Scattering of spatially bounded X-ray beams in lateral periodic structures

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Abstract. The dynamical theory of X-ray diffraction is developed to the case when the incident and reflected X-ray beams are spatially bounded. X-ray diffraction in complicated lateral periodic structures is considered. Effects, due to periodic regular elastic deformations of a crystal lattice on an angular distribution of the scattered intensity, are investigated. Using the found solutions, numerical simulations of reciprocal space maps for crystals with periodically distributed elastic strains were performed. It was established, that for crystals modulated by a surface acoustic wave, diffraction orders consist of the main reflection vertical band and a pair of inclined bands, induced by spatially bounded X-ray beams. In the case of diffraction in crystals with the surface grating, one observes additional satellites along inclined bands caused by the spatial modulation of incident X-ray wave. Results of X-ray diffraction on a crystal modulated by a surface acoustic wave and on a crystal with a metal surface grating are presented.

1. Introduction
Semiconductor systems based on lateral periodic structures (LPS) have found wide application because of their high efficiency and play key role in different modern electronic devices. LPS of different types and origins, including multilayer and crystal diffraction gratings, systems modulated by an external influence (for example, by an ultrasonics), are successfully used in nano- and optoelectronics, as well as in X-ray optics due to their high stability, reliability and compactness. Still, to fully realize potential of LPS-based devices one face a sophisticated problem to determine specific LPS features of source semiconductor materials. To solve the problem it is common to use an experimental X-ray diffraction method [1] in conjunction with adequate theoretical model. Usually, X-ray scattering on LPS is described by means of a model of an incident plane wave, that is spatially unbounded in lateral direction. Such a traditional approach, however, is not entirely appropriate, since in any experiment X-ray beams are always spatially bounded, no matter what kind of X-ray source is used and diffraction geometry type is applied. What is more, within the framework of the plane wave model, it is totally impossible to perform a numerical calculation of the scattering intensity distribution in vicinity of a reciprocal lattice node, since an angular dimension of diffraction orders is described by the Dirac delta function and tends to infinity at zero. Therefore, to remove the contradiction between the conditions of a real experiment and the mathematical model, in this work, we generalize the theory of x-ray diffraction to the case of spatially bounded x-ray beams.
Figure 1. Geometry of diffraction for spatially bounded X-ray beams on a crystal modulated by a surface acoustic wave.

Figure 2. Geometry of diffraction for spatially bounded X-ray beams on a crystal with a surface grating.

2. Basic equations

Let us consider a general case of diffraction of spatially bounded X-ray beams in a crystal which surface consists of deformed sections periodically distributed in a lateral direction. Such a lateral periodical distribution of elastic deformations in crystal can be obtained, for instance, under influence of an acoustic wave (Figure 1) spreading in a surface layer [2], or as a result of an elastic interaction on heterogeneous boundary between a crystal surface material and a surface grating (periodically located strip-like cap layer, Figure 2).

According to the model, a width of a crystal surface area illuminated by an incident X-ray beam depends on a size of the slit $S_1$, that restricts an incident wavefront, and is equal to $l_x^{(in)}$. The transverse size of the reflected wave is limited by the exit slit $S_2$, which defines a lateral size of $l_x^{(ex)}$ at the crystal surface. We assume that the propagation distance between the particular slit and the crystal surface is small enough to satisfy the geometrical optics approximation. The X-ray diffraction at the edges of the slits $S_1$ and $S_2$ of incident and reflected beams is neglected.

For simplicity, we constrained our problem to the case of symmetric Bragg diffraction. The amplitude reflection coefficient (ARC) of a spatially bounded X-ray beam from the crystal with LPS is written as follows:

$$ R(q_x, q_z) = \frac{a_h}{2\pi l_x^{(in)}} \int_{-\infty}^{+\infty} d\kappa \ R_\infty(\kappa, q_x, q_z) \hat{Y}_1(\kappa) \hat{Y}_2(\kappa - q_x), $$

(1)

where $R_\infty(\kappa, q_x, q_z)$ is the ARC of a spatially unbounded plane wave [2] and "hatted" functions are

$$ \hat{Y}_1(\kappa) = \frac{\sin(\kappa l_x^{(in)}/2)}{\kappa/2}, $$

(2)

$$ \hat{Y}_2(\kappa - q_x) = \frac{\sin((\kappa - q_x) l_x^{(in)}/2)}{(\kappa - q_x)/2}. $$

(3)

For more details see [3]. The tricky part in (1) is to calculate ARC of crystal with periodically distributed deformations and depends on exact shape of an atomic displacement filed.

3. Numerical simulations

In order to conclude numerical simulation and illustrate the above theory of X-ray diffraction, we must first define concrete expression for an atomic displacement field and find expression for
Using the solution (1) and expressions for atomic displacement fields we performed numerical simulations of reciprocal space maps for crystals with periodically distributed elastic strains Figure 5 and Figure 6. It was established, that for crystals modulated by a surface acoustic wave, diffraction orders consist of the main reflection vertical band. Comparing with results of numerical simulations in [2] and those, shown on Figure 5, one can observe, that spatially
bounded incident and reflected X-ray beams induces symmetric inclined streaks (with respect to the vertical axis) in the RSMs. The length of these streaks depends on the size of slits $S_1$ and $S_2$: the narrower the slit, the wider and longer the intensity streak in the RSM. The direction of the streaks in reciprocal space coincides with the direction of the monochromator and analyzer pseudo-peaks in the triple-crystal diffraction scheme [3].

In the case of diffraction in crystals with the surface grating, one observes satellites along inclined bands. Those additional peaks are caused by lateral modulation of atomic displacement field and by the spatial modulation of incident X-ray wave Figure 6. Namely, If there is a system of thin-film lines of another material on the surface of the crystal, then, in general, the incident X-ray beam, before it reaches the surface of the substrate, will experience absorption in the sites of these lines. The presence of lines leads to a periodic deformation of the near-surface region of the crystal [4]. As in the previous case, there are symmetric inclined streaks induced by spatial restriction of incident and reflected X-ray beams.

4. Conclusion
The dynamical theory of X-ray diffraction of spatially bounded X-ray beams [3] is applied to crystals with laterally periodic structures. Within the framework of the theory of elasticity, numerical calculations of atomic displacement fields for lithium niobate (modulation period of 4 $\mu$m) and silicon crystals with wolfram surface grating (modulation period of 0.5 $\mu$m) are performed. Using the found solutions, numerical simulations of reciprocal space maps for crystals with periodically distributed elastic strains were performed. The theory developed explains the experimentally observed features in the angular distributions of the intensity of scattering from a crystals with periodic spatial modulation and can be used to describe the dynamical X-ray diffraction in crystals with different LPS types.

References
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