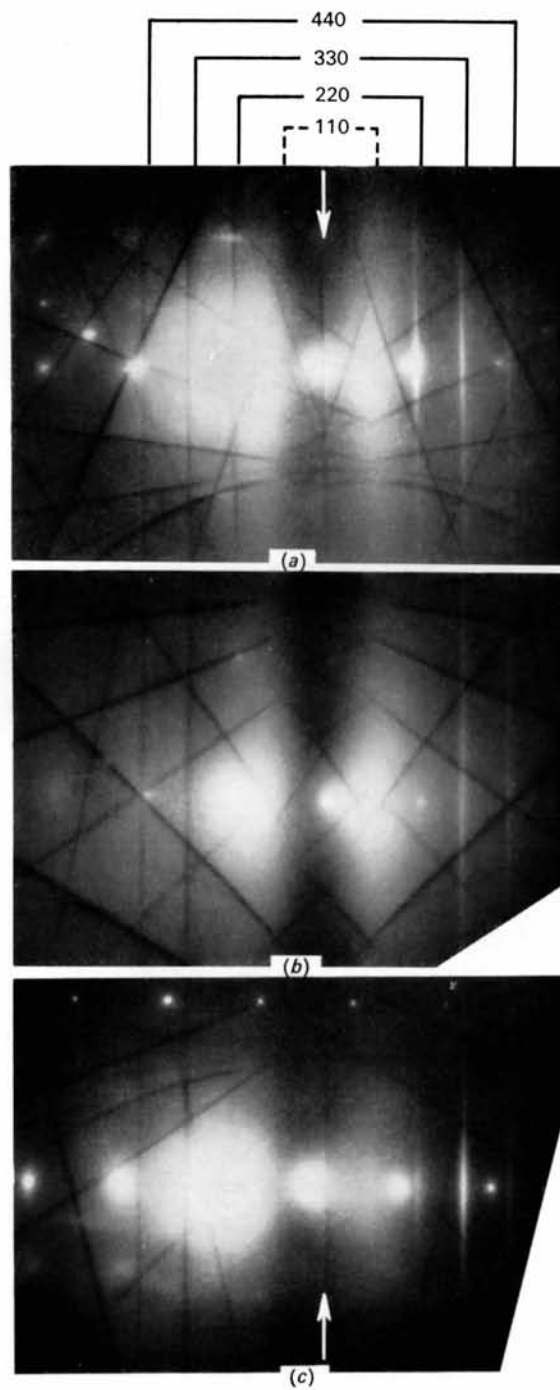
Fig. 1. Electron diffraction patterns from iron – 20 at.% aluminum alloy taken at 200 kV (*a*), 340 kV (*b*) and 380 kV (*c*). Arrows in (*a*) and (*c*) show the middle line of the Kikuchi band.

$$U'_h(E) = \left(1 + \frac{eE}{m_0c^2}\right)$$

$$\times \left[U_h(0) - \left(1 + \frac{eE}{m_0c^2}\right) \sum_g {}'' \frac{U_g(0)U_{h-g}(0)}{\kappa^2 - k_g^2} \right] \quad (2),$$

where h is the index of the main reflexion and g those of weak ones; κ is the mean wave number in the crystal and k_g the wave number for the gth reflexion; $\sum_g {}''$ means the summation over all the reciprocal lattice points except for 0 and h. Provided strong simultaneous reflexions are not excited, it is sufficient to limit the summation over the systematic interactions (*e.g.* Uyeda, 1968). For the second order reflexion the summation term in formula (2) is positive and large, provided $U_1(0)$ of the first order is large and all $U_g(0)$'s are positive (Raether, 1962; Kimoto & Nishida, 1967). When the accelerating voltage is increased, $U'_2(E)$ for the second order decreases, vanishes at a certain voltage E_c, then changes the sign and increases the absolute value. Nagata & Fukuhara (1967) and Uyeda (1968) observed this effect in the extinction distance of the second order reflexion. The present note describes an experimental study of this effect including the change of the sign of $U'_2(E)$.

Fig. 1 shows the diffraction patterns from a single crystal of iron–20 at.% aluminum alloy taken at 200 kV (*a*), 340 kV (*b*) and 380 kV (*c*), where the accelerating voltages were determined by Kikuchi lines (Uyeda, Nonoyama & Kogiso, 1965). The 220 Kikuchi lines become gradually weak with the accelerating voltage, vanish at $E_c = 340$ kV, and then become gradually strong again. This intensity variation is in accordance with that of the absolute value of $U'_{220}(E)$. Moreover, the change of the sign of $U'_{220}(E)$ can be proved as follows. The middle line of the Kikuchi band, which was recently explained by Kainuma & Kogiso (1968),

is clearly visible for the 110 band in Fig. 1(*a*) and (*c*), and vanishes in (*b*). It has an asymmetric excess-deficient profile. Note that the asymmetry of the profile is reversed at the voltage E_c. This implies the change of the sign of $U'_{220}(E)$. It is concluded, therefore, that the sign of the factor $U'_h(E)$ can be determined by observing the asymmetry of the middle line.

The same effect was also observed for the 200 reflexion of iron, the 222 of aluminium, nickel and silver, and the 400 of silver. The observed values of E_c are roughly in accordance with those calculated by formula (2). For the exact comparison of experiment with theory, calculations by many-beam theories must be carried out. It should be added that the experimental value of E_c can be determined quite accurately. Thus many-beam version of formula (2) at $E = E_c$ gives a relation between V_g's ($g = 1, 2, \ldots$). Since V_g of high order can be calculated accurately, the relation will be useful for the determination of V_g of low order.

Detailed experimental results and discussion will be reported in the near future.

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Die Ewald'sche Konstruktion im Vorlesungsversuch.

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The Ewald construction is easily demonstrated by means of a simple X-ray counter diffractometer for teaching crystallography.

Im Vorlesungsversuch lässt sich das Zustandekommen des reziproken Netzes als zweidimensionaler Modellfall für das reziproke Gitter leicht mit Röntgenstrahlung demonstrieren (Riechert & Weiner, 1964). Die hierzu erforderliche Anordnung hat die Bragg'sche Gleichung in ihrer vektoriellen Form

$$\frac{\sigma - \sigma_0}{\lambda} = n \cdot \frac{n}{d},$$

welche bekanntlich auf P. P. Ewald zurückgeht, zu ihrer Grundlage. Beim Auftreten von Röntgenreflexen werden die zugehörigen reziproken Netzpunkte durch den Eckpunkt P eines beweglichen Parallelogramms bezeichnet, dessen Seitenpaare durch die Vektoren σ_0/λ und σ/λ gebildet werden (Fig. 1).

Der Strecke OP entspricht dann der reziproke Vektor $(\sigma - \sigma_0)/\lambda$. Durch $\theta/2\theta$-Bewegungen – unter Koppelung von

reziproker Ebene und Parallelogrammführung – sowie durch Drehen von Kristall und reziproker Ebene gegenüber der Beugungsanordnung lässt sich das reziproke Netz punktweise aufbauen.

Röntgenröhre, Kristall, Detektor sowie $\theta/2\theta$-Führung befinden sich auf der Rückseite der reziproken Scheibe. Deren Vorderseite enthält nur die beschriebene Parallelogrammkonstruktion aus Plexiglaslinealen.

Die Anordnung basiert letzlich auf der Ewald'schen Konstruktion und lässt sich daher leicht zu deren Demonstration benutzen. Hierzu wird eine Scheibe aus Plexiglas mit aufgezeichnetem Ewaldkreis (Radius $AO \equiv \sigma_0/\lambda$) im Punkte A befestigt (Fig. 2). Das Ende des Vektors OP liegt – *per definitionem* – immer auf diesem Kreis. Nach Einstellen der – für einzelne Reflexserien spezifischen Glanzwinkel Θ – tritt beim Drehen des Kristalls und seiner reziproken Ebene Röntgenintensität in der Beugungsrichtung nur dann