Genetic algorithm application for solving X-ray diffraction inverse problem

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Abstract. For solving inverse problem of scattering of X-ray with transversely restricted wavefront from the ideal crystal within the dynamical theory of X-ray diffraction taking into account the effect of the diffractometer’s instrumental function the Genetic Algorithm in the form of Differential Evolution method was used. The calculations were performed.

Introduction

Today, the actual tasks are to increase quality control and improve the production of elements of nanoelectronic devices. The most effective method for analyzing the structure of this objects is X-ray diffraction. This method is sensitive to the fine details of the nanometre range. In addition, this method is non-destructive and rapid. The information on the structure of the object under study is obtained in the form of the scattering intensity distribution map in the reciprocal space, and to get the required parameters the inverse problem need to be solved. In addition to developing a theory describing the interaction of X-ray with matter, an effective algorithm for minimizing the residual functional is needed. The feature of this problem is in the large number of local minima in the parameter space and large number of parameters. Therefore, traditional iterative optimization methods are not well suited due to the considerable time required to find a solution. Evolutionary algorithms, including genetic ones [1], showed their high efficiency for searching solutions in the space of a large number of parameters in a wide range, particularly in problems of X-ray scattering [2, 3].

An experiment on X-ray scattering is simulated and an approach to the solution of the inverse problem is proposed.

Diffraction theory

In the X-ray scattering experiment, the total intensity obtained at the output of the detector is written as

\[ I_{\text{sim}}(q_x, q_z) = K \cdot I_h(q_x, q_z) + I_{bg}, \]

where \( I_{bg} \) – background intensity, \( K \) – intensity scaling parameter. The expression for the scattering intensity at the input of the detector, taking into account the influence of the instrumental function of the monochromator and the analyzer, has the form [1]

\[ I_h(q_x, q_z) = \frac{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dq_x dq_z M(q_x'q_z') R^A(q_x'q_z') R^M(q_x'q_z) \delta(q_x-q_x') \delta(q_z-q_z')}{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dq_x dq_z M(q_x'q_z') R^A(q_x'q_z')}, \]
where $R_M$, $R_A$ – monochromator and analyzer reflection coefficients, $I_h$ – beam scattering intensity. It can be represented as two terms, reflecting the nature of the scattering, connected through the Debye-Waller factor $f$

$$I_h(q_x, q_z) = (1 - f^2)I_h^c(q_x, q_z) + f^2I_h^d(q_x, q_z),$$

(3)

$I_h^c$ – the coherent part, describing the ideal crystal scattering. It contains information on the thicknesses and periods of the layers in the crystal structure; $I_h^d$ – the diffuse part. It contains information on the parameters of structural defects, such as quantum dots, pores, dislocations of different types (their size, shape, orientation, distribution in the sample, etc.).

The scattering intensity calculations were performed within the dynamical theory of X-ray diffraction expanded to the special case of transversely restricted wavefronts of the incident and reflected waves taking into account the effect of the diffractometer’s instrumental function [4]. In that case the intensity of the diffracted X-ray wave (in the Bragg geometry) near the reciprocal lattice point $\mathbf{h}$ depends on the illuminated area of the crystal top surface $f^{(in)}_x$ and crystal thickness $l_x$ as [4]

$$I_h^c(q_x, q_z) = \left| a_n \frac{\exp(i\hat{\mathbf{h}}l_x)}{\hat{Q}} \sin\left(\frac{q_x f^{(in)}_x}{2}\right)\right|^2,$$

(4)

where

$$\hat{\mathbf{h}} = 2a_0 - q_x \cot\theta_B - q_z,$$

$$\hat{Q} = \xi_1 \exp(i\xi l_z) - \xi_2,$$

$$\xi_1, \xi_2 = (-\hat{\mathbf{h}} \pm \hat{\Gamma})/2,$$

$$a_0 = \pi \chi_d/\left(\lambda \sin\theta_B\right),$$

$$a_n = C \pi \chi_d/n/\left(\lambda \sin\theta_B\right).$$

Here $\lambda$ – X-ray wavelength, $\chi_d$ – Fourier component of X-ray polarizability (determined by h), $C$ – polarization factor.

To model the experiment, Poisson noise function in the form of

$$n(q_x, q_z) = \sqrt{\frac{l_h(q_x, q_z)}{6\theta_B}} \text{rand}[-1, 1],$$

(5)

where rand([-1, 1]) – random value produced by pseudorandom number generator within the [-1,1] diapason, was also added to the expression (1) as a multiplier [3].

Residual functional

For the minimization procedure in the paper we considered the following types of residual functional

$$\rho_{abs}(q_x, q_z) = \frac{1}{N_f} \sum_{i=1}^{N_f} |I_{sim}(q_x, q_z; x) - I_{exp}(q_x, q_z)|,$$

(6a)

$$\rho_{sqr}(q_x, q_z) = \frac{1}{N_f} \sum_{i=1}^{N_f} \left| \frac{I_{sim}(q_x, q_z; x) - I_{exp}(q_x, q_z)}{I_{sim}(q_x, q_z; x)} \right|^2,$$

(6b)

$$\rho_{log}(q_x, q_z) = \frac{1}{N_f} \sum_{i=1}^{N_f} \left| \log I_{sim}(q_x, q_z; x) - \log I_{exp}(q_x, q_z) \right|,$$

(6c)

$$\rho_{log}(q_x, q_z) = \frac{1}{N_f} \sum_{i=1}^{N_f} \left| \log I_{sim}(q_x, q_z; x) - \log I_{exp}(q_x, q_z) \right|^2,$$

(6d)

where $x$ – vector of parameters in the parameter space, $I_{sim}$ – diffracted intensity theoretical data, $I_{exp}$ – experimental data.

The comparison between theoretical and experimental data in absolute value (6a) is effective for analysis at high values intensity, as well as for small-angle scattering in undeformed crystals. That is, in the cases when the data on the curve have the same order.

The root-mean-square deviation (6b) should be effective in cases similar to (6a). In addition, if it is used, the accuracy of the solution is slightly affected by the statistical noise and such approach is effective for analyzing highly noisy signals.
The logarithms comparison (6c) is effective for data analysis at low intensity values or when the peaks of the investigated curve differ by an order of magnitude, especially by several orders. This is true for large scattering angles, when the scattering intensity contains information on the smallest (of the order of the incident wavelength) structural features and the spectrum contains peaks of higher orders. It can also be used effectively for small-angle scattering, but when the diffuse scattering channel is considered, which also contains information on small deformations.

In addition, by analogy with (6b), the residual functional in the form of the root-mean-square deviation of the logarithms (6d) was added.

**Differential Evolution algorithm**

Differential Evolution (DE) algorithm is described in detail in [5]. For calculation DE-strategy in the form “rand/1/exp” was used. That means that population vector to be mutated was chosen randomly, one difference vector was used and trial vector was generated using exponential crossover.

For our task in obtaining mutant vectors, the absolute values of the corresponding expression were taken in order to exclude the search for a solution among the parameter vectors with negative parameters.

**Results**

In the work, the experiment of X-ray scattering on an ideal 100 μm thickness Si crystal near a lattice site (111) was simulated. The width of the slit before the sample (the wave’s transverse width) \( w = \frac{\lambda}{2\pi} \sin(\theta_B) = 100\mu m \), the background intensity value \( I_{bg} = 1 \), intensity scaling parameter \( K = 10^6 \). The wavelength of the incident beam \( \lambda = 1.54 \AA \). The statistical noise was added (as in a real experiment) according to the formula (5). Calculations were performed using C++. Program was based on the algorithm template from the Differential Evolution homepage [6].

Structure parameters using for modeling of the scattering experiment, their search ranges and DE algorithm parameters using for the inverse problem solving and are shown in the table 1. DE algorithm parameters were chosen as the best for searching. DE algorithm parameters \( F \) and \( C \) were chosen according to the lowest goodness of fit (residual functional) \( \rho_{log}^{abs} \) [3]. In table 1 “\( x_0 = \) random” means that target vector chosen randomly from the population.

| Structure parameters | Search ranges | DE algorithm parameters |
|----------------------|---------------|-------------------------|
| \( L_x = 100 \mu m \) | (10-200) \( \mu m \) | \( F = 0.1 \) |
| \( w = 100 \mu m \) | (10-200) \( \mu m \) | \( C = 0.4 \) |
| \( I_{bg} = 1 \) | (0-10) | \( x_0 = \) random |
| \( K = 10^6 \) | (0.1-10)x10^6 | \( N = 40 \) |

Table 1. Structure parameters, their search ranges and DE algorithm parameters, using for search.

The results of solving the inverse problem of X-ray diffraction within the framework of the proposed approach are presented in Figure 1. For every residual functional form (6a-6c) the inverse problem was solved. On figure 2 the dependences of the corresponding residual functional values on the number of DE algorithm cycles are presented. For curves having the same color, the same pseudo-random number generator seed was chosen. In table 2 the average values of the relative deviations from the unknown structural parameters specified in the numerical experiment are presented.

| Structure parameters | Search ranges | DE algorithm parameters |
|----------------------|---------------|-------------------------|
| \( L_x = 100 \mu m \) | (10-200) \( \mu m \) | \( F = 0.1 \) |
| \( w = 100 \mu m \) | (10-200) \( \mu m \) | \( C = 0.4 \) |
| \( I_{bg} = 1 \) | (0-10) | \( x_0 = \) random |
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Table 1. Structure parameters, their search ranges and DE algorithm parameters, using for search.

It is clearly seen that the best solution (most precise) was found for the \( \rho_{log}^{abs} \) residual functional (figure 2b) given by expression (6b). With the residual functional in the form (6a) the less accurate result was obtained (figure 2a). It should be mentioned that the use of the residual functional \( \rho_{log}^{abs} \) in the form (6d) allows solving the problem faster but with the worst accuracy. That makes it possible to use it for the initial narrowing of the parameter range and the subsequent search using the solution (6b). The same applies to the (6c), which is not far behind in speed (6d).
Figure 1. (a, b, c). (a) X-ray scattering intensity distribution map in reciprocal space - the result of the inverse problem solve; (b) X-ray scattering intensity distribution map in reciprocal space - experiment simulation; (c) scattering curves for $q_x = 0$ and $q_y = 0$: black - minimization of the residual functional, gray - simulation of the experiment with Poisson noise considering.

Figure 2. (a, b, c, d). Dependences of residual functional on the number of algorithm cycles in log scale. Residual functional in the form of (a) absolute value, (b) root-mean-square value, (c) absolute logarithmic value, (d) root-mean-square logarithmic value. Curves having the same color have the same seed for pseudo-random number generator.
Table 2. The average values of the relative deviations obtained after solving diffraction inverse problem with using DE algorithm.

|                  | $\rho_{abs}$ | $\rho_{sqr}$ | $\rho_{abs}^{log}$ | $\rho_{sqr}^{log}$ |
|------------------|--------------|--------------|--------------------|-------------------|
| $\Delta L_z / L_z$ | 0.1          | 0.01         | 0.07               | 0.008             |
| $\Delta w / w$    | 0.03         | 0.06         | 0.16               | 0.1               |
| $\Delta l_{bg} / l_{bg}$ | 1.6e-4     | 2.6e-4       | 9.2e-4             | 20.0e-4           |
| $\Delta K / K$    | 3.1e-2       | 3.0e-2       | 1.6e-2             | 5.3e-2            |

Conclusion

The approach for solving the inverse problem in the analysis of model X-ray scattering reciprocal space maps is developed. The proposed approach based on using DE algorithm for analysis the results of numerical simulation and experimental data of X-ray diffraction is useful and effective for nondestructive diagnostics of nanostructured media.

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