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Analysis X-ray diffractograms from near-surface layers of monocrystals: development of models, algorithms and software

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An algorithm for analyzing double-crystal rocking curves from the near-surface layers of monocrystals has been proposed, and corresponding software has been developed. It is taken into account that to obtain correct results, both coherent and diffuse components of X-ray scattering need to be considered. The possibility of simultaneous analysis of rocking curves from several reflections is provided. To approximate experimental rocking curves with theoretical ones, an approach that simultaneously uses three different approximation methods has been utilized. The effectiveness of the proposed approach is confirmed by verifying the uniqueness of the obtained results.

Keywords: computer simulation, algorithm, X-ray diffraction, crystal structure, surface layer, strain profiles, rocking curve, defects.

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Introduction

X-ray structural analysis is a primary source of information about the crystalline structure of materials. Additionally, this analysis is one of the main methods for studying the structure of near-surface layers of monocrystalline materials after various types of processing [1, 2].

Most types of surface treatment or modification of crystals lead to changes in the crystalline structure of their near-surface layers. For example, ion implantation results in the incorporation of implant ions into the structure and the generation of radiation defects, which are unevenly distributed throughout the thickness of the disturbed layer [3]. This leads to changes in the interplanar distances in the near-surface layer (formation of a strain profile). These changes in interplanar distances cause additional peaks and humps (additional oscillatory structure) to appear on the X-ray diffractograms near the main Bragg peak from the ideal part of the monocrystal. Analyzing this additional oscillatory structure allows obtaining information about the state of the ion-implanted layer of monocrystals and, accordingly, about the quantity, characteristics, and depth distribution of radiation defects that cause changes in the interplanar distances of the near-surface layer.

I. Analysis of the state of the problem

Unlike the analysis of polycrystalline materials, which has a wide range of both commercial and free software [4, 5], as well as the possibility of using more complex [6] or simpler approaches [7], there are significantly fewer programs in the field of analyzing the defect structure of monocrystals and their near-surface layers.

Existing programs for the analysis of near-surface layers and layered structures are mainly focused on the study of reflectometry data (XRR), and their analysis is periodically conducted in scientific publications, for example [8-10]. However, regarding diffractometry with the implementation of scans in various modes (XRD), such programs are practically unavailable for free access. This is because each scientific group creates its own software and does not make it publicly available. These programs reflect the current and optimal approaches to X-

ray diffraction modeling and solving specific scientific problems relevant to the particular research group. There are also specialized programs for analyzing superstructures, layered structures, and ion-implanted layers on the surfaces of monocrystals in respective industries, but their commercial use is significantly limited.

Nevertheless, different approaches to analyzing X-ray diffraction patterns from surface layers of monocrystals and thin films are described in detail in the literature. Therefore, for those who need to analyze and account for various effects, it is necessary to develop appropriate software themselves. Thus, we will examine the main approaches to analyzing the surface layers of monocrystals and thin films described in the literature in more detail.

At present, the analysis of surface layers of monocrystals is performed using kinematic [11] and dynamic [12-14] X-ray scattering theories.

Over the past decades, there have been many publications on this topic, but the approaches to analysis, fitting methods, the degree of uniqueness of the results, and other important aspects of interpretation are usually not specified. Work [15] is one of the few works that details the logic of finding strain profiles from the perspective of software architecture and describes the minimization algorithms and analyzes them. The genetic algorithm [16] and the annealing simulation algorithm [17] are also used to determine strain profiles. These methods allow for the determination of the strain profile even without "assuming" its shape. However, when analyzing the results provided by the program, one must critically assess the physical validity of the obtained dependencies.

It should be noted that in the determination of strain profiles, diffuse X-ray scattering on defects is not taken into account in a significant number of publications.

In general, most publications on the study of the structure of surface-disturbed layers are limited to determining deformation profiles. The diffuse component of X-ray scattering on defects is also not considered, and thus, defect parameters are not determined. Many works define the parameters of the disturbed layer using a single reflection or several reflections, but with a separate analysis, which does not allow for the unambiguous determination of the structural parameters of the surface-disturbed layers of monocrystals and films. Therefore, there are reasons to believe that existing approaches only partially cover all the tasks involved in X-ray structural analysis of surface-disturbed layers of monocrystalline materials and films. This is why further work is needed in the direction of developing approaches and software for the correct determination of the structure of the surface-disturbed layers of monocrystalline materials.

The aim of this work is to develop algorithms, models, and software for the analysis of X-ray diffraction patterns in the study of surface-disturbed layers of monocrystalline materials or films after various types of treatment, including ion implantation.

II. Approaches to modeling X-ray diffraction in crystals

To analyze experimental rocking curves for determining the parameters of the crystal structure of near-surface layers in monocrystals and films, X-ray diffraction modeling is used.

The development of software for X-ray diffraction modeling is a labor-intensive and complex task. Without delving into the specific formulas for calculations, we will present a general scheme that describes the logic of the modeling process.

When analyzing diffraction patterns from mono-crystals, direct modeling of X-ray diffraction is performed based on the parameters of the crystal structure and parameters that characterize X-ray scattering by atoms.

In the modeling, it was taken into account that the intensity of X-rays reflected from the crystal consists of coherent R_{coh} (takes into account X-ray scattering on an "ideal" crystal lattice) and diffuse R_{diff} (takes into account X-ray scattering on crystal structure defects) component [18]:

$$R(\Delta\theta) = R_{coh}(\Delta\theta) + R_{diff}(\Delta\theta).$$

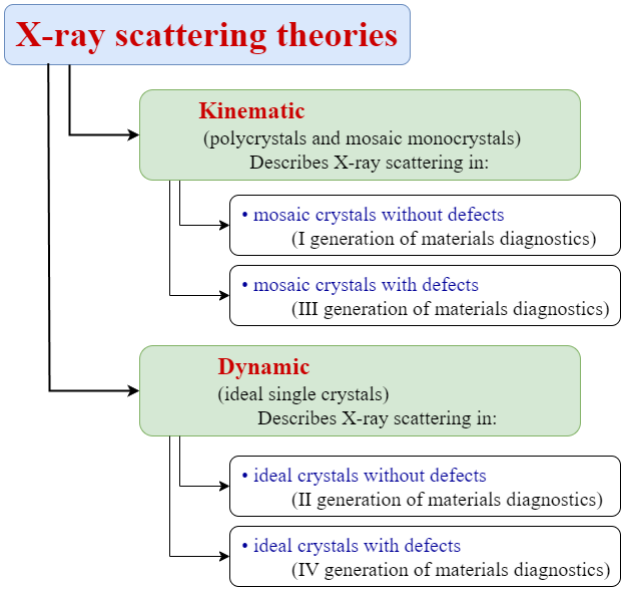


Fig. 1. Scheme of X-ray scattering theories application.

From the perspective of X-ray crystallography for analyzing crystal structures, various X-ray scattering theories can be applied to the analysis of diffraction patterns (Fig. 1). In the developed software, the analysis of near-surface layers of monocrystals is performed using the kinematic theory of X-ray scattering [19], dynamic theories based on the Takagi equations [20-24], and the statistical dynamic theory of X-ray scattering [25-27]. Special attention is given to the highly detailed and rigorous model of X-ray diffraction in monocrystals with defects of any type and size – the statistical dynamic theory developed by V.B. Molodkin (G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine) [28-30]. All of these approaches were utilized in the development of the software for the analysis of near-surface layers of monocrystals.

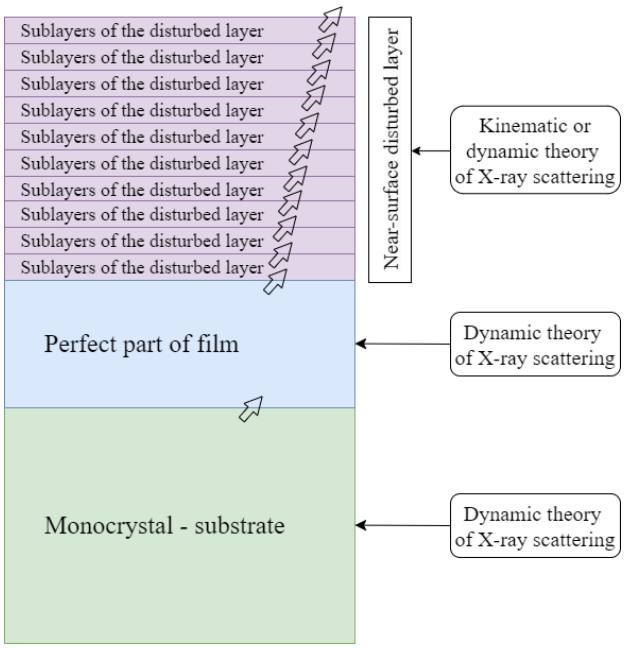


Fig. 2. Crystal structure used for modeling.

The use of different theoretical approaches allows for modeling with varying degrees of speed, complexity, and detail, both in terms of diffraction description and the complexity of the crystal structure of the studied near-surface layers.

In the general case, the model of the investigated system consists of a monocrystal substrate, an ideal part of the film, and a near-surface disturbed layer, which is divided into sublayers for the implementation of an iterative procedure (Fig. 2). In each sublayer, defects are assumed to be uniformly distributed, and the defect parameters, deformation, and degree of amorphization are considered constant. Thus, the intensity calculated from the substrate serves as the input intensity for the ideal part of the film, and the output intensity from the ideal part of the film becomes the input intensity for the lowest sublayer of the disturbed layer, and so on. The experimentally observed intensity is the result of the last sublayer of the disturbed layer.

In crystals, various types of defects are considered, which can be described using parameters of specific types of defects as well as parameters that indirectly describe the defect subsystem. The schematic of the defect subsystem used for X-ray diffraction modeling in dynamic case in

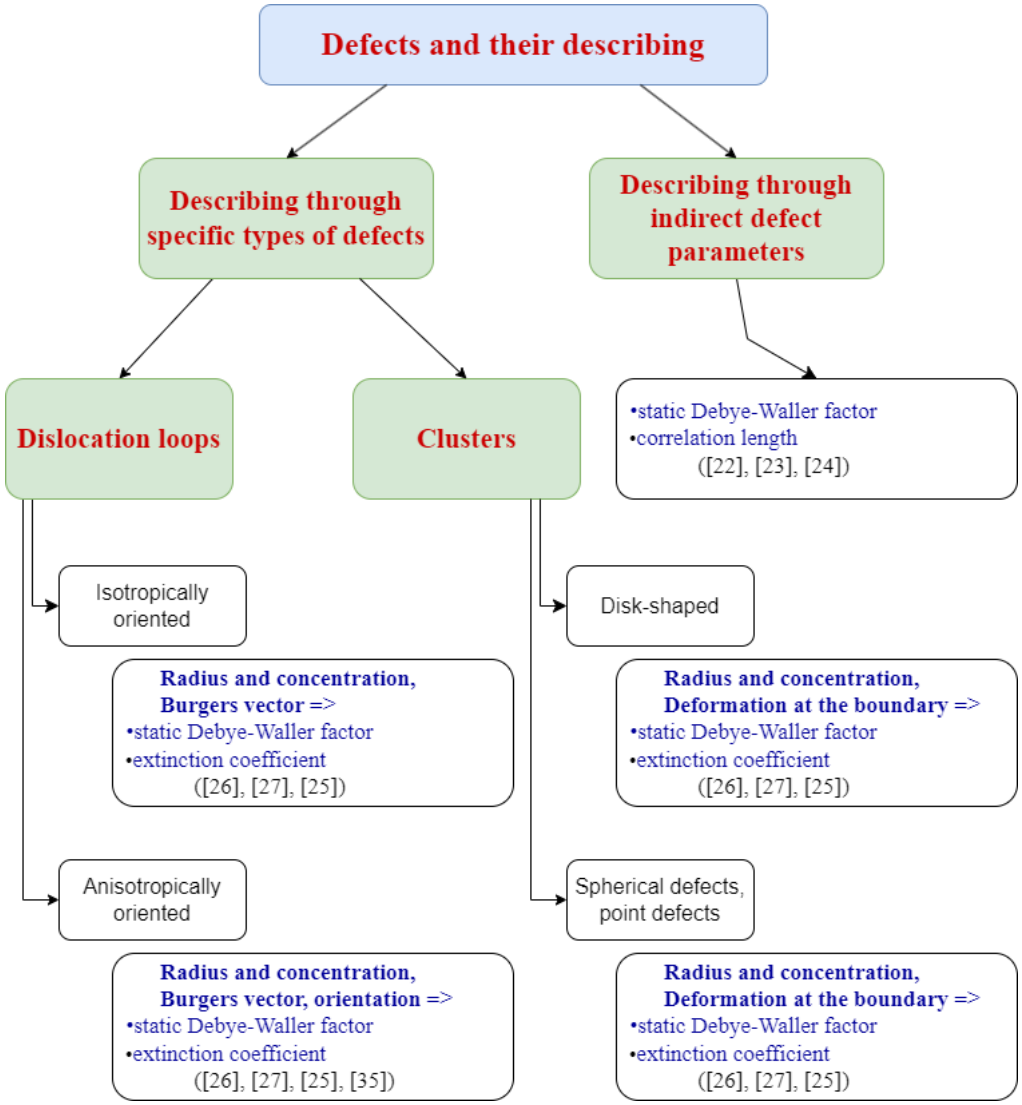
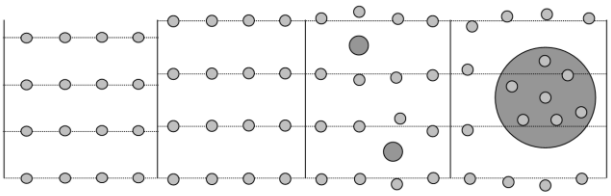


Fig. 3. Scheme of the defect subsystem of the crystal considered in the modeling.

this work is shown in Fig. 3. This diagram also presents the main parameters of the theory and the corresponding publications.

The disturbed layer can be described within different models, as shown in Fig. 4. For each of these models, both kinematic and dynamic theories of X-ray scattering can be applied. Given that the inhomogeneous near-surface layer is divided into sublayers for modeling purposes, the distribution of various disturbed layer parameters with depth (including the strain profile) is represented as a step function (it can also be depicted as an averaging line in the figures). A more detailed description of the structure of the ion-implanted layer is provided in [31]. The use of various models of the disturbed layer, scanning methods, and approaches to obtaining information from them are considered in [32-34].



$\Delta d/d = 0$	$\Delta d/d \neq 0$	$\Delta d/d \neq 0$	$\Delta d/d \neq 0$
$E = 1$	$E = 1$	$E \neq 1$	$E \neq 1$
$\mu_{ds} = 0$	$\mu_{ds} = 0$	$\mu_{ds} \approx 0$	$\mu_{ds} \neq 0$
$\tau = 0$	$\tau = 0$	$\tau \approx 0$	$\tau \neq 0$
$R_{coh} \neq 0$ $R_{diff} = 0$	$R_{coh} \neq 0$ $R_{diff} = 0$	$R_{coh} \neq 0$ $R_{diff} \approx 0$	$R_{coh} \neq 0$ $R_{diff} \neq 0$

a *b* *c* *d*

Fig. 4. Models of the disturbed layer:
a) perfect monocrystal, b) deformed monocrystal, c) deformed monocrystal with disorder (with point defects), d) deformed monocrystal with disorder (with nonpoint defects).

For dislocation loops, possible orientations are also taken into account. In the case of an equally probable orientation of defects in all crystal equivalent directions, most of the terms that arise when deriving the final mathematical ratios are mutually compensated and a relatively simple final mathematical expression is obtained. The mathematical model that accounts for anisotropy in the orientation of non-spherically symmetric defects was developed by us and described in [35]. To obtain the analytical expression considering anisotropy in defect orientations, the terms mentioned above are not zero and are not mutually canceled, so the computer algebra system Maple was used to facilitate the derivation of formulas and avoid errors.

A simplified scheme of the algorithm for modeling the coherent component from monocrystals with a near-surface disturbed layer is presented in Fig. 5. The purpose of most modules is clear from their names.

The disturbed layer is divided into sublayers, in each of which all the crystal structure parameters are considered to be constant. The subdivision into sublayers is meaningful as long as it affects the theoretical rocking curves. The modules covered by the "Sublayer Iteration" section are repeated in a cycle tens or even hundreds of times.

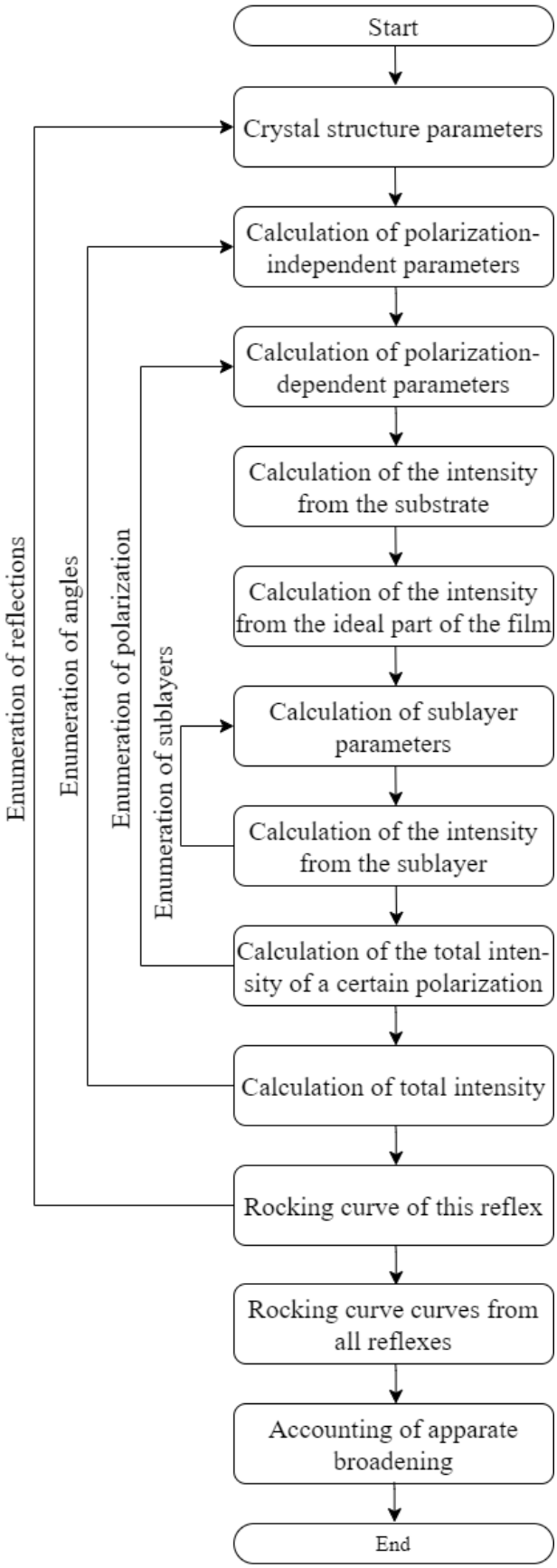


Fig. 5. Structural diagram of the algorithm for modeling the coherent component of the rocking curves from monocrystals (substrate-film-disturbed layer system).

The model considers two types of X-ray polarization, which is why most calculations (covered under "Polarization Iteration") are performed twice.

It is important to note that calculations from the "Calculation of Polarization-Independent Parameters" module to the "Total Intensity Calculation" module pertain to a single point on the rocking curve, that is, the intensity at a specific angle. Therefore, "Angle Iteration" means that all calculations covered by this iteration are repeated in a loop thousands of times.

The calculation of the diffuse component follows a structural scheme for modeling that is somewhat similar but significantly more complex because it involves calculating the diffuse components for many types of defects. Consequently, the computation time increases by several orders of magnitude. Additionally, accounting for anisotropy in the orientation of non-centrosymmetric defects further complicates the calculations and increases the computation time by hundreds of times.

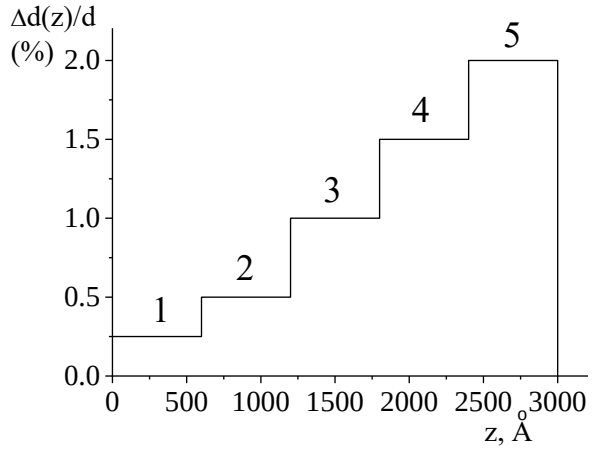


Fig. 6. Strain profiles.

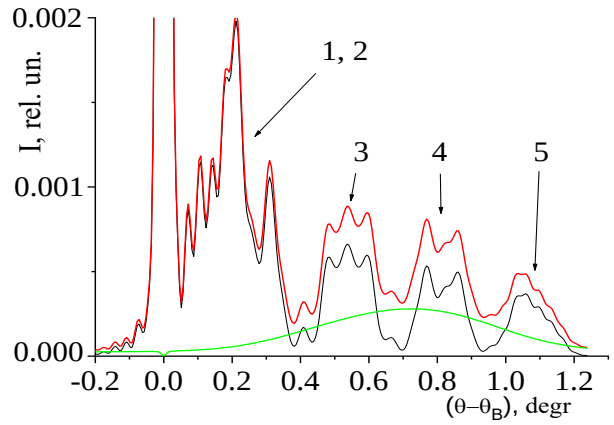


Fig. 7. Diffraction rocking curves
(black – coherent, green – diffuse, red – total).

As an example, we present the result of modeling X-ray diffraction on a monocrystal with a surface-disturbed layer, where the strain profile is shown in Fig. 6, and defects are present. The calculated rocking curve and its components are presented in Fig. 7. Scattering on the defects results in the formation of a diffuse component, while scattering on the quasi-ideal part results in the coherent component. The coherent component clearly indicates diffraction from specific sublayers where there is a large deformation difference between them (sublayers 3-5), and interference effects in the case of smaller deformation differences (sublayers 1 and 2).

III. Software design and development for analyzing X-ray diffraction data from monocrystals

Based on the analysis of literature data and the needs arising from the analysis of experimental X-ray diffraction patterns, it was determined that the software should have the following main functionalities and features:

–modeling of X-ray diffraction in crystals taking into account the coherent and diffuse components of X-ray scattering;

–taking into account when modeling the parameters of monocrystals, including defects of various types;

–modeling of X-ray diffraction using the main currently existing theoretical approaches;

–implementation of a mathematical and computer model of X-ray diffraction, taking into account anisotropy in the orientation of non-centrosymmetric defects within the framework of the statistical dynamic theory of X-ray scattering;

–simultaneous consideration in the analysis of several reflexes with methods of assessing the degree of coincidence of theoretical diffractograms with experimental ones;

–availability of a powerful method of approximating theoretically calculated diffractograms to experimental ones.

Based on the aforementioned functionality, a software package for analyzing monocrystals, monocrystals with disturbed near-surface layers, film-substrate systems, and multilayer structures has been developed using the C++ programming language (Builder). This software enables the modeling of theoretical rocking curves given specific parameters for the crystal defect subsystem. The interface of the developed program is shown in Fig. 8.

When developing software, a lot of useful information can be taken from the book [36]. The algorithm for minimizing the deviation of theoretically calculated rocking curves from experimental ones combined three methods, a detailed description of which is given in [31, 37]. To compare the experimental and theoretical KDV, the convolution of the calculated theoretical KDV was made with the apparate function of the spectrometer.

The main stages of using the developed approach in the previous version of the software are shown in the work [31]. In particular, it demonstrates the sequential stages of simultaneous analysis of several experimental rocking curves, starting from the modeling of ion implantation and ending with the consideration of anisotropy in the orientation of radiation defects.

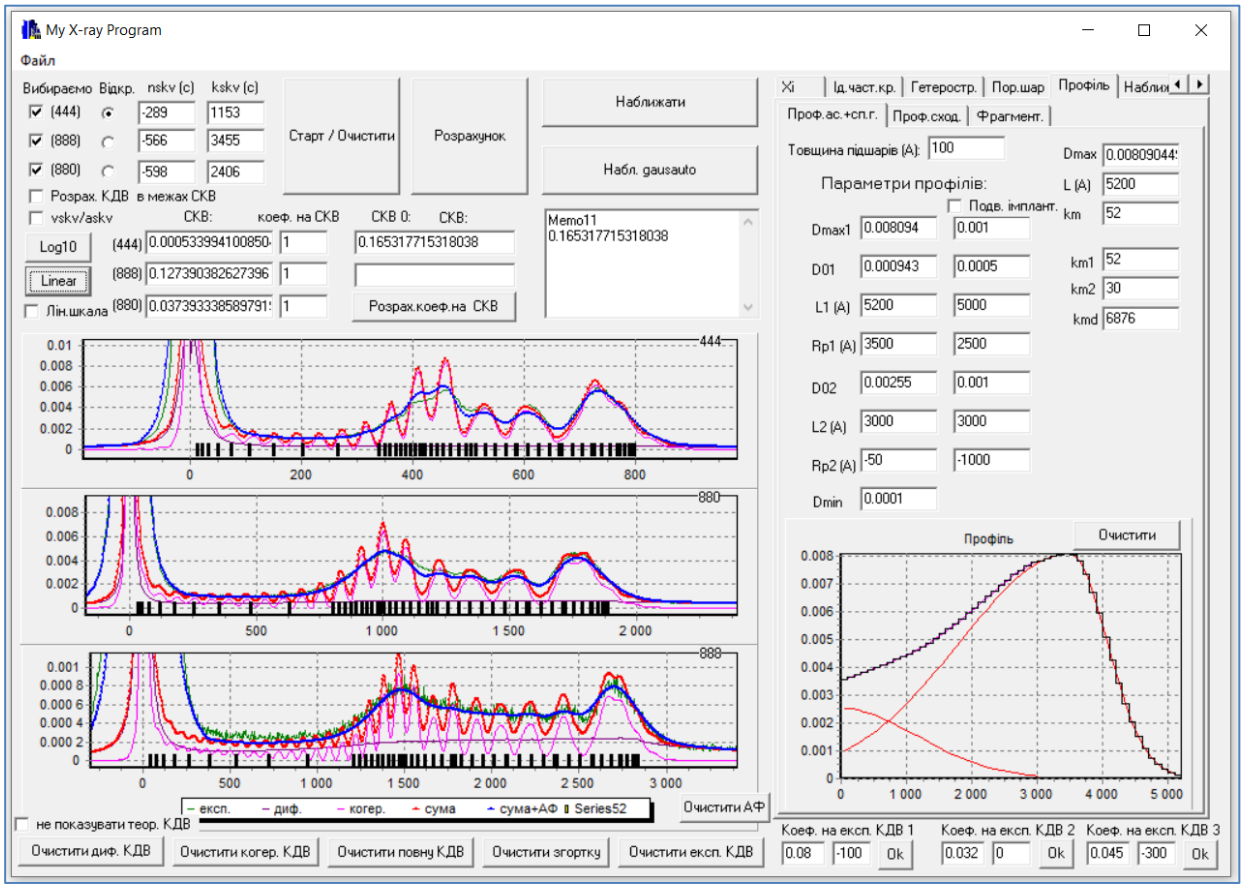


Fig. 8. The interface of the developed program for modeling X-ray diffraction in real crystals.

Conclusions

1. An algorithm and its software implementation have been developed for analyzing monocrystals, films, and near-surface layers of monocrystalline materials after various types of processing.

2. Using the developed software, X-ray diffraction in monocrystals (both ideal and real) can be modeled using various theoretical approaches, including the calculation of coherent and diffuse components of X-ray scattering.

3. The developed software has the capability of simultaneously processing experimental rocking curves from a series of symmetric and asymmetric reflections. It accounts for the presence of various types of defects and deformations in all structural elements of the investigated sample, which distinguishes it from its analogs with great quality.

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Аналіз Х-променевих дифрактограм від приповерхневих шарів монокристалів: розробка моделей, алгоритмів та програмного забезпечення

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Запропоновано алгоритм аналізу двокристальних кривих дифракційного відбиваня від приповерхневих шарів монокристалів та розроблено відповідне програмне забезпечення. Враховано, що для отримання коректних результатів необхідно враховувати як когерентну так і дифузну складові розсіяння Х-променів. Передбачена можливість одночасного аналізу кривих дифракційного відбивання від кількох рефлексів. Для наближення експериментальних кривих дифракційного відбивання теоретичними використано підхід, який одночасно використовує три різні методи наближення. Ефективність запропонованого підходу підтверджується перевіркою отриманих результатів на однозначність.

Ключові слова: комп'ютерне моделювання, алгоритм, рентгенівська дифракція, кристалічна структура, поверхневий шар, профілі деформації, крива гойдання, дефекти.