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Surface Studies of II-VI compound semiconductors

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**Report:** The (00 1) CdTe surface has been extensively investigated by grazing incidence X-ray diffraction (GIXD)[1] and STM<sup>[2,3]</sup>. The surface structure of the c(2x2) has been successfully solved[1] and a strong anisotropy observed on the reconstructed domain size for the c(2x2) and (2x1)<sub>HT</sub>. The fks results of in-situ sputtering of the CdTe(OO) surface have shown very interesting surface phenomena, These findings together with Monte Carlo simulation of the island distribution for different coverages were submitted to publication in Europhys. Lett.<sup>[4]</sup> A brief resume of the major results follows.

X-ray diffraction was used to investigate in-situ the Ar<sup>+</sup> ion sputtering of the CdTe(OO) surface. The correlation lengths on the surface were estimated from the widths along the h and k directions of an integer order reflection close to anti-Bragg condition (at  $1 \approx 0$ ) to be about 400 Å (evaluated as  $L = a_s / \Delta h(\Delta k)$ ). The (1 20. 1) reflection intensity (close to the out-of-phase condition) was used to follow the roughness evolution during the removal which is characteristic of a layer-by-layer behaviour at substrate temperatures below 280°C and of an almost step flow above 300°C. The evolution of the de-growth mode from a layer-by-layer to an almost step-flow can be understood considering the high mobility of the Cd and Te atoms at these temperatures.<sup>[5]</sup> The more surprising result, however, appears in the diffraction peak profiles recorded along the h ([1 -1 0]) and k ([1 1 0]) directions (Fig. 1-a , b). The sample temperature was kept constant at 270°C during the sputtering and the peak profile measurements were performed after quenching the system by simultaneously stopping the ion gun and the sample heater after removal of a given coverage. A very different behaviour is observed along the h and k directions. A broad peak at 0.016 reciprocal lattice units (r.l.u.) from the (1 20. 1) peak is observed (Fig. 1-b) along the [1 1 0] direction. The intensity of this peak remains almost constant for the different coverages although it shows a shallow minimum 'at integer layer removal. The position of this peak (P<sub>2</sub>) corresponds to a surface lattice parameter 0.8 % smaller than the bulk one. Its width is related to a domain size along the [1 1 0] direction of only 40 Å. This value is similar to the one determined for the periodical fault distance of the CdTe(OO) c(2x2) structure<sup>[6]</sup>. The deconvolution of the peak profile requires the knowledge of the resolution function orientation (Fig. 2) and of its path during h and k scans. The measured profile is a convolution between the resolution function and the peak intensity distribution in reciprocal space. Unfortunately the h scans were not done around the P<sub>2</sub> position (surface lattice) but around the P<sub>1</sub> position (bulk lattice). Two satellites (S<sub>1</sub> and S<sub>2</sub>) are visible and the knowledge of the orientation and size of the resolution function allows us to determine the precise satellite positions. These satellites are characteristic of a regular distribution of islands along the [1 -1 0] direction<sup>[6]</sup>. From their position an average island distance of

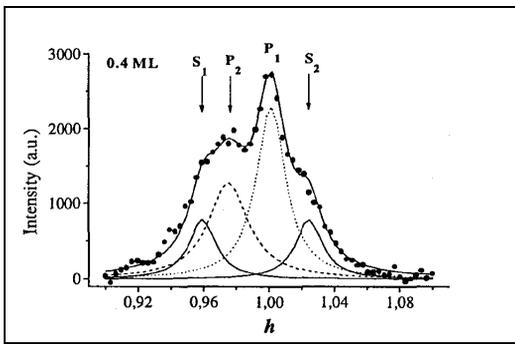


Fig. 1-a) Hscan profile.

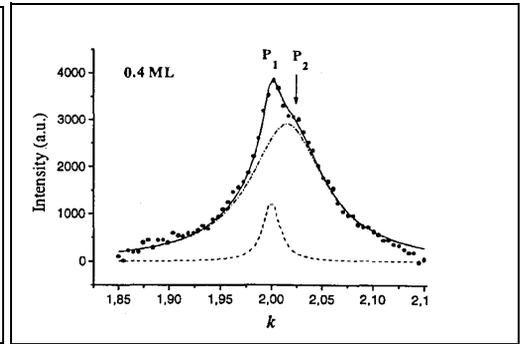


Fig. 1-b) Kscan profile.

100 Å was determined. To understand these findings it is necessary to take into account the surface energy minimisation during the sputtering and to consider the microscopic structure of the CdTe(001) surface. The  $c(2 \times 2)$  structure is formed by 0.5 ML of Cd atoms bounded to a full Te layer and arranged such that a strong lattice distortion is produced in the CdTe bulk structure down to the 6th atomic layer inwards<sup>[1]</sup>. The heating of this surface under UHV above 280°C produces a structural transition to a  $2 \times 1$  surface which is supposed to have the same atomic pattern as the  $c(2 \times 2)$ <sup>[3]</sup>. However the  $2 \times 1$  symmetry does not allow the bond rotation around the Cd atoms in the third layer which is, in the  $c(2 \times 2)$  structure, essential for strain propagation. An alternate possibility to release the strain is to allow a surface lattice contraction along the  $[1 \ 1 \ 0]$ . The deformation produced in the tetrahedron by the motion of the two Te atoms along the  $[1 \ -1 \ 0]$  direction can be compensated by the lateral contraction measured along the  $[1 \ 1 \ 0]$  direction. To summarise the sputtering processes: the first few atoms removed in the beginning produce rows 40 Å apart along the  $[1 \ 1 \ 0]$  direction and the surface can re-order to a  $2 \times 1$  structure. The relaxed surface layer gives the broad peak visible in the  $k$  scans. The system is then composed of two-dimensional islands of  $40 \times 400 \text{ Å}^2$  and the next step will take place independently within these islands.

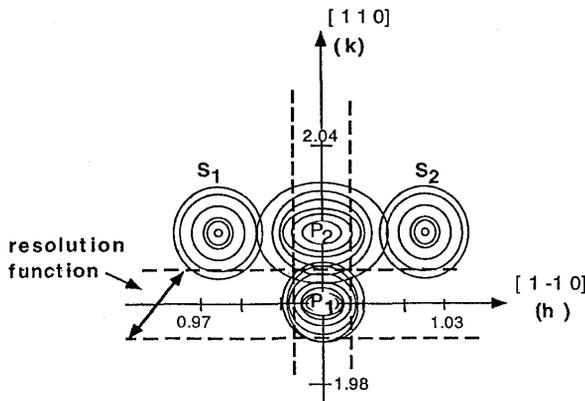


Fig. 2 - Reciprocal space and resolution function

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