P-03

Atomic and electronic struture of Bi-Te films grown at various conditions by MBE method

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Topological insulators (TI) are new remarkable materials that have band gap in the bulk but can conduct electricity on their surface via special surface electronic states^[1]. A unique feature of these states is the postulated "topological protection" towards electrons scattering, leading to high electrical conductivity. In addition, a direct relationship between spin direction and the wave vector of surfcae electrons results in a spin polarization electric current. All of these remarkable properties of TI make them the promising candidates for applications ranging from spintronics to quantum computing.

One of the known TI's is bismuth telluride Bi_2Te_3 , which for which the specific properties also retain in the thin films form. The bulk component of the Bi_2Te_3 electronic structure is characterized by a narrow energy band gap which has the value close to 0.16 eV (reported in high quality undoped samples)^[2]. The Fermi level formed by the surface states is then placed roughly in the middle of the bulk gap. Bi_2Te_3 crystallizes in the rhombohedric structure belonging to the R3m space group. The unit cell is built by quintuple layers (QL) – a sequence of five atomic layers consisting of covalently bonded Te(1)-Bi-Te(2)-Bi-Te(1). The QLs are weakly bonded each-together by van der Waals interactions. The thickness of the QL in Bi_2Te_3 is about 1 nm, while the lattice constant extends for 3 QLs in the [001] direction.

 Bi_2Te_3 layers were synthesized on the silicon (100) and mica (001) substrate by molecular beam epitaxy MBE in the co-deposition mode^[3]. The growth process was realized at the ultra-high vacuum conditions (5·10⁻⁹ mbar). The thicknesses of the deposited films were from 10 to 30 nm. The layers had polycrystalline (silicon substrate) and mono-crystalline (mica substrate) structure.

Further studies were carried out *in-situ*. The structure of the obtained films were studied immediately after the synthesis process by reflection high-energy electron diffraction (RHEED) and low-energy electron diffraction (LEED). These techniques revealed the hexagonal structure of surfaces.

The analysis of electronic structure was carried out by X-ray photoelectron spectroscopy (XPS), it revealed no additional elements such as oxygen, carbon and other contaminants, even after several days of storage samples in a vacuum chamber. The analysis of the chemical state based on Bi 4f and Te 3d lines was in the agreement with the literature data for this compounds. In the case of polycrystalline samples the electronic structure was tested for different stoichiometries (tellurium-rich layer, the correct stoichiometry Bi₂Te₃ and sample depleted in tellurium). For monocrystalline films the chemical states of tellurium and bismuth were studied for two different ways of growth process. In the first case sample growth was realized in assumed correct flux ratio of bismuth to tellurium (Bi/Te ratio 2/3). In the second one, the film was deposited in the environment rich in tellurium. Moreover, the XPS was used in order to specify the termination of the Bi₂Te₃ films. The valence band structure of the Bi₂Te₃ films was also investigated by XPS and UPS techniques.

The topography of selected films was measured *ex*situ by atomic force microscopy AFM, thus the sample was shortly (< 5 min) introduced to the external atmosphere. The typical topography indicated the Stranski-Krastanov like growth. The flat areas constitute relatively small part of the total area of film surface. The RMS was found to be of about 9.0(1) Å. The surface is mostly formed by characteristic triangular-shaped islands reflecting the hexagonal crystal structure in the [001] direction. A number of pyramidal-shape terraces with 1 nm high was detected which is in agreement with the thickness of a single QL.

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