Formation of *Rocksalt*-PbTe Quantum Dots Embedded in *Zincblende*-CdTe

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We recently reported the formation of highly symmetric quantum dots (QD) during annealing of a heteroepitaxial PbTe single quantum well clad between CdTe. The formation of these dots is driven by the mismatch of the lattice types of the involved materials. We investigated the QDs with conventional transmission electron microscopy (TEM), which reveals a strong influence of the layer thickness and annealing conditions on the resulting QDs. We perform high resolution TEM investigation combined with multislice simulation for the characterization of the new types of interfaces between the two cubic materials. One effect is the formation of two differently terminated {001} interfaces due to the polar properties of CdTe.

Introduction

We recently reported the formation of highly symmetric quantum dots (QD) during annealing of a heteroepitaxial PbTe single quantum well clad between CdTe layers [1], [2]. The mechanism relies on the mismatch of the two lattice types. The ionic IV-VI compound PbTe possesses *rocksalt* (*rs*) structure; the more covalently bonded II-VI compound CdTe has a *zincblende* (*zb*) crystal structure. Both tellurides show a face-centered cubic (*fcc*) translation symmetry with almost the same lattice constants. This leads to a continuous Te *fcc* sublattice throughout the heterostructure. Although the two heteromaterials are immiscible, coherent layer-by-layer growth is possible far from equilibrium at low growth temperatures around 220 °C. However, during annealing (e.g. 10 min at 320 to 350 °C) the PbTe layer disintegrates into coherent QDs terminated by the three low index {100}, {110} and {111} facets. The resulting QDs exhibit intense room-temperature mid-infrared photoluminescence due to electron-hole pair recombination in the narrow-gap PbTe QDs [1].

Conventional TEM Characterization

We investigated by conventional transmission electron microscopy (TEM) samples with various PbTe layer thicknesses. Mainly bright (BF) and dark field (DF) imaging of the structure-sensitive {002} diffraction spot under two-beam conditions was performed. The specimens were prepared along a <001> zone axis (plan-view sample) or along a <011> zone axis (cross-sectional sample). These investigations give insight into the disintegration of the 2D layer into islands, and show the strong influence of the annealing parameters on the symmetry of the QDs. They reveal also the dependence of the size and density distribution of the resulting PbTe on the epilayer thickness. Figure 1 shows several samples with epilayers of different thickness annealed under different

conditions. Figures 1(a) and 1(b) show a similar PbTe pattern (BF image, dark areas image PbTe). It has, however, to be mentioned that (a) was recorded from a 5 nm thick epilayer annealed at 320 °C for 10 min, whereas (b) is from an as-grown 3 nm thick epilayer, which started to disintegrate due to heating during the specimen preparation process. Figure 1(c) and 1(b) show a 3 nm and a 1 nm PbTe epilayer annealed under the same conditions.

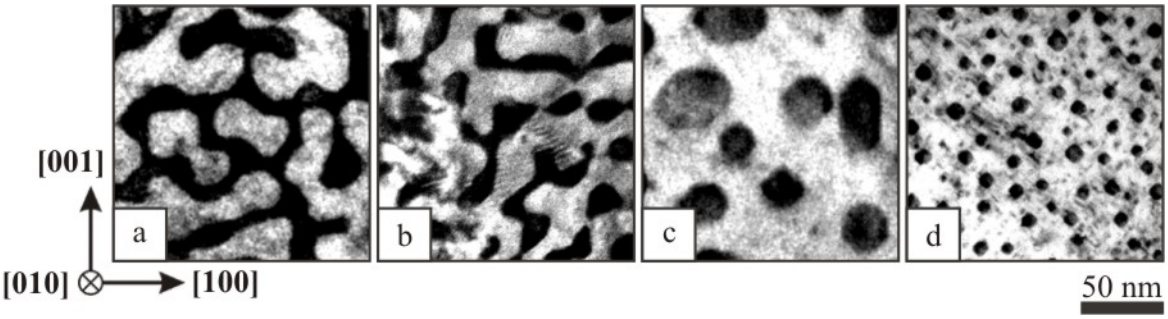

Fig. 1: Bright field (BF) plan-view images of samples with deposited PbTe layers of different thickness. (a) 5 nm PbTe epilayer, annealed at 320 °C for 10 min. (b) as-grown 3 nm thick PbTe epilayer; here the disintegration is induced by the thermal heat transferred during sample preparation. (c) 3 nm PbTe epilayer, annealed at 320 °C for 10 min. The original PbTe layer has already separated into islands with dimensions from 20 to 50 nm and the characteristic set of interface facets. (d) 1 nm PbTe epilayer, annealed at 320 °C for 10 min. The specimen contains only highly symmetric QDs in the range from 5 to 12 nm.

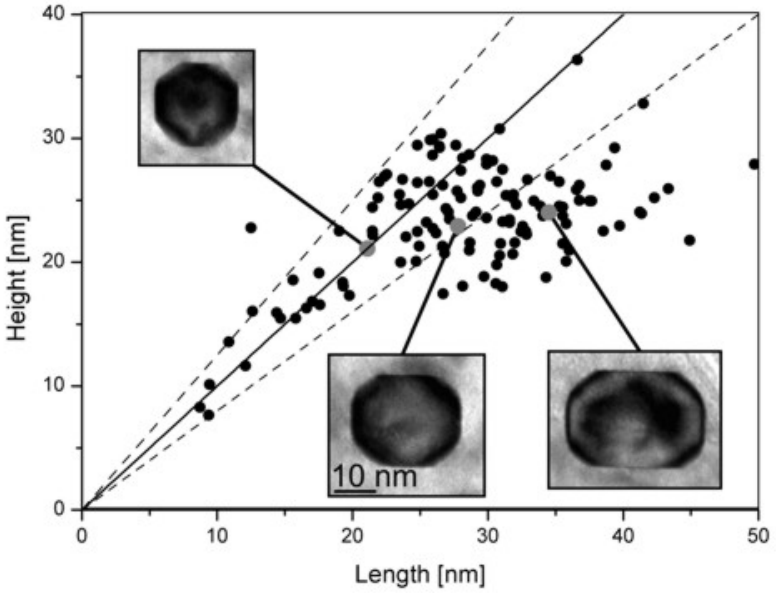

Fig. 2: Evaluation of the dot size distribution form a nominally 5 nm PbTe thick epilayer annealed at 350 °C for 10 min. The height of the dot was measured along the growth direction in a cross- sectional specimen.

Cross-sectional specimens are best suited for statistical evaluation, because both the in-plane and out-of-plane dimensions are visible. Figure 2 shows the size distribution found in a nominally 5 nm thick sample, which was annealed at 350 °C for 10 min. The BF images are from a cross sectional specimen, which means that the plotted height of the dots corresponds to the dimension in growth direction of the SQW. The height ranges form 10 to 30nm, whereas the lateral dimensions can be larger, especially for larger dots. We also evaluated the size of other samples, and found scaling with the initial epilayer thickness. For instance, the resulting QDs from a 1nm SQW are not larger than 12nm.

High Resolution TEM Characterization

HRTEM images of {001} facets prove the coherence and the continuous Te matrix at the interfaces between the two types of crystal structures. It is necessary to perform HRTEM simulations for further insight into the structure of the interfaces. This was done with the JEMS program package. The simulation employs the so-called multislice method, which uses a stack of projected potentials calculated from a thin crystal slice to determine electron transmission through the crystal in connection with the imaging conditions. Theoretical considerations result in two different atomic structures of the {001} interfaces due to the polar character of the {001} CdTe faces (Fig. 3). The figure shows a 3D model of a PbTe SQW with the two kinds of (001) interfaces on opposite sides. As the projection of the crystal structures is different for a 90° rotation of the line of sight along a <011> zone axis, both projections are also shown in Fig. 3.

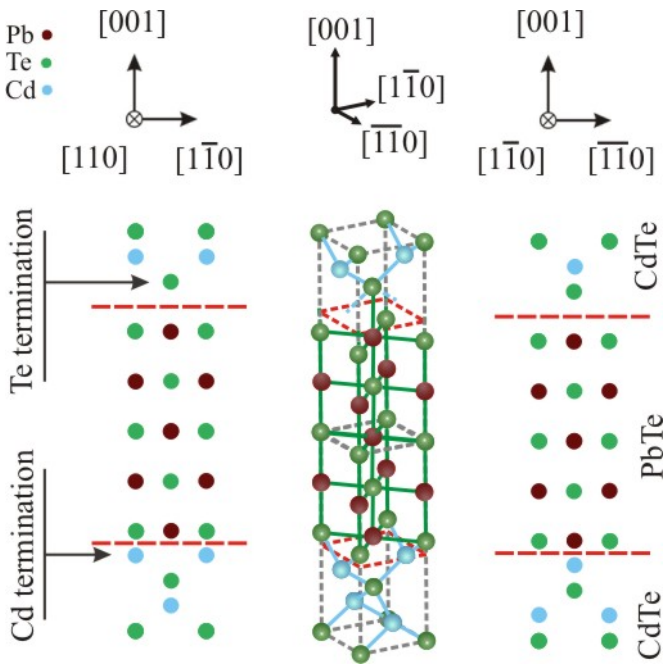

Fig. 3: Model of the {001} interfaces. According to the termination of the polar *zb* CdTe faces, two kinds of {001} interfaces are possible. The Te terminated interface has a lattice plane spacing of ½a at the interface, the Cd terminated has a smaller one of ¼a. Two possible projections of these interfaces can occur in a cross -sectional TEM specimen. The two projections are shown at the left and right hand side of the 3D model.

The identification of these interfaces requires a comparison of simulated HRTEM maps with recorded HRTEM defocus series. This allows an unambiguous allocation of the

projected crystal potentials, which are specifically different for Cd and Te terminated interfaces, to the images. The procedure is necessary, because the relation between the intensity of the recorded images and the projected potential is strongly non linear, and the thickness and defocus conditions of a HRTEM image are only poorly known. This way it was possible to identify both kinds of {001} interfaces in our specimen, as show in Fig. 4. The two HRTEM images of Fig. 4(a) are recorded at opposite interfaces of one and the same QD. Figure 4(b) shows a section of a simulated HR map.

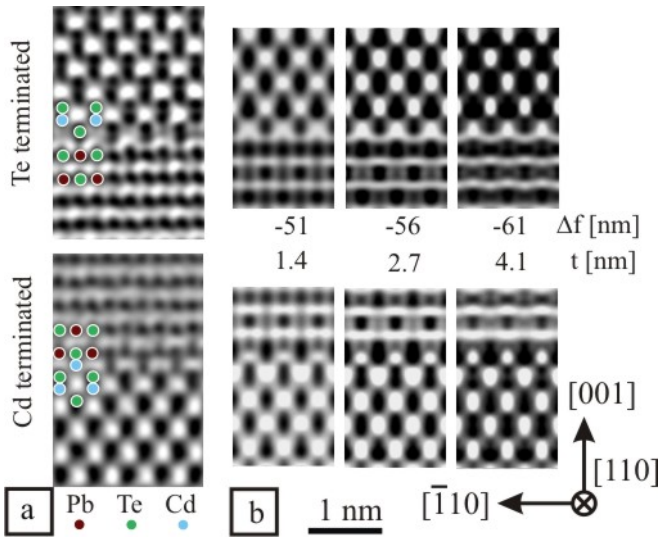

Fig. 4: (a) HRTEM images of a Cd and a Te terminated (001) interface. The respective atomic positions are indicated. (b) A selection of the simulated HR maps for the recorded TEM images. Characteristic for a large range of simulation parameters are the overlapping lattice fringes for the Cd terminated interface and separated lattice fringes for the Te terminated interface.

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