

Table 1. Lattice parameters and structural data for some GdM compounds, where M is Al, Cu, Rh, Ag or Au

Compound	Lattice constant	Structure type	Reference
GdAl	$a = 3.7208 \pm 0.0002 \text{ \AA}$	CsCl + 2nd phase	(a)
GdAl	$a = 9.274 \pm 0.007$ $b = 7.679 \pm 0.008$ $c = 5.584 \pm 0.003$	CeAl	This paper
GdCu	$a = 3.505$	CsCl	(b)
GdCu	$a = 3.503 \pm 0.001$	CsCl	(a)
GdCu	$a = 3.5020 \pm 0.0004$	CsCl	This paper
GdRh	$a = 3.4425 \pm 0.0006$	CsCl	This paper
GdAg	$a = 3.66$	CsCl	(c)
GdAg	$a = 3.653$	CsCl	(d)
GdAg	$a = 3.6476 \pm 0.0008$	CsCl	(a)
GdAg	$a = 3.6491 \pm 0.0002$	CsCl	This paper
GdAu	$a = 3.593 \pm 0.002$	CsCl + 2nd phase	(e)
GdAu	$a = 3.6009 \pm 0.0008$ $a = 4.522 \pm 0.005$ $b = 10.826 \pm 0.008$ $c = 4.734 \pm 0.004$	CsCl and CrB	This paper This paper

(a) Baenziger & Moriarty (1961). (b) Dwight (1959a). (c) Dwight (1959b). (d) Iandelli (1960). (e) Chao, Luo & Duwez (1963).

Examination of the published literature indicates that the rare earth-aluminum compounds, RAl, crystallize with either b.c.c., CsCl type or one of two different orthorhombic structures, *i.e.* CeAl type, which belongs to the space group $Cmc2_1$ (van Vucht, 1957) or CrB type found for YAl (Dagerhamn, 1963). All the lines in the GdAl powder pattern could be indexed on the basis of the CeAl type orthorhombic structure. Although Baenziger & Moriarty (1961) found some b.c.c. lines in their complex X-ray pattern for GdAl while none were found in this research, this does not necessarily indicate that one of the results is incorrect. The difference could be explained by the existence of a high-temperature b.c.c. phase retained upon quenching by Baenziger & Moriarty (1961) but not retained in this research because of either too slow a cooling rate during quenching or too low an annealing temperature, *i.e.* below the orthorhombic \rightleftharpoons b.c.c. transition temperature.

Chao, Luo & Duwez (1963) found that when GdAu was very rapidly quenched, only the b.c.c. lines were observed, but when this compound was slowly cooled both the complex and b.c.c. lines were obtained. No other literature data

are available concerning the structures of the complex phase of any of the rare-earth-gold equi-atomic compounds. All the lines, other than those which were indexed as b.c.c., CsCl type, could be indexed as orthorhombic CrB, B_f type.

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References

- BAENZIGER, N. C. & MORIARTY, J. L., JR. (1961). *Acta Cryst.* **14**, 948.
 CHAO, C. C., LUO, H. L. & DUWEZ, P. (1963). *J. Appl. Phys.* **34**, 1971.
 DAGERHAMN, T. (1963). *Acta Chem. Scand.* **17**, 267.
 DWIGHT, A. E. (1959a). U. S. Atomic Energy Comm. Rept. ANL-6099.
 DWIGHT, A. E. (1959b). *Trans. Met. Soc. AIME*, **215**, 283.
 IANDELLI, A. (1960). *Atti accad. nazl. Lincei Rend., Classe sci. fis. mat. e nat.* **29**, 62.
 VUCHT, J. H. N. VAN (1957). *Z. Metallk.* **48**, 253.

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Infinite slit height corrections in small angle X-ray scattering*. By B. CHU and D. M. TAN CRETU, *Chemistry Department, The University of Kansas, Lawrence, Kansas, U.S.A.*

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The problem of correcting for the effect of beam height on scattering curves, which will be referred to as 'unsmearing' (Entschmierung), has been considered by many authors (Guinier & Fournet, 1947a, b, 1955; DuMond, 1947; Shull & Roess, 1947; Yudowitch, 1949; Franklin, 1950; Kratky, Porod & Kahovek, 1951; Schmidt, 1955; Gerold, 1957; Kratky, Porod & Skala, 1960; Schmidt & Hight, 1960; Heine & Roppert, 1962; Heine, 1963; Kent & Brumberger, 1964; Rausell-Colom, 1963). However, numerical calculations are tedious without the aid of a computer and col-

limation correction has often become a time-consuming obstacle for beginners in small-angle X-ray scattering work. It is therefore of interest to point out the simplicity of Schmidt's method (Schmidt & Hight, 1960) which has the advantage of eliminating the need for numerical differentiation or functional fitting of the experimental curve. Furthermore, for an infinitely long and negligibly wide primary beam, his approximate method is applicable to all slit collimated cameras provided that the requirement for infinite slit height approximation is satisfied.

For slits of negligible width and infinite height, the experimental scattered intensity $F(h)$ for a scattering angle h is related to the perfect collimation scattered intensity $I(h)$

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by the equations (Guinier & Fournet, 1947, *a, b*, 1955; DuMond, 1947):

$$F(h) = \int_0^{\infty} I[(h^2 + \varphi^2)^{\frac{1}{2}}] d\varphi \quad (1)$$

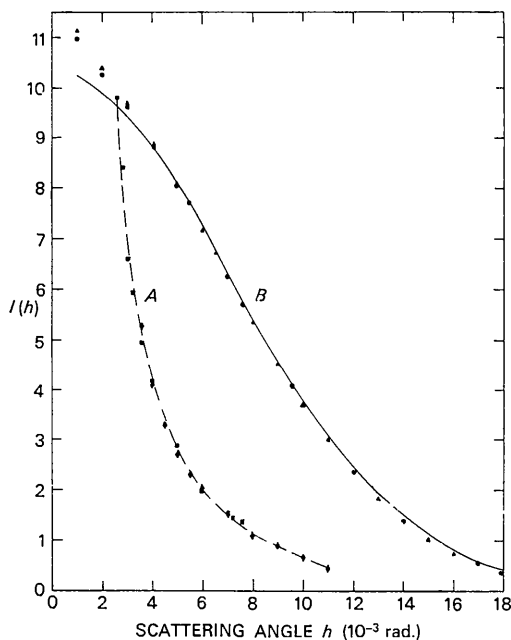


Fig. 1. Plot of perfect collimation scattered intensity $I(h)$ versus scattering angle h . Curve A represents the angular dissymmetry of polystyrene ($M_n = 147,000$, $M_w/M_n = 1.04$) in cyclohexane near the critical mixing point (Chu, 1965). The diamonds are the points calculated by the unsmearing process, using equation (3) with the summation going from $i=1$ to 15. The squares are the points calculated by Brumberger's unsmearing process (Kent & Brumberger, 1964). The solid line (Curve B) gives the perfect collimation scattering proportional to $\exp(-10^4 h^2)$. The points show the results of applying the unsmearing process to $F(h) \propto \exp(-10^4 h^2)$. The circles are the points using equation (3) with the summation going from $i=1$ to 15. The triangles are the points using only ten terms $\sum_{i=1}^{10} T_{ij} F[(i+j)\Delta h]$.

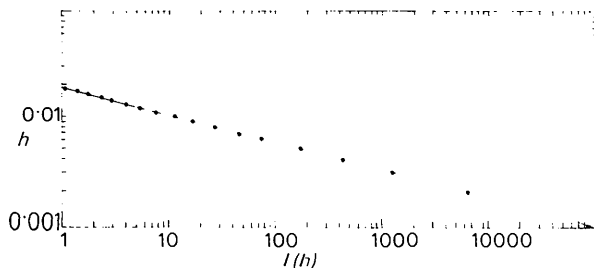


Fig. 2. Plot of scattering angle h versus perfect collimation scattered intensity $I(h)$. The solid line gives the perfect collimation scattering proportional to the inverse fourth power of the angle. The points show the results of applying the unsmearing process to $F(h) \propto h^{-3}$.

$$I(h) = \frac{-2}{\pi} \int_0^{\infty} \frac{dt}{(h^2 + t^2)^{\frac{3}{2}}} F'[(h^2 + t^2)^{\frac{1}{2}}]. \quad (2)$$

Modification of equation (2) leads us to (Schmidt & Hight, 1960):

$$I(h) \propto \frac{1}{j^2} [j(2j+1)^{\frac{1}{2}} F(j\Delta h) - \sum_{i=1}^{\infty} T_{ij} F\{(i+j)\Delta h\}] \quad (3)$$

with

$$T_{ij} = (\Delta h)^{-1} (j+i)(\Delta^2 ij)$$

$$\Delta_{ij}^2 = -R_{i+1} + 2R_i - R_{i-1}$$

$$R_i = \Delta h(i^2 + 2ij)^{\frac{1}{2}}$$

$$h = j\Delta h$$

$$h_i = (i+j)\Delta h.$$

Equation (3) is suitable for numerical evaluation and computer programming. (FORTRAN source programs for IBM 1620 and 7040 computers are available.) The authors can supply the table of T_{ij} ($i=1$ to 20, $j=1$ to 120). As these values are the same for all experimental curves, regardless of the type of slit collimated camera one uses, a point on the unsmear curve can be computed with a desk calculator if a table of T_{ij} is available. Figs. 1 and 2 show tests of the unsmearing process. We used $\Delta h = 10^{-3}$ radian, and found that the errors amount to about a few per cent except at the smallest angles ($h \sim 10^{-3}$ rad.).

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References

- CHU, B. (1965). *J. Chem. Phys.* **42**, 426.
 DUMOND, J. W. M. (1947). *Phys. Rev.* **72**, 83.
 FRANKLIN, R. E. (1950). *Acta Cryst.* **3**, 158.
 GEROLD, V. (1957). *Acta Cryst.* **10**, 287.
 GUINIER, A. & FOURNET, G. (1947a). *J. Phys. Radium*, **8**, 345.
 GUINIER, A. & FOURNET, G. (1947b). *Nature, Lond.* **160**, 501.
 GUINIER, A. & FOURNET, G. (1955). *Small-angle Scattering of X-rays*. New York: John Wiley.
 HEINE, S. (1963). *Acta Phys. Austriaca*, **16**, 144.
 HEINE, S. & ROPPERT, J. (1962). *Acta Phys. Austriaca*, **15**, 148.
 KENT, P. & BRUMBERGER, H. (1964). *Acta Phys. Austriaca*, **17**, 18.
 KRATKY, O., POROD, G. & KAHOVEK, L. (1951). *Z. Elektrochem.* **55**, 53.
 KRATKY, O., POROD, G. & SKALA, Z. (1960). *Acta Phys. Austriaca*, **13**, 76.
 RAUSELL-COLOM, J. A. (1963). *Brit. J. Appl. Phys.* **14**, 31.
 SCHMIDT, P. W. (1955). *Acta Cryst.* **8**, 772.
 SCHMIDT, P. W. & HIGHT, R. (1960). *Acta Cryst.* **13**, 480.
 SHULL, C. G. & ROESS, L. C. (1947). *J. Appl. Phys.* **18**, 295.
 YUDOWITZ, K. L. (1949). *J. Appl. Phys.* **20**, 174, 1232.