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

R.N.Kyutt¹, N.S.Sokolov¹, A.G.Banshchikov¹, S.M.Suturin¹, M.Tabuchi², Y.Takeda²
¹Ioffe Physico-Technical Institute, St. Petersburg, Russia
²Venture Business Laboratory, Nagoya University, Japan

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, CaF₂ has cubic fluorite structure and MnF₂ has tetragonal unit cell of the rutile type. It was earlier shown that thin, below 3 monolayers (ML) MnF₂ films grow in metastable fluorite structure [1]. It has been recently demonstrated that using CaF₂ buffer layer on Si substrate MnF₂ 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 MnF₂/CaF₂ superlattices (SLs) with a MnF₂ 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 CaF₂ 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 MnF₂ and “thick”, over 4 MLs of MnF₂ in each period. The SLs were grown at room temperature and covered with thin (2-3nm) CaF₂ 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 MnF₂-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 d₁ and d₂ in CaF₂ and MnF₂ sublayers correspondingly, numbers n₁ and n₂ of monolayers in them and ratio of structural factors \( \frac{F(MnF₂)}{F(CaF₂)} \) (5 parameters in total).

Results

Two typical measured θ–2θ-scans are presented in Fig. 1a,b. For samples with very thin MnF₂-sublayers (n=2-3 ML) the well resolved satellites and thickness fringes are observed on the diffraction curves (Fig. 1a). When the MnF₂-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” MnF₂-sublayers.

As follows from parameters obtained, for the sample 863 the values of the (111)-interplanar spacing are the same as for the CaF₂ and MnF₂ fluorite structure films fully strained relative to Si-substrate. The d-values for the sample 5386 characterize the strained CaF₂-layer and relaxed MnF₂ layer with orthorhombic α–PbO₂-structure. The ratio \( L \) of structural factors corresponds also to their values of the fluorite and a-PbO₂ structure of MnF₂.

References