

(see Table 2). Calculations were not performed for aluminium since its rocking curve showed the existence of two peaks in the mosaic block distribution a few minutes of arc apart.

Table 2.

Interfering reflecting planes	[(N - N'(0))/N] × 100 for copper (111)	
	Measured	Calculated
(115) ($\bar{3}\bar{3}\bar{3}$) ($\bar{2}\bar{2}\bar{4}$) ($\bar{2}\bar{2}\bar{4}$)	14.5	17.5
(113) (004)	23.5	21.5 (23.0)
($\bar{1}\bar{3}\bar{3}$) ($\bar{3}\bar{1}\bar{3}$)	13.0	13.0
($\bar{2}\bar{2}\bar{2}$)	9.4	11.4

Calculated values obtained using equation (16). Values in brackets for (113) and (004) obtained by graphical integration of equations (12) and (13).

Finally it should be pointed out that the density of inverted peaks and their magnitude effectively

prohibit the use of the crystal monochromator for precise measurements of neutron spectra. There would appear to be no simple valid method of correcting for these effects. Suitable choice of reflecting plane and plane of reflection could result in a reduction of the number of peaks observed.

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Diffusion Centrale des Rayons X par des Particules Filiformes

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The asymptotic form of the intensity scattered by an assembly of filiform particles is determined for large values of s and the geometrical parameters it depends on are given.

The influence of certain types of configuration on this asymptotic behaviour is discussed.

Introduction

Le problème mathématique que nous traitons ici nous a été suggéré par l'analyse de données expérimentales, tant de diffusion centrale des rayons X, que de diffusion de la lumière, obtenues avec des solutions de particules longues et rigides, notamment d'acide dés-oxyribonucléique et de certains polypeptides de synthèse. Bien souvent, en effet, nous avons constaté d'une part que la fonction $i(s)$ expérimentale a, pour s grand, la forme typique de bâtonnets:

$$i(s) = Ks^{-1} \quad (1)$$

$s \rightarrow \infty$

(K est une constante, $s = 2 \sin \theta \cdot \lambda^{-1}$, 2θ étant l'angle de diffusion), mais d'autre part que l'écart entre $i(s)$ et sa forme asymptotique Ks^{-1} devient parfois important à mesure que l'on se rapproche des petites valeurs de s .

Or on sait que si un échantillon est formé de bâtonnets longs et rigides, $i(s)$ admet un développement asymptotique dont le premier terme, d'ordre s^{-1} , ne dépend que de leur masse linéaire spécifique (Kratky, 1956; Luzzati, 1960). Nous nous sommes proposé

d'étendre ce développement asymptotique en déterminant les paramètres structuraux dont dépendent les termes d'ordre supérieur à s^{-1} . Pour cela nous avons choisi un modèle plus général que celui des bâtonnets, mais dans lequel la matière est toujours distribuée uniformément le long d'un fil.

Ce modèle est analogue à la 'worm-like chain' dont Porod (1949) s'est servi pour traiter un problème analogue à celui que nous nous proposons de résoudre ici: nous discuterons plus loin ses résultats.

Bien que le traitement mathématique soit formulé ici dans le cas de la diffusion des rayons X, il s'applique également à la diffusion de la lumière.

Traitement mathématique

Nous admettons dans la suite que toute la matière de l'échantillon est localisée dans un ou plusieurs filaments de dimensions transversales négligeables, dont la masse spécifique linéaire est partout la même. L est la longueur totale des filaments de l'échantillon, M leur masse ($\mu = M/L$). Nous supposons en outre que l'échantillon est isotrope.

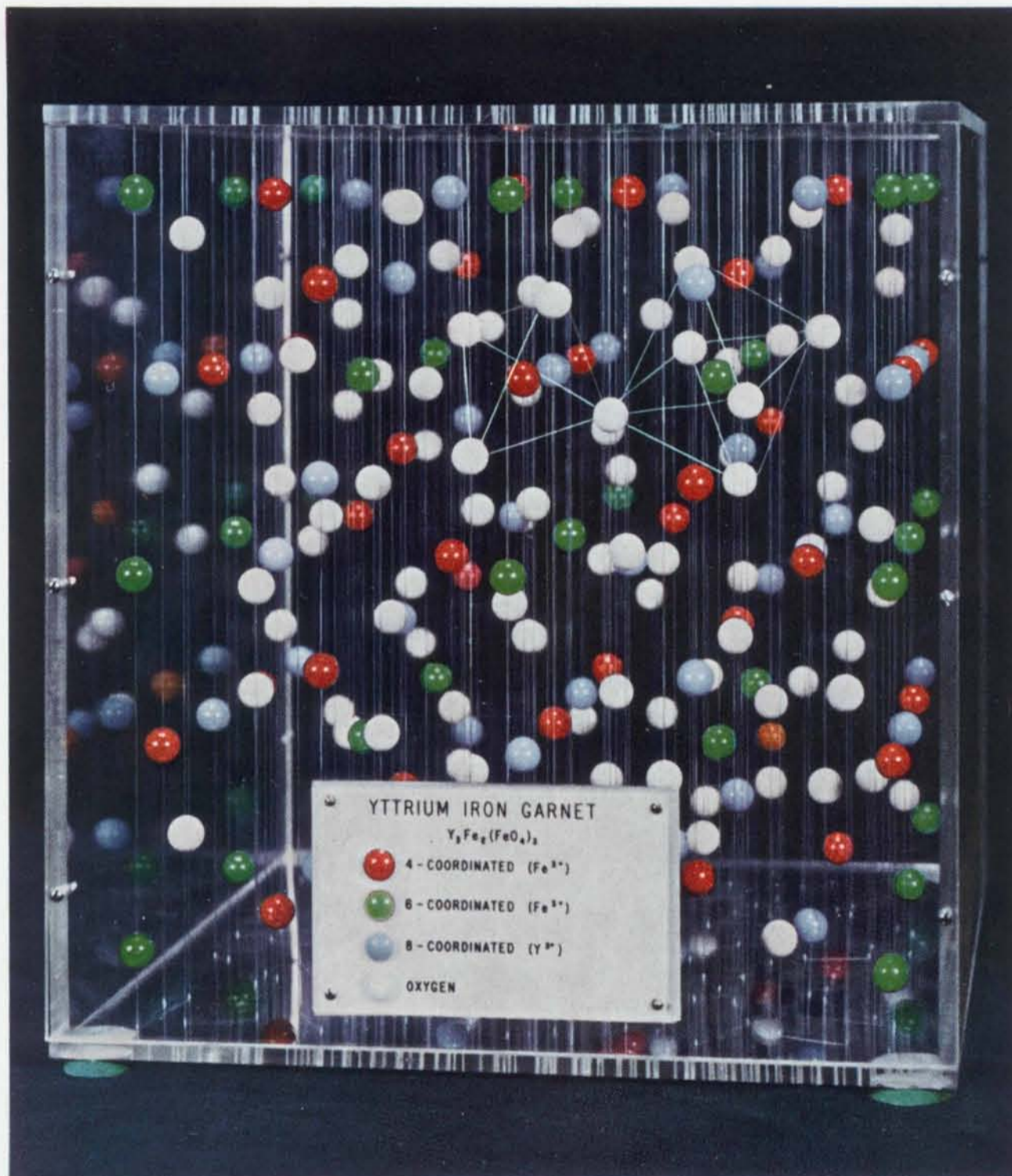


Fig. 2. Finished model of yttrium iron garnet having 160 atoms in the unit cell.

is made. The positions may be tabulated from the data in the *International Tables for X-ray Crystallography* (1952) arranging it in such a way that the order of stringing the balls on each thread is obvious. For triclinic crystals a displacement of top and bottom plates with threads running at an angle other than 90° to the base will represent the unit cell successfully.

The $\frac{1}{2}$ inch diameter plastic balls* must be drilled to accommodate the nylon thread. A straight hole through the center of the ball will allow the ball to drop freely out of position. To prevent this the hole is made with a bend in the interior of the ball as shown in Fig. 1(a). This can be accomplished by drilling in from two opposite ends of a diameter at an angle of 24° using the jig shown in Fig. 1(b). Two brass blocks $\frac{3}{4} \times 1 \times 2$ inches each with spherical hollows of the radius of the plastic ball are slotted on the sides to take phosphor bronze springs to hold the ball firmly. The drill #70 (0.028 inch) is guided in a hardened steel bushing first from one side and then from the other.

To string the nylon thread, the front and back of the plastic box are removed, and the nylon cord is passed through the holes in the top and bottom, adding the required balls on each string in their proper order according to the tabulated crystallographic data. This stringing may be done with one continuous piece of thread or perhaps more conveniently in sections, starting at the center of the box, and securing each thread with a knot at the bottom. After stringing loosely, the tension on each thread is adjusted and all balls pushed to the top. The balls are then set to the proper height in sequence using a toolmaker's

* Obtained from Allied Plastics Corp., 75 Cliff Street, New York.

surface height gauge. To leave room for knots and the nylon cord on the underside of the box, four $\frac{1}{4}$ inch thick felt disks—approximately 1 inch in diameter are glued on for feet.

Example

The general effect of the model can be seen from the photograph of Fig. 2, where a model of Yttrium iron garnet is shown. The colors of the balls represent different types of coordination of oxygen around the metal atoms in this model. For emphasis the coordination can be conveniently represented by attaching threads to the appropriate balls to form the coordination figure. In the photograph of Fig. 2 it is possible to see the octahedral and tetrahedral coordination figures which have been outlined this way. If cotton thread is used for this purpose, the segments are sometimes loose after being glued in place. They can be tightened by wetting with water, after which they will shrink an appreciable fraction of their length. One successful glue is collodion which dries quickly enough that the thread can be held in place by hand until set.

The example shown for this crystal with 160 atoms in the unit cell was fabricated easily enough to suggest that no serious study of a crystal need be carried out without the aid of an appropriate model.

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