ESRF	**Interface structure analysis of the Rashba-Dirac hybrid system BiTeI/Bi_2Se_3(0001)**	**Experiment number**: HC-2926
Beamline: **ID03**	**Date of experiment**: from: 13/06/2017 to: 18/06/2017	**Date of report**: February. 2018
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Report:

We have successfully carried out the proposed experiments. First, the Bi_2Se_3 (0001) single crystal was cleaned by mild Ar+ ion sputtering followed by annealing up to about 500◦C leading to a clean surface and to a sharp contrasted (1×1) low energy electron diffraction (LEED) pattern. Subsequenty BiTeI was evaporated from a Knudsen cell at 380◦C. Owing to the presence of a high Z element (Bi) spin-orbit (SOC) coupling is important and new functionalities can be expected by reducing the crystal's dimensionality to the ultra-thin film limit thereby also breaking the inversion-symmetry which is a prerequisite to observe exotic new phenomena such as the appearance of free electron Rashba-type splitting and the emergence of topological quantum phenomena. Owing to the weak vdW bonding between the BiTeI TL's and between the film and the substrate the maximum film thickness achieved was found to be only 1.5 TL's when the substrate is kept at room temperature.

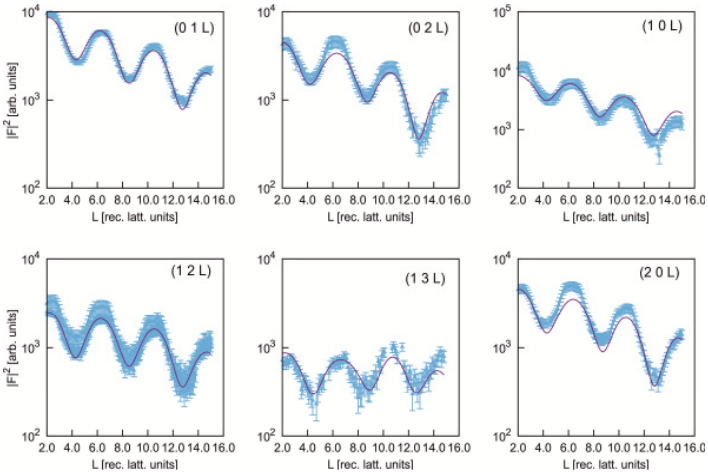

Fig. 1 Data (symbols) and fit (lines) for BiTeI/Bi_2Se_3(0001)

During deposition new LEED spots appear closely corresponding to a √3×√3-R30◦ superstructure. The detailed SXRD analysis indicated that the first order spot is located at h=k=0.316 units of the hexagonal Bi_2Se_3 reciprocal surface lattice rather than at h=k=1/3 for the ideal √3×√3-R30° superstructure, i.e. the BiTeI film is incommensurate with the substrate. In total 1042 symmetry independent reflections were collected along six lattice rods which are shown as symbols in Fig. 1.

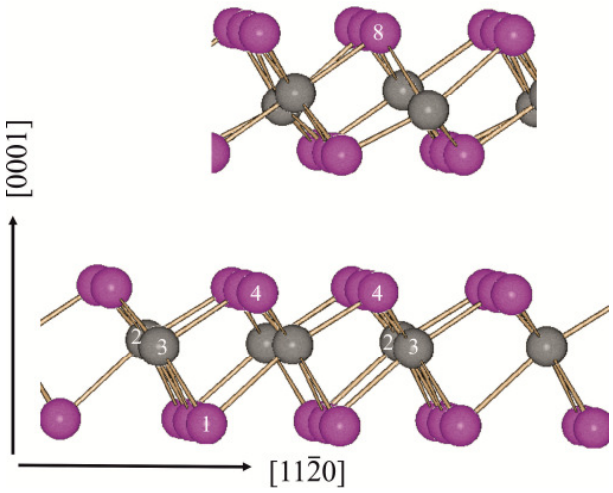

Fig. 2 shows in side view a schematic structure model derived from the fitting of the data. Pink and grey balls represent iodine (tellurium) and bismuth atoms, respectively. The analysis shows that there is one complete and approximately one half of a TL on the Bi_2Se_3 surface. Since this corresponds to the saturation coverage it can be concluded that the inter- layer interaction is very weak. We find strong vertival relaxations, especially a significant increase of the vdW gap. The data analysis is still in progress.