Scanning Tunneling Microscopy Investigations of Surface Undulations in Lattice-Mismatched Heteroepitaxy

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The surface structure of relaxed IV-VI heteroepitaxial layers is studied using scanning tunneling microscopy. For bilayer structures consisting of highly relaxed EuTe layers covered by thick PbTe buffer layers, huge surface undulations with amplitudes as large as 50 Å are observed. These undulations are completely decoupled from the surface step structure and can be observed even for large cap thicknesses. The deconvolution of the surface profiles shows that the surface undulations are purely caused by the nonuniform misfit dislocation network at the EuTe/PbTe interface.

1. Introduction

Strained-layer heteroepitaxy is of considerable importance for semiconductor devices, offering more degrees of freedom in design and fabrication of modulated heterostructures and superlattices. In such structures, strain-engineering can be utilized as an additional method for adjustment of the electronic properties [1]. This is usually accomplished by predeposition of highly relaxed buffer layers as “virtual substrates” prior to the active layers. However, the strain relaxation often results in pronounced surface undulations of the buffer surface [2] – [8], such as the so-called “cross hatch” surface pattern on InGaAs [2] or SiGe [3] , [5] – [8] buffers. The origin of these undulations has remained a controversial issue. While some groups have proposed nonuniform growth due to localized dislocation strain fields [3], [7], [8], other groups have favored glide steps and lattice deformations [4] – [6]. Up to now, most studies have not been able to distinguish between these effects. In the present work, the evolution of the surface structure of highly relaxed IV-VI epitaxial layers was studied using scanning tunneling microscopy. These materials have been used extensively for the fabrication of mid-infrared diode lasers [9]. To circumvent the problems associated with the interdependence of strain relaxation and epitaxial growth, we have designed a bilayer structure, where first a highly lattice-mismatched layer is deposited to produce a dense network of misfit dislocations, followed by a nearly pseudomorphic second layer. In this two-step process, the dislocation formation within the first layer is completely decoupled from the growth of the subsequent layer.

2. Experimental

The bilayer EuTe/PbTe samples were grown by molecular beam epitaxy on 3 µm PbTe buffer layers predeposited on (111) BaF_2 substrates. Both compounds crystallize in the rock salt crystal structure and their lattice-mismatch is 2.1%. First thick PbTe buffers were deposited on the substrate, which yields high quality epitaxial layers with very smooth surfaces [10]. Onto these buffers, EuTe layers with thicknesses exceeding the critical thickness were grown in order to form a network of misfit dislocations with well defined dislocation density. Although the critical thickness for misfit dislocation formation is 18 monolayers (ML) for the EuTe/PbTe case [4], significant strain relaxation does not occur before 40 ML when dislocation multiplication sets in. The highly dislocated layers were overgrown by PbTe cap layers with thicknesses varying from 0.1 to 3 µm. For the study of the evolution of surface morphology, the samples were rapidly cooled and transferred to an UHV-STM chamber for surface imaging. The strain state of the layers and corresponding overall misfit dislocation densities were determined by high x-resolution x-ray diffraction. To access the large scale surface morphology, the samples with thick cap layers were also studied by AFM under ambient conditions.

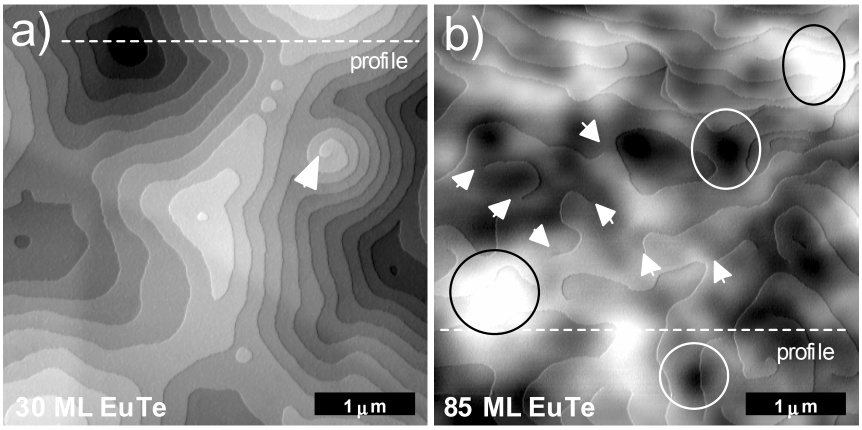

Fig. 1: STM surface images of two PbTe/EuTe bilayer samples with an EuTe layer thickness of (a) 35 ML and (b) 85 ML, but with identical 1000Å PbTe cap thickness. The arrows indicate the penetration points of threading dislocations and the surface profiles along the dashed lines are shown in Fig. 2. The strong surface contrast observed for the highly relaxed sample (b) and indicated by the circles arises from large scale surface undulations that are not correlated with the monolayer step structure.

3. Results

The STM images of two bilayer samples with different EuTe layer thicknesses but identical 1000 Å PbTe cap thickness are shown in Fig. 1. The first sample with an EuTe thickness of d_{EuTe} =30 ML is a nearly pseudomorphic structure with a negligible number of misfit dislocations (relaxed strain of less than 0.01% from x-ray diffraction). As shown in Fig. 1 (a), the surface of this sample exhibits an evenly spaced terrace structure that is essentially identical to that of the underlying PbTe buffer layer [10], with occasional threading dislocations (see arrow) that remain from the growth on the lattice-mismatched BaF_2 substrates. The measured threading dislocation density is about 10^7 cm^{-2} in this sample, which is typical also for the PbTe buffer layers [10].

In contrast, the STM image of the highly relaxed sample (Fig. 2 (b)) with d_{EuTe} = 85 ML (six times the critical thickness) reveals a completely different surface structure. The highly irregular surface steps consists of many short segments terminated by threading dislocations. In fact, the threading dislocation density of 10^9 cm^{-2} in this sample is a factor of 100 larger than that of the PbTe buffer layers. This is a clear indication for the formation of misfit dislocations at the EuTe/PbTe interfaces, with a corresponding increase of the threading dislocation density due to dislocation nucleation and multiplication processes.

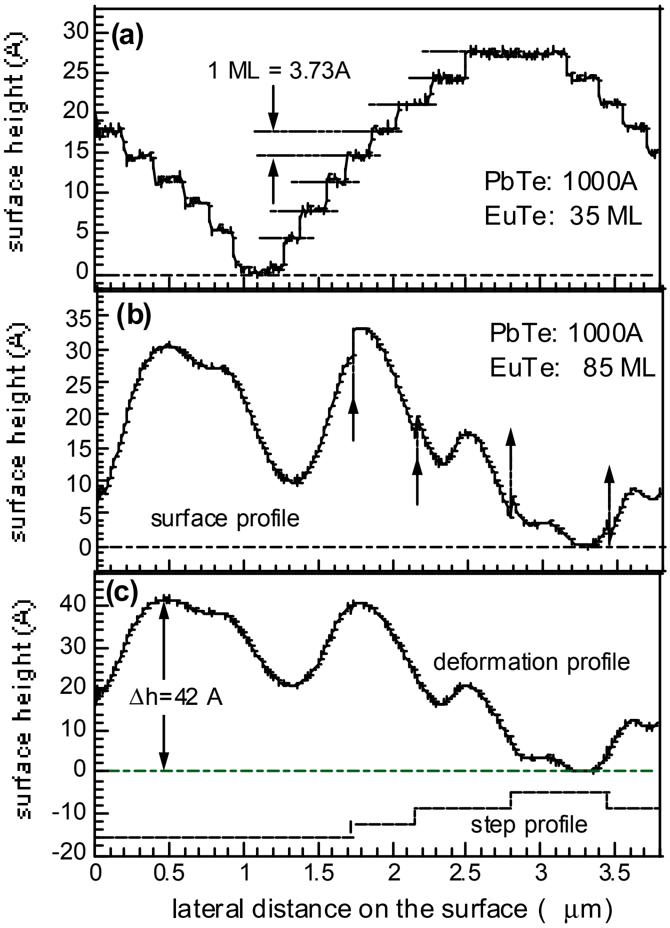

Fig. 2: Measured scanning tunneling microscopy surface profiles along the dashed lines in Fig. 1: (a) pseudomorphic structure with d_{EuTe}=30 ML, and (b) relaxed sample with d_{EuTe} = 85 ML. (c) shows the deconvoluted deformation profile (full line) and the step profile (dashed line) derived from the measured profile (b).

Even more, however, a very strong black and white contrast appears in the STM images, as is indicated by the circles in Fig. 1 (b). The corresponding local depressions and elevations of the surface of up to 50 Å by far exceed the changes in surface height due to the monolayer steps, and their lateral extent is typically between 0.5 and 1 μm. Apparently, these large scale surface undulations are not correlated to any steps on the surface, but appear on the flat terraces as well as across single monolayer steps that separate adjacent terraces. Therefore, they cannot be related to growth effects but must arise from large inhomogeneous strain fields within the misfit dislocation networks at the buried heterointerfaces.

The completely different surface structure of the two samples is even more evident from the comparison of the STM surface profiles measured along the dashed lines in Fig. 1.

Whereas for the pseudomorphic structure (Fig. 2 (a)), the surface profile consists only of a train of monolayer surface steps with 3.73 Å step height, the profile of the highly relaxed sample (Fig. 2 (b)) exhibits large scale *continuos* undulations superimposed on the surface steps. Since the individual surface steps in the STM profiles are well resolved, this surface profile can be deconvoluted into two contributions: one from the usual surface step structure (arrows in Fig. 2 (b)), and one from continuos wave-like deformations of the epitaxial surface. Figure 2 (c) shows the deconvoluted step and deformation profiles (dashed and full lines, respectively), clearly indicating that the contribution of the lattice-deformation by far exceeds that of the usual surface steps. Thus, most part of the observed surface morphology is not related to growth features.

The origin of the large-scale surface undulations can be explained as follows. As shown by our previous STM work [11], each *individual* subsurface misfit dislocation gives rise to a local deformation of the surface with an amplitude of the order of the dislocation Burgers vector (4.4 Å). The width of the deformation profile increases linearly with layer thickness, but its amplitude remains constant. Consequently, the factor ten larger surface undulation observed in the present samples must arise from the constructive overlap of the deformation fields of many individual misfit dislocations concentrated at certain areas of the interface. For a *regular* network of misfit dislocations, the surface displacements from evenly distributed dislocations would cancel out completely as soon as the depth of the dislocations is about three times larger than the dislocation spacing because the width of the individual deformation profiles is equal to the dislocation depth [11]. For *irregular* dislocation networks this is not necessarily the case. Considering a period of the surface undulations of the order of 1 µm, the existence of bunches of up to 10 individual dislocations explains the observed large scale surface undulations. Such bunches of dislocations are indeed consistent with the measured average dislocation densities of 75 μm^{-1} in our samples.

4. Conclusions

In conclusion, we have shown that the large lattice distortions in highly dislocated lattice-mismatched heteroepitaxial layers give rise to large scale continuous undulations of the epitaxial surface. We do not find any indication that the corresponding inhomogeneous elastic strain fields influence the growth processes on the surface. This general conclusion should apply also for most other strained-layer heteroepitaxial systems.

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