Contribution to the Method for Approximation of X-Ray Diffraction Line Profile

The methods at present commonly used for the investigations of fine intragranular structure of polycrystalline materials are the Fourier-analysis method and integral method (approximation method).

The diffraction line profile being the complex function depending on many factors, approximation using a small number of parameters cannot be an adequately accurate one. Increasing the number of parameters used, the precision of approximation becomes greater. So HALDER[1] obtained the improved approximating functions inserting additional parameters in the Gaussian function and Cauchy function. But employing these functions involves complicated and tedious calculations.

A simpler approximating function is taken in the present work:

$$y = f(x) = \alpha\, x^{\gamma} \cdot \exp(-\varepsilon\, x), \qquad \text{(I)}$$

where α, γ, ε are parameters, obtained by the mean-value method with the use of 'rectifying' method[2]; x is a coordinate expressed in terms of Θ-angles.

For the above function, when the given x-values make up a geometric progression having denominator q, the variables $Y = \Delta_1 \lg y$ and x will be linearly related according to expression:

$$Y = \gamma \lg q + [\varepsilon\,(q-1)\lg e] \cdot x \qquad \text{(II)}$$

Here $\Delta_1 \lg y$ is the difference between the 2 successive values of y with x varying according to the geometric progression[3].

As the criterion for the evaluation of accuracy of the approximation suggested, the centroid position was taken of the calculated line profile, which can be expressed by the well-known analytical relation:

$$X_c = \frac{\int x\, f(x)\, dx}{\int f(x)\, dx}$$

or, inserting the values of $f(x)$ from (I):

$$X_c = \frac{\int_0^{\infty} \alpha\, x^{\gamma+1} \exp(-\varepsilon\, x)\, dx}{\int_0^{\infty} \alpha\, x^{\gamma} \exp(-\varepsilon\, x)\, dx}.$$

On integration one gets:

$$X_c = \frac{\Gamma(\gamma+2)\,\varepsilon^{\gamma+1}}{\varepsilon^{\gamma+2}\,\Gamma(\gamma+1)},$$

which after transforming becomes:

$$X_c = \frac{\gamma+1}{\varepsilon}. \qquad \text{(III)}$$

In order to test experimentally the validity of formula (III), with the use of this formula calculations were made[4] of the Bragg angles from the X-ray diffraction pattern taken from the annealed pure aluminium (99.99%) on the diffractometer URS-501 with CuK_α – radiation.

For purposes of comparison, the calculations of the corresponding Bragg angles using the wellknown formula

$$X_p = \frac{\sum_{i=1}^{n} J_i\, X_i}{\sum_{i=1}^{n} J_i} \qquad \text{(IV)}$$

were also made.

The data obtained by the use of both the above methods, together with the data from [5], are listed in the Table. Analysing these data, one can see that the values calculated with the use of formula (III) are adequately close to the data[5] calculated with great accuracy (using many correction factors).

From the above considerations it follows that the approximation taken in the present work yields fairly good accuracy in Bragg-angle calculations, i.e. the approximating function proposed gives the line profiles closely approaching the experimental ones.

From Eq. (I) one can also derive the expressions for the line profile peak position:

$$X_p = \frac{\gamma}{\varepsilon} \qquad \text{(V)}$$

and for the relative integral breadth of diffraction line:

$$B = \frac{2\,\alpha\,\Gamma(\gamma+1)}{\varepsilon^{\gamma+1}}. \qquad \text{(IV)}$$

As is evident from the article, the relations (III), (V) and (VI) obtained in the present work are very simple. Therefore these can be recommended for rapid calculations yielding high accuracy.

Выводы. Предложена функция для аппроксимации дифракционного профиля рентгеновских линий. Получены формулы для расчета максимума, центра тяжести профиля и интегральной ширины линии. Проведена экспериментальная проверка метода на примере алюминия.

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hKL	Calculated values of $X_c = 2\Theta$ for *Al* pattern taken with CuKα-radiation		
	From formula (IV)	From formula (III)	According to DELF[5]
III	38° 34′	38° 31′	38° 30′
200	44° 50′	44° 48′	44° 48′
220	65° 13′	65° 14′	65° 12′
311	78° 20′	78° 20′	78° 18′

[1] N. C. HALDER, Physica, *30*, 1044 (1964).
[2] B. P. DEMIDOVICH, I.A. MARON and E. Z. SHUVALOVA, *Tchislennyeh Methody analiza*, F. M. L. (1963).
[3] Eq. (II) serves for determination γ and ε.
[4] No corrections were introduced in calculation, and the parameters ε and γ obtained by the mean-values method were used.
[5] B. W. DELF, Brit. J. Appl. Phys. *14*, 345 (1963).