THE SIMULATION OF BRAGG-CASE SECTION IMAGES OF DISLOCATIONS AND INCLUSIONS IN ASPECT OF IDENTIFICATION OF DEFECTS IN SiC CRYSTALS

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Bragg-case section topography is the important method of X-ray diffraction topography allowing to reveal fine details of strains defects thanks to appearing of the interference effects. It also provides the possibility of effective simulation of the images of topographical defects based on the numerical integration of the Takagi equations. The formation of contrast in the method seems to be equivalent to the diffraction of the spherical wave from a certain number of closely located excitation points.

In the present paper the conventional section topography supported by numerical simulation of defects is applied for studying of the images of dislocation and pipe-formed cavities in SiC bulk crystals. The important goal of the paper was also studying of the elements of the contrast of the dislocations to check the possibility of using simple approximations of extinction contrast, often dominating in the Bragg-case section images of dislocations.

The numerical analysis of the Bragg-case section images was performed for the case of screw dislocation perpendicular to the crystal surface in an arbitrary asymmetrical reflection. It is well known that this kind of dislocations is particularly important in the case of SiC, because it is relatively common and was also suggested by Dudley and coworkers [1] as the possible source of micro-pipes, where many single screw dislocations may join in forming one hollow-core super-screw dislocations with a large Burgers vector.

The present simulation became more realistic and better corresponding to the experimental dislocation images by adding many shifted spherical images, filing the area irradiated by the narrow beam, analogously at it was proposed by Epelboin and Soyer [2] in the case of transmission projection topography. The obtained simulated images were compared with two adapted simplified models of extinction contrast described by Miltat and Bowen [3]. The results evidently indicated that the extinction contrast in the simulated images and topographs is very similar to the contours limiting the effective change of the diffracting conditions and differs substantially from the contours representing the condition of the wave-field decomposition.

For studying of the strain field of some pipe-formed cavities and rod like defects, we revealed a method of approximate evaluation of the strain field of rod like inclusion, integrating the contribution from a very large number of point like inclusions filling the assumed volume of inclusion. The model allowed taking into account the relaxation of strains on the free surface using the initial formulae given by Sen [4], and calculation of strains for differently inclined rods. The application of the model enabled obtaining realistic test simulation of topographic images of some solute trails in garnet, and some similarity to the Bragg-case section topographic images of some pipe formed inclusions in SiC.

References

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