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Structural study of novel epitaxial heterostructures with manganese fluoride layers on silicon

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Introduction

It is known that crystalline structure of epitaxial films can differ from that of bulk materials. In a state of the bulk single crystals, CaF_2 has cubic fluorite structure and MnF_2 has tetragonal unit cell of the rutile type. It was earlier shown that thin, below 3 monolayers (ML) MnF_2 films grow in metastable fluorite structure [1]. It has been recently demonstrated that using CaF_2 buffer layer on Si substrate MnF_2 epitaxial films can be grown in metastable orthorhombic phase [2]. These films are attractive for studies of very important in numerous applications exchange bias effect in ferromagnet – antiferro-magnet heterostructures. In the present work, we have studied the crystal structure of short period MnF_2/CaF_2 superlattices (SLs) with a MnF_2 layer thickness from 3 to 6 ML.

Experimental

The structures were grown on Si(111) by molecular beam epitaxy (MBE). Before the growth of SL CaF_2 buffer layer was deposited on atomically clean Si surface. All grown SLs can be divided into two groups – "thin" with no more than 3 MLs of MnF_2 and "thick", over 4 MLs of MnF_2 in each period. The SLs were grown at room temperature and covered with thin (2-3nm) CaF_2 cap layer.

The XRD measurements were carried out at the BL-4C using radiation with the wavelength of 1.54 Å. Intensity distribution in θ–2θ scanning mode near the 111 and 222 symmetrical Bragg reflections was measured.

Simulation of rocking curves was performed according to semi-kinematical approximation in which a scattering kinematical amplitude from the SL was calculated by summing over molecular monolayers in SL period and added with dynamical diffraction from substrate and kinematical amplitudes from the buffer and cap layers [3]. Because the structure of MnF_2-sublayer and relaxation state of the epitaxial system were unknown beforehand in the first step of a fitting procedure the SL was characterised interplanar spacing d_1 and d_2 in CaF_2 and MnF_2 sublayers correspondingly, numbers n1 and n2 of monolayers in them and ratio of structural factors $F(MnF_2)/F(CaF_2)$ (5 parameters in total).

Results

Two typical measured θ–2θ-scans are presented in Fig. 1a,b. For samples with very thin MnF_2-sublayers (n=2-3 ML) the well resolved satellites and thickness fringes are observed on the diffraction curves (Fig. 1a). When the MnF_2-sublayer thickness is 6 ML the thickness fringes disappear and wider satellites are detected only. Besides the diffraction pattern is broadened in direction normal to diffraction vector that follows from θ–scan curves (are not shown). Such difference in diffraction from two groups of SLs is most probably the evidence of relaxation process occurred in SLs with "thick" MnF_2-sublayers.

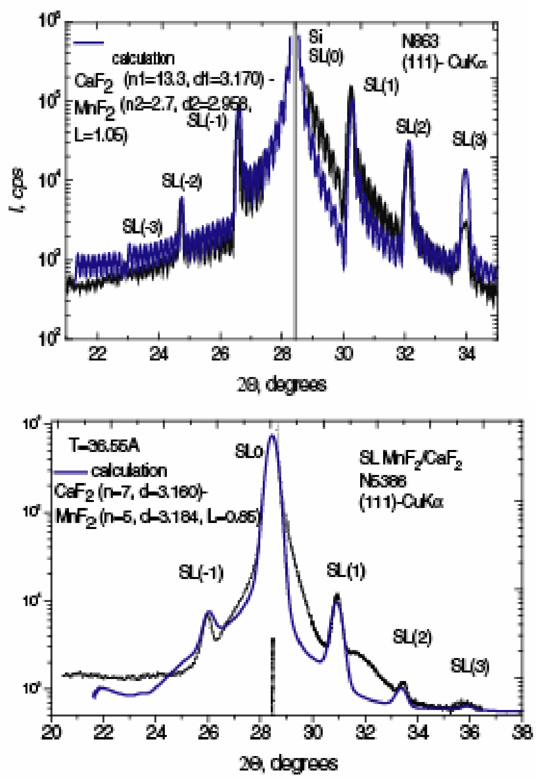

Fig.1. Measured (black) and simulated (blue) θ–2θ-scans for 3/13 (a) and 5/7 (b) MnF_2/CaF_2 SLs. Refined parameters are shown in the graphs.

As follows from parameters obtained, for the sample 863 the values of the (111)-interplanar spacing are the same as for the CaF_2 and MnF_2 fluorite structure films fully strained relative to Si-substrate. The d-values for the sample 5386 characterize the strained CaF_2-layer and relaxed MnF_2 layer with orthorhombic α–PbO_2-structure. The ratio L of structural factors corresponds also to their values of the fluorite and a-PbO_2 structure of MnF_2.

References

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