Monte Carlo Simulations of X-Ray Diffraction from Dislocations in Epitaxial Films

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Main building blocks of electronic and optoelectronic devices are heteroepitaxial structures consisting of crystalline materials with different lattice parameters. Relaxation of the lattice mismatch gives rise to misfit dislocations at the interface and threading dislocations going from the interface to surface.

Distortions caused by dislocation strain fields are revealed by x-ray diffraction and can be precisely evaluated, due to weak interaction of x-rays with the matter. In kinematical x-ray diffraction, scattered intensity is described by the Fourier integral

$$I(\mathbf{q}) = \int G(\mathbf{r}) \exp(i\mathbf{q}\cdot\mathbf{r}) d\mathbf{r}$$

of the pair correlation function

$$G(\mathbf{r}) = \langle \exp\{i\mathbf{Q}\cdot[\mathbf{U}(\mathbf{r}_1) - \mathbf{U}(\mathbf{r}_2)]\}\rangle .$$

Here $\mathbf{Q}$ is the scattering vector and $\mathbf{q}$ is its deviation from the nearest reciprocal lattice vector, $\mathbf{U}(\mathbf{r}) = \sum_j \mathbf{u}_j(\mathbf{r})$ is the total displacement field due to all dislocations in the crystal, the homogeneous dislocation distribution is assumed so that $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, and the angular brackets $\langle \ldots \rangle$ denote statistical average over dislocation distribution. The integration is performed over the crystal volume.

We calculate the x-ray diffraction peak profiles from distributions of misfit dislocations in the whole range of their positional correlations, from completely random to periodic. Both the spatial integration and the integration over the dislocation ensemble are performed by Monte Carlo techniques. The diffraction peaks from thin relaxed films consisting of a narrow coherent and a broad diffuse component are explained. Correlation functions are calculated analytically for different types of positional correlations between dislocations [1]. We model the screening of the long-range strain fields of threading dislocations by arrangement of dislocations with opposite Burgers vectors in pairs. Any screening can be modeled by appropriate distribution of the dislocation pairs. Analytical description of the peak profiles is compared with the Monte Carlo results [2]. We compare diffraction profiles for different models of dislocation arrangements calculated directly by the Monte Carlo method with the strain distributions for the same arrangements, which corresponds to the StokesWilson approximation. The strain distributions and the diffraction profiles are found to be in a close agreement as long as the long-range order is absent [3].

References

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