11-Surfaces, Interfaces and Thin Films

PS-11.01.22 THE DIFFUSE X-RAY SCATTERING FROM A CRYSTAL SURFACE POSSESSING SOME ROUGHNESS

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Recently one of the present authors (J.H) has discussed the intensity modulation on the crystal truncation rod (CTR) scattering due to the surface roughness of a crystal on the basis of the kinematical diffraction theory [Acta Cryst.(1992).A48, 764-771]. If the crystal surface possesses some roughness, the intensity of the sharp CTR scattering falls off by a Roughness Damping Factor with the increase of the distance from the Bragg point but diffuse scattering comes out around the CTR scattering. In this paper we show that the rough state on a crystal surface is represented by introducing a similar short range order parameter α_{mn} to that defined by Warren-Cowely for local order arrangement of a binary alloy, if the surface is well represented by a two level model. The short range order parameter α_{mn} is given by $1 - P^{01}_{mn}/\gamma_1$, where P^{01}_{mn} is the probability of finding a vacancy at the lattice site which is separated by $r_{mn} = a \cdot m + b \cdot n$ from the reference lattice site occupied by an atom and $\gamma_0(\gamma_1 = 1 - \gamma_0)$ is the coverage of the surface by atoms on the 0-th level. In terms of the α_{mn} parameters the diffuse scattering is expressed as

$$I(q_x, q_y, q_z) = MN\gamma_0\gamma_1 f^2 \sum_m \sum_n \alpha_{mn} \cos\{2\pi(q_x \cdot m + q_y \cdot n)\},$$

where the summation m,n are taken to be in the two dimensional surface and MN is the number of the effective lattice sites illuminated by X-rays. On the basis of this relation we discuss the intensity distribution of the diffuse scattering in the reciprocal space for several cases of some α_{mn} parameters.

PS-11.01.23 **X-RAY CHARACTERIZATION OF THE MBE GROWN SrF_2/CaF_2 SUPERSTRUCTURES ON Si(111) SUBSTRATE.**

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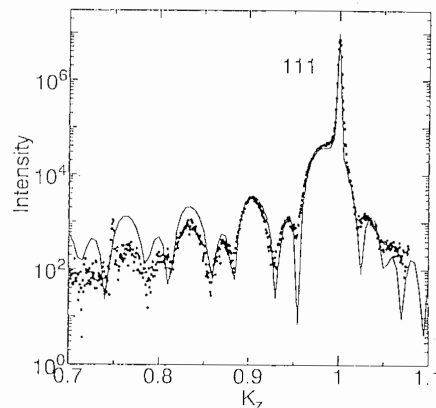
Much attention has been paid for the epitaxy of superstructure of fluorite-type crystals grown on the semiconductor substrates from the standpoint of its potential applications to semiconductor device. In order to understand the initial stage of such a hetero-epitaxial growth of this system on an atomic scale, we prepared several samples of different molecular layers of SrF_2 in 3[SrF_2 Xml/CaF_2 10ml at 773K]/[CaF_2 2ml at 1045K]/Si(111); X= 1, 2 in A F Ioffe Physico-Technical Institute, and characterized them by using X-ray crystal truncation rod(CTR) techniqe. X-ray measurements were performed at Beam Line $6A_2$ in Photon Factory KEK, Tsukuba. Oscillation photographs were taken by imaging plate(IP) detectors so as to observe a range from 0 to 23 degree. The CTR scattering around 111 and 311 Si Bragg points and also 131 CaF_2 Bragg point was observed as well as the X-ray reflectivity near the reciprocal space orign. From the geometrical relation between the three peaks in reciprocal space, it was confirmed that the present CaF_2 epi-layer was grown in so called the B-type configuration on the Si(111) substrate. Figure shows the observed and calculated integrated intensity along the *lll* direction(normal to the crystal surface) near the 111 point obtained from a sample of 2 molecular layer of SrF_2. A sharp peak in k_z=1.0 is the 111 Bragg scattering from Si substrate where k_z is the component of the scattering vector. Characteristic interference fringes consisting of two kind of peaks with different half width are due to the complex multi-layer structure, and are well reproduced by a simulation where lattice spacings and the number of layeres were refined. Disagreement between the observation and the calculation suggests the existence of interface roughness on an atomic level.



Observed and simulated intensity modulation along the 111 CTR scattering

PS-11.01.24 TWINNING IN A HgTe SEMICONDUCTOR

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Twinning in materials with the sphalerite structure is of particular importance because this represents the structure of most of the III-V and II-VI semiconductor compounds. The electrical and optical properties are known to depend on these twin lamellae. Two models of the {111} twin, the so-called para- and ortho-twin, have been reported so far. In the para-twin case an atom has a similar atom as its nearest neighbour at the boundary. Thus, wrong bonds are induced whereas in the ortho case no wrong bonds are formed. The atomic distances in these two cases have previously been taken to be 1/4[111]. The two twin types result in different electrical properties; perfect ortho-twin boundary does not contain any electrically active centres, whereas the wrong bonds at the interface in the para case act as such centres. The microstructure of HgTe films grown on CdTe substrates by the MBE method have been investigated by means of high resolution electron microscopy. Multiple (111) twin lamellae and a co-existing lateral twin with (112) plane as twin interface have been observed. The atomic positions at the {112} boundary are found to be displaced in the [111]-direction from this assumed perfect positions. To explain this effect the observed contrast has been simulated for different relative shift in the [111]-direction. A new model for the para-twin is suggested using coincidence site lattice (CSL), in which there is an extra 1/12[111] displacement of the atoms at the boundary. Thus, the distance becomes 1/3[111] (0.374nm) instead of the original 1/4[111] (0.28nm) that seems to be too short for two neighbouring anions. The predicted shift leads to a good correspondence between the observed and the simulated high resolution images.

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