

Taking into Account the Orientation of Disc-Shaped Clusters in the Static Debye-Waller Factor Calculation

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Presence of defects in crystals affects their physical properties. It is important to know not only the type, size and concentration of existing defects, but in the case of spherically asymmetric defects (dislocation loops, disk-shaped clusters) also their spatial orientation. X-ray diffractometry enables to define these characteristics. A powerful theoretical tool is statistical dynamical theory of X-rays scattering [1]. The presence of defects oriented perpendicular to the diffraction vector, leads to higher intensity of X-rays diffuse scattering than presence of defects oriented at some angle to the diffraction vector [2]. The lowest diffuse scattering values are observed when defects are located in parallel to the diffraction vector planes. In X-ray diffractometry it leads to a change in values of the crystallographic parameters such as static Debye-Waller factor $L_{dcl} = \exp(-L)$ and the absorption coefficient due to diffuse scattering on defects μ_{dd} . In the presence of a disc-shaped clusters in a crystal static Debye-Waller factor can be given by the formula:

$$L_{dcl} = \frac{2\pi c R_0 \varepsilon (H h_p)^{3/2}}{4\pi V_c} \eta(\vec{H}_0, \vec{n}_{cl})$$

where c is a clusters concentration, V_c – crystal unit cell volume, h_p – cluster thickness, R_0 – an average cluster radius, ε – cluster boundary deformation, $\Gamma = \frac{1}{3}(1+\nu)(1-\nu)^{-2}$, ν – Poisson's ratio, H – module of diffraction vector, $\vec{H}_0 = H/H$ – unit vector in the diffraction vector direction, \vec{n}_{cl} – unit normal to the cluster surface. The assumption that the disk-shaped clusters are formed in all equivalent crystallographic planes with equal probability and averaging over all their probable orientations lead to values of $\eta(\vec{H}_0, \vec{n}_{cl})$ close to 0.5. Since the value of $\eta(\vec{H}_0, \vec{n}_{cl})$ depends only on the relative orientation of the vectors \vec{H}_0 and \vec{n}_{cl} , then for calculating the static Debye-Waller factor in the case of a presence in a crystal of disc-shaped clusters only certain orientations one can use the values obtained by the authors of [2].

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