Nano-Scale Dislocation Patterning in PbTe on PbSe (100) Heteroepitaxy Studied by Scanning Tunneling Microscopy

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Heteroepitaxial growth of PbTe on 5.2% lattice mismatched (100) oriented PbSe is investigated using UHV-scanning tunneling microscopy. A 2D growth mode is found, and it is shown that strain relaxation occurs by pure edge type misfit dislocation formation. The early stages of strain relaxation show a lateral injection of dislocation half loops from monolayer step edges on the surface. A rapid increase of the dislocation density with PbTe layer thickness indicates a very effective strain relaxation mechanism with a critical layer thickness below 1 monolayer (ML). At PbTe layer thicknesses above 4 ML we observe the formation of a highly regular network of misfit dislocations with a dislocation spacing of around 10 nm, and a smallest variation of the dislocation separation of only ±12%. Thus, this nano-scale dislocation patterning can serve as template for the fabrication of self-assembled, ordered nanostructures.

1. Introduction

Strain relaxation is a critical process in lattice-mismatched heteroepitaxy. For highly mismatched heteroepitaxial systems, two different strain relaxation mechanisms exist, namely (1) the spontaneous formation of strain-induced coherent 3D islands on the surface, or (2) by misfit dislocation formation at the layer/substrate interface. For the latter, recent work has shown that the formation of interfacial dislocations strongly modifies surface morphology of the epitaxial layers, due to long-range elastic deformations of the lattice and in many cases due to monolayer surface glide steps [1]. In semiconductors, misfit dislocations are usually distributed in a irregular way within the layers, but for special growth geometries highly periodic dislocation arrays occur [2], [3]. This dislocation pre-patterning has been demonstrated as a tool for spatial manipulation of the nucleation sites of self-assembled quantum dots [4], [5], based on the local perturbation of the total free energy of the surface by the subsurface misfit dislocations.

In the present work, we have studied the strain relaxation mechanisms of PbTe on 5.2% lattice-mismatched (100) oriented PbSe substrates, using UHV scanning tunneling microscopy (STM). The non polar (100) surface has the lowest surface free energy in the rocksalt crystal structure, other than the polar (111) surface, where strain relaxation is found to occur by Stranski-Krastanow growth.

2. Experimental

The samples were grown by molecular beam epitaxy using compound sources for PbSe and PbTe. On polished PbSe (100) substrates, a several μm thick PbSe buffer layer was deposited at a temperature of 380 °C, followed by a PbTe layer, where the PbTe layer thickness was varied from 0.3 to 22.5 ML. After growth, the samples were rapidly cooled down to room temperature and transferred to a separate UHV-STM chamber without breaking ultra-high vacuum conditions.

3. Results

In contrast to (111) oriented growth we find for the growth of PbTe on (100) oriented PbSe substrates a 2D growth mode that persists throughout the heteroepitaxial growth process (Fig. 1). Strain relaxation occurs purely by the formation of misfit dislocations that appear as dark surface depression lines in large-scale STM images (Fig. 1(b) – (d)). Studies of layers with varying PbTe layer thicknesses give a critical layer thickness h_c for the onset of misfit dislocation formation of only 0.8 ML, and STM images of very early relaxation stages show that misfit dislocation half loops are injected laterally from monolayer step edges on the surface (Fig. 1(b)). With increasing PbTe layer thickness the misfit dislocation density increases rapidly, and above about 4 ML PbTe a highly regular, square grid of misfit dislocations with a spacing of the order of 10 nm develops. By measuring the dislocation line density in STM images the relaxed strain in the layers was determined as a function of layer thickness, indicating a very rapid strain relaxation with more than 90% of the 5.2% misfit strain already relaxed at a PbTe layer thickness of 9 ML.

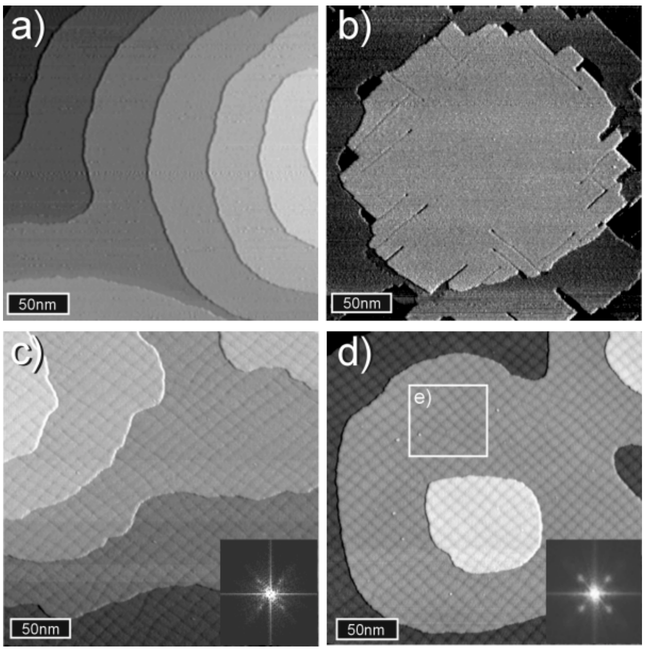

Fig. 1: STM images of PbTe layers on PbSe (100) for different layer thicknesses of (a) 0.3, (b) 0.8, (c) 4.5 and (d) 9 ML. Insert in (c) and (d): FFT power spectra of the STM images. The marked area (e) is shown in Fig. 2 (a) on an enlarged scale.

Atomically resolved STM images of an endpoint of a misfit dislocation (see Fig. 2(b)) show that the Burgers vector **b** is of ½<011> type, as expected for the rocksalt crystal structure of PbSe and PbTe. The Burgers vector is parallel to the heterointerface, and thus, the misfit dislocations cannot be formed by glide but only by climb processes. In addition, **b** is perpendicular to the misfit dislocation lines that run along the fourfold <1-10> directions. Therefore the misfit dislocations are of pure edge character.

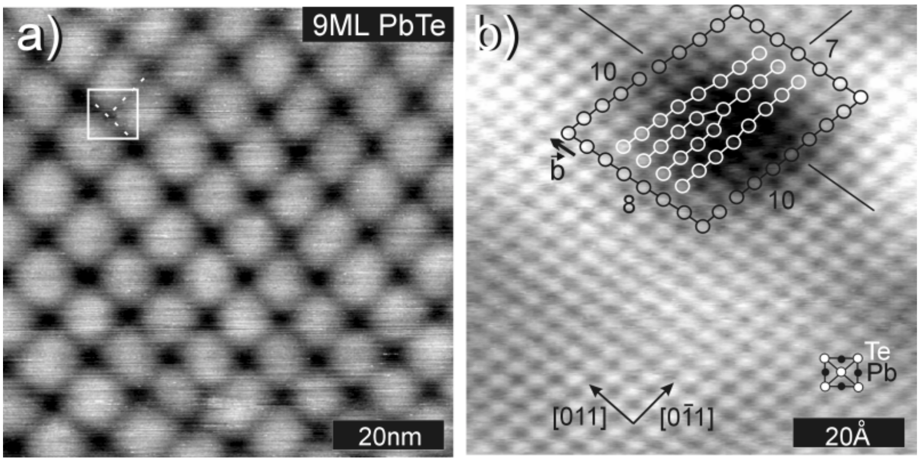

Fig. 2: STM images of a 9 ML PbTe layer on PbSe (100). As shown in (a) a very regular quadratic dislocation array is formed. The atomically resolved STM image of the area in (a) is shown in (b). As indicated by the Burgers circuit, the Burgers vector is equal to ½<011> and the dislocations are formed along the <0-11> directions.

The remarkable regularity of the dislocation network is evidenced by the appearance of satellite peaks in the FFT power spectra of the STM images (insert in Fig. 1(c) and (d)). A statistical analysis of the dislocation spacings for the 4.5 and 9 ML PbTe samples (Fig. 3) indicates a narrowing of the distribution of the dislocation spacings, i.e. a higher regularity of the dislocation network with a variation of the dislocation separation of only ±12% for the 9 ML sample. This is less than the typical variations in size and spacing of self-assembled quantum dots formed by the Stranski-Krastanow growth mode. The high regularity of the dislocation network is explained by the repulsive force between the dislocations and the high dislocation mobility within the heterointerface.

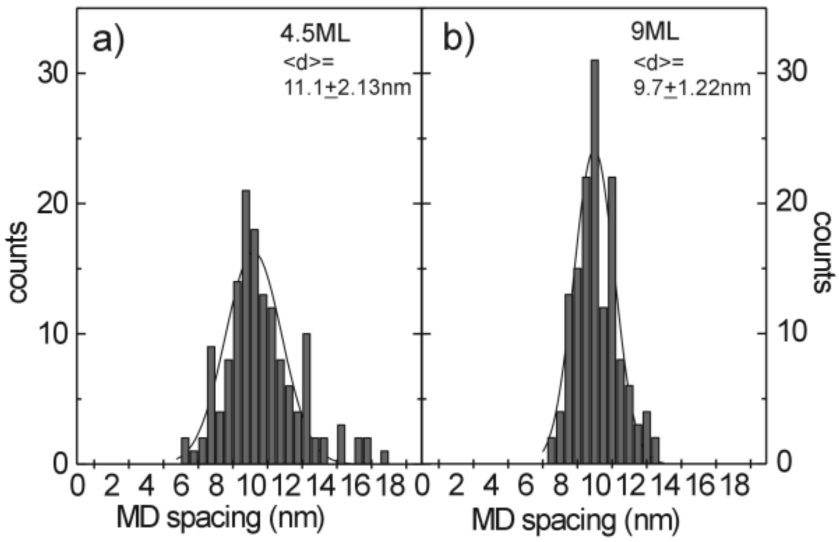

Fig. 3: Histograms of the lateral misfit dislocation spacings for PbTe layer thicknesses of (a) 4.5 ML and (b) 9 ML, indicating that the distributions narrow with increasing layer thickness.

4. Conclusions

For the growth of PbTe on (100) oriented substrates we find a 2D growth mode and a very effective strain relaxation process by the formation of pure edge type misfit dislocations that are formed by a climb process. With increasing PbTe layer thickness, the dislocations form a highly regular, square grid along the fourfold <1-10> directions with a period of the order of 10 nm. Due to the high uniformity of the dislocation network, this dislocation patterning can serve as template for the fabrication of self-organized ordered nanostructures. Because the interaction between dislocations depends strongly on the dislocation separation, similar results can be expected for other highly mismatched heteroepitaxial systems.

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