

Fig. 2.

Wie in Fig. 2 gezeigt, kann der Neutronenleiter aus zwei entgegengesetzt gekrümmten Teilstücken 'einfacher direkter Sichtweite' zusammengesetzt werden. Durch die Richtungsänderung treffen Neutronen, die im ersten Abschnitt noch unter sehr kleinen Winkeln nur an der gekrümmten Aussenfläche reflektiert wurden (girlandenreflektiert), im zweiten Abschnitt mit zu grossem Winkel auf und gelangen nicht mehr durch den Leiter. Die über den Querschnitt gemittelte Durchlässigkeit für den doppelt gekrümmten Neutronenleiter, zeigt ebenfalls Fig. 1. Für $k_z \geq \sqrt{2}k_{z,m}$ ist die Durchlässigkeit Null. Wählt man $k_z = 0,8 k_{z,m}$, dann ist der Verlust gegenüber einem geraden Neutronenleiter nur 30%. Die in z-Richtung austretenden Neutronen haben am linken und rechten Rand die maximale Wellenzahl $k_z = k_{z,m}$ in der Mitte die maximale Wellenzahl $k_z = \sqrt{2}k_{z,m}$. Die Impulsraumbreite in der k_x -Richtung ist ebenfalls in der Mitte des Strahls am grössten. Der Neutronenstrahl ist bezüglich seiner Impulsraumverteilung symmetrisch zur Mitte

des Strahls, im Gegensatz zum einfach gekrümmten Neutronenleiter (siehe auch Maier-Liebnitz, 1965).

Wie man aus Fig. 2 ersieht, gelangen schnelle Neutronen und γ -Strahlen bestenfalls nach zweimaliger Streuung aus dem Neutronenleiter. Die Anordnung könnte symmetrisch verkürzt werden bis zu $(\frac{1}{2} + \sqrt{\frac{3}{4}})L_{II}$, jedoch ist dieser Gewinn nicht wesentlich und aus Abschirmungsgründen ist es auf jeden Fall zweckmässig die Baulänge gleich L_{II} zu belassen, auch gilt die Kurve in Fig. 1 exakt nur für $L \geq L_{II}$.

Ein Dimensionierungsbeispiel für 4 Å - Neutronen möge den Sachverhalt noch veranschaulichen: Gewünscht sei eine Strahlbreite von 3 cm. Mit $k_z = 0,8 k_{z,m}$ berechnet sich nach voriger Gleichung der Krümmungsradius und damit nach Fig. 2 die Länge zu 45 Meter. Der Divergenzwinkel α am Ausgang des Neutronenleiters ist für beide Richtungen senkrecht zum Strahl 50 Winkelminuten bei 4 Å - Neutronen.

Herrn Professor Maier-Liebnitz danke ich für fruchtbare Diskussionen.

Literatur

- MAIER-LEIBNITZ, H. (1966). *Nukleonik*. Erscheint demnächst.
 MAIER-LEIBNITZ, H. & SPRINGER, T. (1963). *J. Nuclear Energy*, A/B 17, 217.

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Separation of particle size and lattice strain in integral breadth measurements*. By N. C. HALDER and C. N. J. WAGNER, *Hammond Laboratory, Yale University, New Haven, Connecticut, U.S.A.*

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In the Warren & Averbach (1950, 1952) analysis of line broadening, the Fourier coefficients $A^D(L)$ of the line profiles broadened by lattice strains ϵ_L can be represented to a good approximation by a Gaussian function for small values of ϵ_L , i.e., $A^D(L) \approx \exp[2\pi^2 L^2 \langle \epsilon_L^2 \rangle / d^2]$ where L is the distance normal to the planes of interplanar spacing d . The particle size D_e is the reciprocal of the negative slope of the particle size coefficients $A^P(L)$ versus L curve at $L=0$, and $A^P(L)$ can be approximated by $A^P(L) \approx \exp[-L/D_e]$. The Fourier transforms of $A^D(L)$ and $A^P(L)$ lead to Gaussian and Cauchy line profiles respectively. Recently Schoening (1965) has demonstrated that the integral breadth of a line profile produced by the convolution of a Gaussian profile with a Cauchy profile is

$$b(s) = b^D \exp[-(b^P/\sqrt{\pi}b^D)^2][1 - \text{erf}(b^P/\sqrt{\pi}b^D)], \quad (1)$$

where

$$\text{erf}(b^P/\sqrt{\pi}b^D) = (2/\sqrt{\pi}) \int_0^{b^P/\sqrt{\pi}b^D} \exp(-t^2) dt; \quad (2)$$

b^D and b^P are the integral breadths due to strain and particle size and are given by

$$b^D = 1/\int_{-\infty}^{\infty} A^D(L) dL = 2\epsilon_1/d = \sqrt{2\pi} \langle \epsilon_L^2 \rangle^{1/2} / d \quad (3)$$

and

$$b^P = 1/\int_{-\infty}^{\infty} A^P(L) dL = 1/D_e = 1/2D_e, \quad (4)$$

Table 1. Values of particle sizes and strains in cold-worked silver-10% indium and pure tungsten fillings

Particle size		Warren-Averbach	Equation (5)		Equation (6)
Material	$[hkl]$	D_e	D_e^P	D_e	D_e^G
Ag-10%In	[111]	120 Å	210 Å	105 Å	185 Å
Ag-10%In	[100]	70	155	76	120
W	Isotropic	210	430	215	350
Strains		Warren-Averbach	Equation (5)		Equation (6)
Material	$[hkl]$	$\langle \epsilon_L^2 \rangle^{\frac{1}{2}}$	ϵ_L^P	$\langle \epsilon_L^2 \rangle^{\frac{1}{2}}$	ϵ_L^G
Ag-10%In	[111]	0.0038	0.0042	0.0034	0.0051
Ag-10%In	[100]	0.0050	0.0083	0.0066	0.0091
W	Isotropic	0.0020	0.0037	0.0030	0.0041

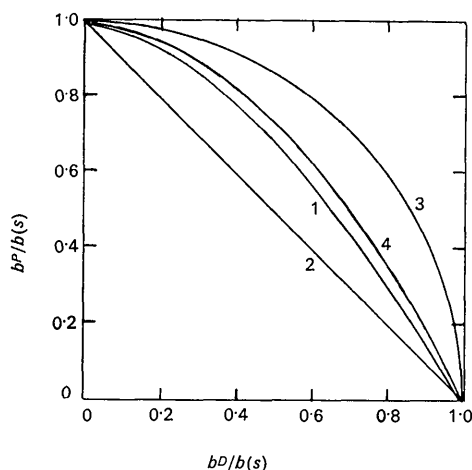


Fig. 1. Plots of $b^P/b(s)$ versus $b^D/b(s)$
 Curve 1: $b(s) = b^D \exp [-(b^P/\sqrt{\pi}b^D)^2]/[1 - \text{erf}(b^P/\sqrt{\pi}b^D)]$
 Curve 2: $b(s) = b^P + b^D$
 Curve 3: $b(s) = [(b^P)^2 + (b^D)^2]^{\frac{1}{2}}$
 Curve 4: $b^P/b(s) = 1 - [b^D/b(s)]^2$

where ϵ_I and D_I are the integral breadth strain and particle size, respectively. Equation (1) is too complicated and cannot be handled conveniently to estimate the particle size and strain. We suggest that the equation

$$b^P/b(s) = 1 - [b^D/b(s)]^2 \quad (5)$$

is a very good approximation to equation (1) and can be employed without difficulty. We plot $b^P/b(s)$ versus $b^D/b(s)$ from equations (1) and (5) and see that the difference between the two curves is at most 10%. This is illustrated in Fig. 1.

We analyzed the broadening of cold-worked pure tungsten and Ag-10% In alloy by the Warren-Averbach analysis, by applying equation (5) and also by applying

$$b^2(s) = (b^D)^2 + (b^P)^2 \quad (6)$$

Equation (6) is obtained when both the particle size and strain profiles are approximated by Gaussian functions.

Pure tungsten and Ag-10% In filings were prepared at room temperature (23°C) and powder pattern peaks were

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Composition and crystallographic data for the highest boride of tungsten. By P. A. ROMANS and M. P. KRUG, *U. S. Bureau of Mines, Albany Metallurgy Research Center, Albany, Oregon, U.S.A.*

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Chretien & Helgorsky (1961) have described the highest boride of tungsten, which they called WB₄, as tetragonal with $a_0 = 6.34$ and $c_0 = 4.50$ Å. Goldschmidt, Catherall, Ham & Oliver (1963) also observed this compound but reported slightly different parameters ($a_0 = 6.36$ and $c_0 = 4.42$ kX). We have now made a detailed study of this compound and found the unit cell to be hexagonal with $a_0 = 5.200$ and $c_0 = 6.340$ Å. We have also found evidence that while the ideal formula is WB₄, the compound we studied

recorded on a Norelco diffractometer using the nickel-filtered copper radiation. The Fourier analyses of the powder pattern peaks were carried out by the Warren-Averbach technique and the instrumental correction for the integral breadths was made with the use of a parabolic relationship after Wagner & Aqua (1963). The particle size and strain calculated from the Warren-Averbach analysis, present method and pure Gaussian (considering both strain and particle size distribution as Gaussian) approximation are shown in Table 1.

Of the two materials investigated, Ag-10% In is highly faulted and tungsten is free of faults. The particle sizes D_I^P for Ag-10% In obtained by the present method are about twice as high as those obtained by Warren-Averbach analysis. As shown by Mitra & Halder (1964) and Wagner & Aqua (1965) in the case of h.c.p. metals and by Wagner & Aqua (1963) in the case of f.c.c. and b.c.c. metals, if fault broadening predominates, $D_I \approx 2D_e$. The particle size D_I^G calculated from Gaussian approximation for both strain and particle size distribution is only slightly smaller than D_I^P .

For tungsten filings the integral breadth particle size D_I^P is also twice as large as the particle size $D_e = \bar{D}$. This is in agreement with the definitions of D_I and \bar{D} since

$$D_I = \overline{D^2}/\bar{D} > \bar{D}.$$

As shown above, the approximation $A^P(L) \approx \exp[-L/D_e]$ leads to the relation $D_I = 2D_e$.

The lattice strains calculated with equation (5) are lower than those obtained with equation (6), and are in rather good agreement with the root-mean-square strains $\langle \epsilon_L^2 \rangle^{\frac{1}{2}}$ averaged over the dimensions of the coherently diffracting domains, i.e. $\epsilon_I^P \approx 1.25 \langle \epsilon_L^2 \rangle^{\frac{1}{2}}$.

References

- MITRA, G. B. & HALDER, N. C. (1964). *Acta Cryst.* **17**, 817.
 SCHOENING, F. R. L. (1965). *Acta Cryst.* **18**, 975.
 WAGNER, C. N. J. & AQUA, E. N. (1963). *Advanc. X-ray Anal.* **7**, 46.
 WAGNER, C. N. J. & AQUA, E. N. (1965). *J. Less Common Metals*, **8**, 51.
 WARREN, B. E. & AVERBACH, B. L. (1950). *J. Appl. Phys.* **21**, 595.
 WARREN, B. E. & AVERBACH, B. L. (1952). *J. Appl. Phys.* **23**, 1059.

may contain more than stoichiometric amounts of boron.

There are two problems in determining the composition of this compound. First, it is very difficult to produce a single-phase sample large enough for conventional methods of analysis. Second, owing to the large difference in atomic weight, very accurate analysis is necessary to distinguish between WB₄ and WB₅.

We solved the first problem by electron microprobe analysis of several individual grains in three-phase samples