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# Challenges of the inverse problem of the diffraction X-ray Topo-tomography: Theory, formulas and computer iterative algorithms towards the 3D reconstruction of elastic statical displacement field around the point-defects in a crystal

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In the recent 10 years, the Diffraction X-ray Topo-Tomography (DXTT) is widely applied to the structural analysis of real crystals. In the DXTT method the crystal plate is rotated around an axis perpendicular to the reflecting planes net, usually the rotation axis 0X is selected along the diffraction vector h. Then, the 2D-projection set (the diffraction X-ray image topograms-DXITs) is collected for different rotation (inclination) angles $\Phi$, each of which is related to some inclination of the diffraction X-ray plane with respect to the intrinsic coordinate system of the crystal sample, the axis 0S is along the wave vector kh of the diffracted wave propagation. An idea of the computer restoration of the spatial defect positions in a crystal and, what is more important, the local 3D static displacement fields around defects in crystalline materials according to the DXTT data is of a special interest. such a problem is equally, if not more, directly related to the quantitative interpretation of defect imaging on the DXITs. The latter is due to the different defect imaging mechanisms in the near and far regions surrounding the crystal lattice defects. In the present report, the semi-kinematic analytical solution of the dynamical Takagi-Taupin equations for the diffracted wave amplitude Eh(r) is built that allows in general to develop the consequent theoretical approach for resolving the inverse DXTT problem. As an example, using the one 2D projection data with inclination angles $\Phi$=0, the results of the computer restoration of the 3D displacement field function $f(r-r^0)=h\cdot u(r-r^0)$ around the Coulomb-type point defect in crystal Si(111) are reported and discussed (diffraction vector h=[2 $\bar{2}$2], the X-ray MoKα1-radiation, the wavelength λ=0.071nm, the Bragg angle θB=10,65°. $u(r-r^0)$ is the near field of elastic static displacements around the Coulomb-type point defect at the point $r^0$). Respectively, to computer restoration of the 3D displacement field function $f(r-r^0)$ the simulated annealing and Quasi-Newton gradient descent algorithms are applied to our problem. To obtain a good solution convergence, some physical constraints onto the type of functions $\{f(r-r^0)\}$ searched are imposed. The 2D numerically simulated and then, used for the computer 3D restoration of the theoretical function $f(r-r^0)$ is by using the Quasi-Newton descent algorithm, the cross-section pictures of the theoretical function $f(r-r^0)$ and the ones restored from the 2D projection in planes z=const. z(dimensionless units)=(A) 6, (B) 8, (C) 10, in are depicted The case (B) is related to the mid-thickness of Si(111) plate.

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