

Table 1. *Unit-cell constants of divalent metal chlorides* (Å)
Hexagonal cell, space group $R\bar{3}m$ (D_{3d}^5)

Compound	Ferrari <i>et al.</i> *		Grime & Santos, 1934 (CoCl ₂) Pauling & Hoard, 1930 (CdCl ₂)		Present work			
	a	c	a	c	Graphical method		Least-squares method	
					a	c	a	c
MgCl ₂	3.603	17.627			3.632	17.78	3.632 ± 0.004	17.795 ± 0.016
MnCl ₂	3.682	17.480			3.709	17.59	3.711 ± 0.002	17.59 ± 0.07
FeCl ₂	3.585	17.555			3.593	17.60	3.593 ± 0.003	17.58 ± 0.09
CoCl ₂	3.547	17.385	3.551	17.46	3.553	17.41	3.553 ± 0.001	17.39 ± 0.05
NiCl ₂	3.542	17.355			3.481	17.30	3.478 ± 0.001†	17.41 ± 0.12†
CdCl ₂			3.862	17.495	3.845	17.49	3.8457 ± 0.0003	17.48 ± 0.02

* Bruni & Ferrari (1925, 1926, 1927), Ferrari (1927), Ferrari, Celeri & Giorgi (1929).

† From a single crystal, $a = 3.483 \pm 0.006$ Å, $c = 17.40 \pm 0.03$ Å.

Unit-cell data have been found to be $a = 3.483 \pm 0.006$, $c = 17.40 \pm 0.03$ Å. Calculated and observed density were $\rho_c = 3.537$ g.cm⁻³ and $\rho_o = 3.51$ g.cm⁻³. The ($h0l$) integrated reflexions were recorded by an integrating Weissenberg camera and measured by a microdensitometer. Polarization and Lorentz corrections were introduced. Absorption corrections were calculated by Ferrari, Braibanti & Tiripicchio's (1961) method; a contribution, due to the Lindemann tube, deduced from a curve for cylindrical specimens was added to the transmission factors calculated. Atomic form factors were evaluated graphically from the Thomas & Umeda (1957) data. During refinement, anomalous dispersion (*International Tables for X-ray Crystallography*, 1961) and secondary extinction (Pinnock, Taylor & Lipson, 1956) were taken into account.

Ni is in position (a) and Cl in position (c) of the space group $R\bar{3}m$. Only the positional parameter z_{Cl} and the thermal parameters were refined by the least-squares method.

The resulting chlorine coordinate is $z_{Cl} = 0.2551 \pm 0.0008$. The variations of the thermal parameters from the isotropic value ($B = 2.0 \pm 0.2$ Å²) are within the e.s.d.'s.

The structure (*Strukturbericht*, vol. I, p. 742) is formed by octahedra [NiCl_{6/3}] grouped in layers. The metal-halogen distance is Ni-Cl = 2.426 ± 0.008 Å, which is somewhat shorter than the sum of the ionic radii. The distances between two chlorine atoms are Cl...Cl = 3.385 ± 0.016 Å and 3.483 ± 0.006 Å within each octahedron and Cl...Cl = 3.674 ± 0.016 Å between different octahedra. The latter distance is in good agreement with twice the van der Waals radius of chlorine. The angles Cl-Ni-Cl are $89 \pm 3^\circ$ and $92 \pm 3^\circ$.

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A demonstration of a moiré pattern and a pure twist boundary model. By H. OCKEN and E. N. AQUA, *Hammond Metallurgical Laboratory, Yale University, New Haven, Connecticut, U.S.A.*

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This communication describes interference phenomena resulting from two-dimensional point networks which can be interpreted either in terms of moiré patterns or dislocation models of pure twist boundaries.

Moiré patterns may be described as coarse arrange-

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ments produced by the superposition and, in this case, rotation of identical fine networks. The coarse patterns are enlarged versions of the fine ones. Using Gevers's (1962) notation, the size of the magnified moiré image, A , is related to the separation distance of the fine net-

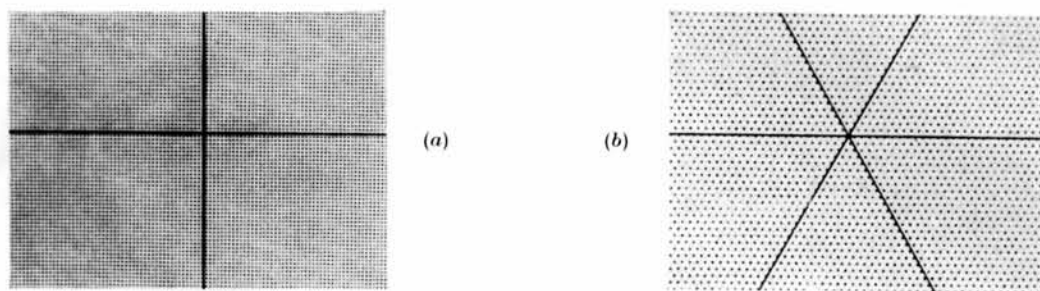


Fig. 1. (a) Elementary square network ($\alpha = \epsilon = 0$). (b) Elementary hexagonal network ($\alpha = \epsilon = 0$).

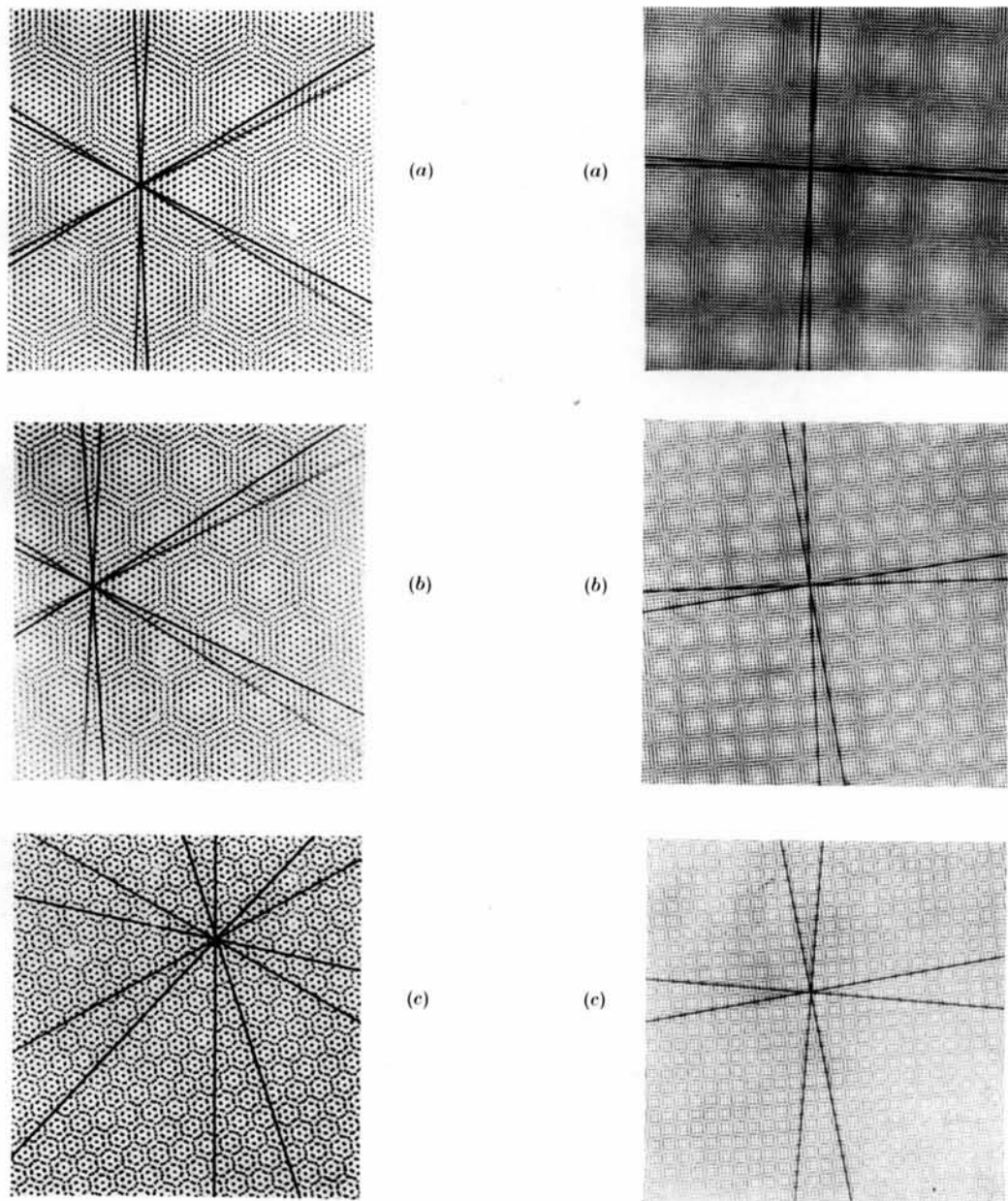


Fig. 2. Interference patterns resulting from hexagonal arrays.
(a) $\alpha = \epsilon = 4^\circ$. (b) $\alpha = \epsilon = 7^\circ$. (c) $\alpha = \epsilon = 18^\circ$.

Fig. 3. Interference patterns resulting from square arrays.
(a) $\alpha = \epsilon = 3^\circ$. (b) $\alpha = \epsilon = 7^\circ$. (c) $\alpha = \epsilon = 15^\circ$.

work, d_g , and the angle of rotation of the networks with respect to each other, ε , by the equation

$$A = d_g/2 \sin \frac{1}{2} \varepsilon . \quad (1)$$

Various dislocation models have been proposed to represent small angle boundaries in metals. For example, a pure twist boundary results from the relative rotation of two grains about an axis normal to the plane of the boundary. The atoms within the two grains comprising the boundary will join together continuously except along a network of screw dislocations. In a twist boundary occurring in a simple cubic structure, the grains may have a common $\{100\}$ plane, which is then the plane of the boundary. A twist boundary in a close-packed cubic structure has a common $\{111\}$ plane, which is also the plane of the boundary. In the former case, the boundary is a square grid of screw dislocations; in the latter case, the screw dislocations form a hexagonal network. Both types of twist boundaries can be analyzed through the use of Frank's (1955) formula,

$$\alpha = 2 \sin^{-1} (b/2h) , \quad (2)$$

which relates the angle of rotation, α , the Buerger's vector, b , of the dislocations comprising the twist boundary, and the distance between mesh centers, h , of the dislocation network.

The above formulas are identical except for notation. The moiré magnification, A , is the same as the separation between mesh centers, h , in the dislocation notation. The magnitude of the Buerger's vector, b , of a dislocation, is given by the separation of atoms in the close-packed direction, and is therefore equal to the dot separation

distance, d_g , in moiré terminology. The angles of rotation, α and ε , are, by definition, equal.

The few illustrations found in the literature, of the interference phenomena described above, have been produced by tedious drafting methods. The authors have developed a simple technique which enables these patterns to be easily generated. The procedure permits the variation of the parameters of interest to be easily effected.

Transparent architectural shading sheets containing uniformly spaced dots were used to obtain the interference patterns. Fig. 1 illustrates the two elementary fine networks. Rotation of one such sheet with respect to another identical one gives a magnified cellular array, *i.e.* a moiré pattern. Photographs were made at representative angles of rotation. Figs. 2 and 3 show the decrease in mesh size with increasing angle of rotation. One can also interpret the elementary networks as models of atomic planes. Viewed in this light, the square arrays of dots are analogous to the $\{100\}$ planes of a simple cubic structure; hexagonal arrays are analogous to the $\{111\}$ planes of a face-centered cubic structure. From the earlier discussion, it is clear that the resulting patterns can also be considered as models of a pure twist boundary.

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X-ray powder diffraction studies of YI_3 . By B. H. KRAUSE, A. B. HOOK and F. WAWNER,* *U.S. Army Engineer Research and Development Laboratories, Fort Belvoir, Virginia, U.S.A.*

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Yttrium triiodide has been prepared by heating high purity (99.995%) yttrium metal in an excess of iodine vapor within an initially evacuated chamber of high purity quartz. The resulting white salt was driven into quartz capillaries and flame-sealed under vacuum. The compound is highly hygroscopic and decomposes in air.

Powder diffraction photographs were taken with $CuK\alpha$ radiation. By comparison of the pattern with that of other triiodides (ASTM Powder Data File; Wyckoff), YI_3 was found to crystallize in the space group $R\bar{3} (C_{3i}^2)$

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with the BiI_3 structure. The lattice constants for the hexagonal unit cell at 20 °C are $a = 7.503 \pm 0.008 \text{ \AA}$ and $c = 20.81 \pm 0.02 \text{ \AA}$. The corresponding X-ray density is 4.617 g.cm.^{-3} .

We would like to thank Mr W. E. Sanburn of the Computer Section for performing the computations.

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