SPECIALIA

X-Ray Research of Polycrystals. X-Ray Diffraction Methods for Precision Determinations of Polycrystal Lattice Parameters over Unsolved Double Lines

The present report considers the possibility of the precise determination of lattice parameters over unsolved and partially solved double lines. The determination of lattice parameters were carried out in this case using 2 points of a diffractional line profile – the middle of a width and the weights-centre. The wave-lengths, corresponding to the above points of the profile of a spectral distribution curve, were used. The values of the wave-lengths were estimated by formulae:

(a) for the point of a weights-centre:

$$\lambda_{\alpha b} = \frac{J_1 \lambda_{\alpha_1 b} + J_2 \lambda_{\alpha_2 b}}{J_1 + J_2}.$$

(b) for the point of a middle width:

$$\lambda_{\alpha av} = \frac{J_1 \lambda_{\alpha_1 av} + J_2 \lambda_{\alpha_2 av}}{J_1 + J_2}.$$

Where J_1 and J_2 are the relative intensities of the components α_1 and α_2 of a doublet, $\lambda_{\alpha_i b}$ and $\lambda_{\alpha_i av}$ ($i = 1.2$) are found from the formulae[1].

The preparation of specimens, exposition and evaluation of angles was carried out as in our earlier work[1]. The parameter of the crystallic lattice of armco-iron was determined over the unsolved double line (2II), using *Cr* K_α-radiation. The mean values of the parameters, estimated over the points of the middle of a width and a weights-centre are equal to 2.86596 ± 0.00008 Å and 2.86599 ± 0.00023 Å, accordingly.

In the case of a partially solved double line, we suggest the following method of the location of a middle-width point.

(1) The lines parallel to the background line are to be drawn through the middle of the height of each component of a doublet.

(2) The segment of a height between these 2 lines is to be divided in ratio $J_2:J_1$ ($\approx 1:2$).

(3) The line parallel to the background line is to be drawn through the above point. The middle of the line obtained is the point to be found.

The lattice parameter of tungsten (W) of 99.95% purity was determined over the middle of the width of the partially solved double line (400), using Cu K_α-radiation. The mean value of the parameter, corrected to 25 °C and for refraction, is equal to 3.16531 ± 0.00008 Å. The lattice parameter of tungsten (W), determined over (420) β-like, is equal to 3.16534 ± 0.00005 Å.

Выводы. Предложена методика рентгенографического прецизионного определения параметров решетки поликристаллов по неразрешенным дублетным линиям. Проведена экспериментальная проверка метода на образцах армко-железа и вольфрама.

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[1] G. V. Davydov, V. P. Dzekanovskaya and N. A. Erokhov, Experientia *23*, 349 (1967).

X-Ray Research of Polycrystals. The Methods for Approximation at Determination of the Real Width of X-Ray Interferentional Lines with the Application of a Standard-Sample

According to the suggested approximating function for the profiles of diffractional lines[1]

$$\varphi(x) = \alpha\, x^\gamma \exp(-\varepsilon\, x)$$

and using the definition of a line width

$$B = \frac{\int_0^\infty \varphi(x)\, dx}{\varphi(x_m)}$$

it is easy to obtain an expression for the absolute meaning of B:

$$B = \frac{c\sqrt{\gamma}}{\varepsilon} \quad (c \approx \sqrt{2\,\pi})\,. \tag{1}$$

It is possible to obtain an expression for the physical broadening of a line due to the blocks dispersity and the second kind of tensions, supposing that the profile of a considered line is described by the function $h(x) = \alpha, x^{\gamma_1}$ $\exp(-\varepsilon, x)$, and the profile of a standard line – by the function $f(x) = \alpha_2\, x^{\gamma_2} \exp(-\varepsilon_2\, x)$. Then

$$\beta = \frac{\gamma_2\, \varepsilon_1 + \varepsilon_2}{\varepsilon_1\, (\varepsilon_2 - \varepsilon_1)} \exp(\varepsilon_1\, \xi_m) \tag{2}$$

where

$$\xi_m = \frac{\varepsilon_2 - \varepsilon_1\, (\gamma_2 + 2)}{\varepsilon_1\, (\varepsilon_2 - \varepsilon_1)}\,.$$

[1] G. V. Davydov, N. A. Erokhov and G. F. Belyaeva, Experientia *23*, 352 (1967).

Taking (1) into account, one obtains:

$$\beta = \frac{B}{c} \cdot \frac{\gamma_2 b + B \sqrt{\gamma_2}}{B \sqrt{\gamma_2} - b} \exp\left[\frac{b (\gamma_2 + 2) - B \sqrt{\gamma_2}}{b - B \sqrt{\gamma_2}}\right] \tag{3}$$

and

$$\xi_m = \frac{B}{c} \cdot \frac{B \sqrt{\gamma_2} - b (\gamma_2 + 2)}{B \sqrt{\gamma_2} - b} . \tag{4}$$

Note that the analythical method, used in present paper to derive the formulae (2–4), can be used for the separation of the effects, induced by the substance dispersity and the microtensions of the second type.

Выводы. Дана формула для определения истинной ширины рентгеновских линий и получена связь между физической шириной и уширениями, обусловленными дисперсностью блоков и напряжениями 2 рода.

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X-Ray Research for Polycrystals. The Formation Geometry of Instrumental Width of the Diffractional Line at the Investigation of the Polycrystals in the Translucent X-Rays

We have solved the tridimensional problem of determination of the instrumental broadening of a line at the study of polycrystals in the reflected rays[1,2].

In the present paper the analogical problem is solved for the study of polycrystals in translucent lighting under the following conditions: the point radiation source: the flat sample, having the definite thickness and the definite area of irradiation, and the reflex recording line is a straight line, parallel to the sample plane (Figure).

Originating from the geometry of the Figure, one obtains the general formula for the position of a reflex:

$$y_1 = y + \frac{(x_0 x - z^2) y + \sqrt{(x_0 x - z^2)^2 y^2 + [(x_0^2 + y^2 + z^2) \cos^2 \beta - y^2] [(x_0 x - z^2)^2 - (x^2 + z^2) (x_0{}^2 + y^2 + z^2) \cos^2 \beta]}}{(x_0^2 + y^2 + z^2) \cos^2 \beta - y^2} \tag{1}$$

where

$$x_0 = x_2 - x .$$

It follows from formula (1), that the maximal and the minimal deviations on the recording line are given by those rays which reflect from the specimen in the points N_1 (x'', m, o) and N_3 (x', $-m$, k) accordingly.

According to the above formula (1) can be expressed as follows:

$$y_{1,m} = m + \frac{x'' [(x_2 - x'')^2 + m^2] \operatorname{tg}\beta + m x'' (x_2 - x'') (1 + \operatorname{tg}^2 \beta)}{(x_2 - x'')^2 - m^2 \operatorname{tg} \sqrt[2]{\beta}} \tag{2}$$

and

$$y_{1,-m,k} = - m + \frac{- m (x_0 x' - k^2) + \sqrt{(x_0 x' - k^2)^2 m^2 + [(x_0^2 + m^2 + k^2) \cos^2 \beta - m^2] [(x_0 x' - k^2)^2 - (x'^2 + k^2) (x_0^2 + m^2 + k^2) \cos^2 \beta}}{(x_0^2 + m^2 + k^2) \cos^2 \beta - m^2} \tag{3}$$

where $x_0 = x_2 - x'$.

From (2) and (3) one obtains the instrumental broadening of a line

$$\Delta l = y_{1,m} - y_{1,-m,k} . \tag{4}$$

If the vertical expansion could be neglected, the minimal deviation on the recording line and the instrumental broadening of a line is described by the formulae in this case:

$$y_{1,-m} = - m + \frac{x^1 [(x_2 - x')^2 + m^2] \operatorname{tg}\beta - m x^1 (x_2 - x^1) (1 + \operatorname{tg}^2 \beta)}{(x_2 - x^1)^2 - m^2 \operatorname{tg}^2 \beta} \tag{3'}$$

and

$$\Delta l' = y_{1m} - y_{1,-m} . \tag{4'}$$

The Table shows the results of estimations of the instrumental width of a line for various experimental conditions at large and small scattering angles are listed.

In this Table, y_{av} and y'_{av} are the positions of the width-middle of a diffractional line in mm and β_{av} and β'_{av} are correspondent scattering angles.

It is seen from the Table, that the instrumental broadening of a line is considerable both at large and at small scattering angles. Nevertheless, the scattering angles, found over the points of the width-middles of lines, coincide rather precisely with the real meanings of the scattering angles at the correct choice of the instrumental factors.

Выводы. Решена задача инструментального расширения линии при исследовании поликристаллов в проходящих рентгеновских лучах при следующих условиях: источник лучей точечный, образец плоский, имеющий определенную толщину и площадь облучения, и линия регистрации