Formation of PbTe quantum dots and their coherent (001) interfaces with the CdTe host crystal

H. Groiss[1], E. Kaufmann[1], S. Kriechbaumer[1], G. Springholz[1], T. Schwarzl[1], G. Hesser[1], F. Schäffler[1], W. Heiss[1], R. Leitsmann[2], F. Bechstedt[2], K. Koike[3], M. Yano[3], T. Wojtowicz[4], P. Werner[5]

1. Institut für Halbleiter- und Festkörperphysik, Universität Linz, 4040 Linz, Austria
2. Institut für Festkörpertheorie und –optik, Friedrich Schiller Universität, Jena, Germany
3. Osaka Institute of Technology, Asahi-ku Ohmiya, Osaka 535-8585, Japan
4. Institute of Physics, Polish Academy of Sciences, Lotnikov 32/46, 02-668 Warsaw, Poland
5. Max Planck Institut für Mikrostrukturphysik, D-06120 Halle, Germany

heiko.groiss@jku.at
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Recently, we have demonstrated a novel approach for the synthesis of epitaxial quantum dots which is based on phase separation between two lattice-type mismatched, immiscible materials in a coherent heterostructure [1]. This principle is applied to the PbTe/CdTe semiconductor system, a combination of the rock salt lattice of PbTe and the zinc blende lattice of CdTe, which show almost identical lattice constants. Upon thermal annealing, 2D PbTe epilayers are transformed into quantum dot (QD) nanoprecipitates with highly symmetric shapes and atomically sharp heterointerfaces [2], (Fig. 1). The QDs show high luminescence efficiency at room temperature in the mid infrared frequency range.

To demonstrate size control of these PbTe QDs, heterostructures with PbTe layer thicknesses of 1 to 10 nm were grown by molecular beam epitaxy. These buried layers were in-situ annealed during the MBE growth and characterized by dark-field TEM. We found an efficient size control with dot sizes from 10 nm to 22 nm (Fig. 1c). The control of the nanocrystal sizes allows also efficient tuning of the photoluminescence properties due to the rapid red shift of the luminescence signal with increasing dot size [3].

To learn more about the formation process we performed annealing experiments with a heatable TEM sample holder to monitor the annealing process. TEM annealing experiments reveal a slow disintegration process of the PbTe epilayer into elongated islands, especially for thicker PbTe layers. This process is followed by a fast transformation of smaller islands into the highly symmetric dots. In addition, also Ostwald ripening of PbTe dots is observed (Fig. 2). The equilibrium shape of the island approaches that of a rhombi-cubo-octahedron, which is defined by atomically sharp {011}, {011} and {111} interfaces (Fig. 1b).

We studied in detail the atomic structure of the polar {001} interfaces between the two tellurides by high-resolution transmission electron microscopy (HRTEM) in combination with multi-slice simulations of phase contrast images. Both the original 2D PbTe epilayers, and the resulting PbTe quantum dots are terminated by distinctively different cation- (Cd) and anion- (Te) terminated (001) interfaces at opposite faces, which can be indentified via simulated HR-maps due their fundamental different lattice spacing at the interface (Fig. 3).

Ab initio simulations reveal that for thin PbTe layers in CdTe different terminated interfaces at opposite {001} interfaces are energetically favorable. This effect is induced by the strong polar bond of the CdTe crystal. It becomes screened by the high dielectric constant of PbTe, which leads to more and more decoupling of the interfaces for thicker layers. Seemingly contradictory findings in recently publish results of the structurally similar

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ErAs/InGaAs [4] heterosystem can be explained by the less polar bonds in the InGaAs compound and the decoupling of the interfaces even for thin layers.

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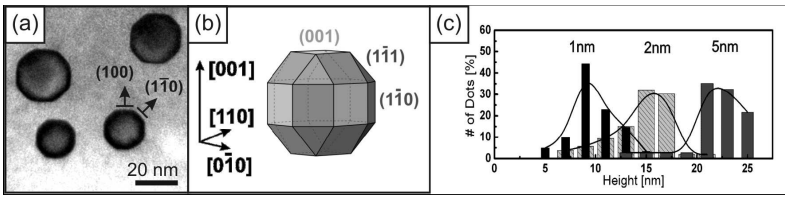

Figure 1. (a) Plan view, bright field TEM image of four PbTe QDs embedded in a CdTe host. (b) The rhombi-cubo-octahedal shape of the highly symmetric QDs. (c) Height histograms of dots originating from PbTe layers with thicknesses of 1, 2 and 5nm before annealing. A substantial increase of the dot size can be seen.

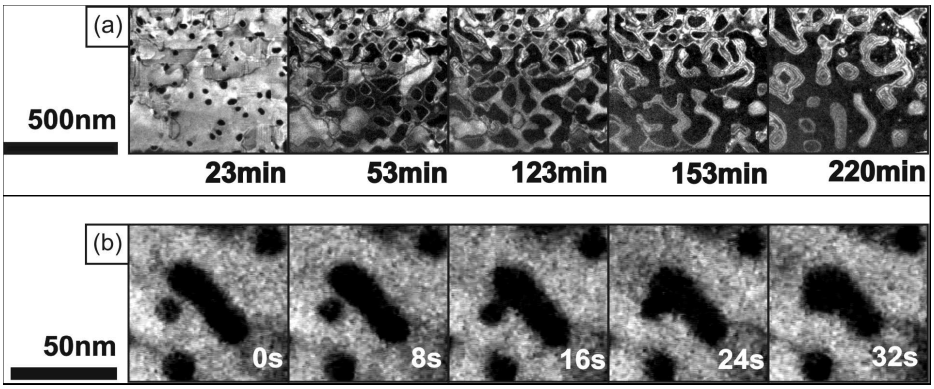

Figure 2. Transformation of an embedded, 5nm thick PbTe epilayer into separated island. The formation was monitored by dark field images (PbTe is bright). The process takes almost 4h, the temperature was increased in this period from 240°C to 340°C. (b) Ostwald ripening of two QDs. Originally the sample contains a 3nm PbTe layer, which was annealed for 30min at 260°C. The aggregation of the small and the large dot happened then within 30 seconds. The images are recorded as bright field images (PbTe is dark).

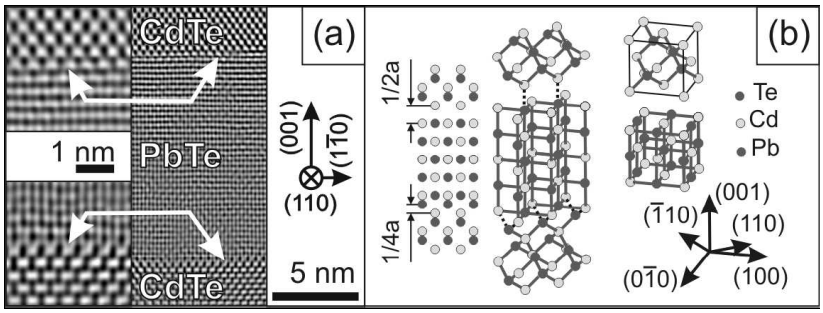

Figure 3. (a) High resolution TEM images of two opposite PbTe/CdTe {001} interfaces. The main difference of an anion- and a cation-terminated interface can be seen in (b). The 3D model shows the atomic configuration of an embedded PbTe slab. The interface spacing changes from ½ to ¼ of the lattice constant *a*, respectively for a Te and a Cd terminated interface.

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