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ScienceDirect
Surface Science 601 (2007) 5441–5444
SURFACE SCIENCE
www.elsevier.com/locate/susc

CdTe and PbTe nanostructures on the oxidized pentagonal surface of an icosahedral AlPdMn quasicrystal

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Received 1 June 2007; accepted for publication 31 August 2007
Available online 15 September 2007

Abstract

By means of congruent evaporation, we have deposited CdTe and PbTe onto the oxidized fivefold-symmetry surface of an icosahedral AlPdMn quasicrystal. This procedure results in the formation of nanocrystals in both cases. While the azimuthal orientations of the crystallites are random, the polar orientations are well defined. The crystalline CdTe and PbTe domains expose their (1 1 1) and (0 0 1) faces, respectively, which are aligned parallel to the pentagonal surface of the quasicrystal. The nanometric size of the domains is not a result of the lattice mismatch between the growing film and the substrate as usually observed in molecular-beam epitaxy, but of the limited size of the oxide domains of the substrate surface.

Keywords: PbTe; CdTe; Al–Pd–Mn; Quasicrystals; Interfaces; Semiconductors; Random orientation

1. Introduction

Properties of semiconductor nanocrystals or quantum dots have received particular attention in the past decades [1]. With decreasing size, solids gradually lose their bulk properties, approaching more and more molecular-like behavior. Due to the confinement of charge carriers to the restricted volume of the small particles, quantum mechanical phenomena are observable for which the range of sizes under investigation is frequently called the size-quantization regime. In the case of semiconductors, size-dependent effects are particularly remarkable. For instance, in the II–VI semiconductor CdS the band-gap energy evolves from 4.5 to 2.5 eV as the size increases from the molecular regime to the macroscopic range [2]. The energy required to add an excess charge carrier above the band-gap decreases by 0.5 eV [3] and the melting point increases from 400 to 1600 °C [4]. During the last few years, a great effort has been spent to achieve the synthesis of well-ordered quantum dots homogenous in size and shape. Besides synthesis in solution and nanolithography, molecular-beam epitaxy has been established as a successful method. Because of the lattice mismatch between the substrate and the deposited material, the growing film breaks up into domains with a typical size in the nm range.

CdTe and PbTe are, in their crystalline forms, direct band-gap semiconductors widely used in the industry. CdTe, a II–VI semiconductor with a wide band-gap of 1.56 eV at room temperature, is considered as one of the most important photovoltaic materials due to its high absorption coefficient and band-gap energy, which is close to the optimum value [5]. It possesses a zincblende structure with a lattice constant of 6.48 Å. PbTe is a IV–VI semiconductor with a narrow band-gap of 0.32 eV at room temperature and one of the most sensitive materials for infrared sensors. Since all technologically important narrow band-gap semiconductors are difficult to fabricate and handle in bulk form, growth of thin films on a dielectric substrate is the preferred solution for large line or area arrays. PbTe possesses a rock-salt structure with a lattice constant of 6.37 Å.

Confinement effects occur in semiconductor quantum dots if their size is smaller or comparable to the exciton

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doi:10.1016/j.susc.2007.08.028

Bohr radius in the material [6]. According to Schmitt-Rink et al. [7], the linear and resonant nonlinear optical properties will exhibit the greatest enhancement when the nanocrystal radius is much smaller than the Bohr radius in the bulk material, the so-called strong-confinement limit. For CdTe and PbTe, the bulk exciton Bohr radii were calculated to be approximately 100 and 500 Å, respectively [6,8], implying that, if the domains are isolated, strong confinement of the charge carriers occurs in all three dimensions. In case of wetting of the substrate by the deposited material, quantum-well states should be observable. Because the size of the nanoparticles normal to the substrate surface can be controlled by choosing the quantity of the evaporated material without any observable structural modification between one and several monolayers, it would be possible to tune the size effects.

Quasicrystals form a third state of atomic ordering besides periodic and amorphous structures. They exhibit sharp electron- and X-ray-diffraction patterns characteristic of long-range orientational, such as five, eight, or tenfold, and quasiperiodic translational order [9]. Crystal–quasicrystal interfaces are of special interest due to the several unexpected phenomena that occur at the conjunction of different, but nevertheless related structural properties. Since preparation methods for the generation of well-defined quasicrystalline surfaces have been established and can be readily applied, quasicrystals became efficient substrates for heteroepitaxy. During the last decade, a great amount of different materials has been deposited on quasicrystalline substrates [10]. Besides pseudomorphic growth and heterogeneous nucleation, the growth of self-size-selecting crystalline domains in the nm range has been observed. In the case of Co deposition, for instance, five body-centered cubic Co domains exposing their (1 1 0) faces parallel to the pentagonal surface of the icosahedral (i-)AlPdMn quasicrystal, rotated by 72° with respect to each other and of a size of about 20 Å are formed [11]. Recently, we have reported the formation of a new kind of crystal–quasicrystal interface by oxidation of the pentagonal surface of the i-AlPdMn quasicrystal. A 5 Å thick, well-ordered aluminum-oxide (Al-ox) film is formed, which consists of five pairs of ℓ-domains rotated by 72° with respect to each other and of a size of about 35 ± 2 Å [12]. The alignment of one pair of ℓ-Al-ox domains along a twofold-symmetry direction of the pentagonal surface of i-AlPdMn is illustrated in Fig. 1.

Here, we present the results obtained for the deposition of CdTe and PbTe onto the oxidized pentagonal surface of i-AlPdMn. We observe the formation of crystallites in the nm range. While their azimuthal orientations are random, the polar orientations are well defined.

2. Experimental

An i-quasicrystal with a nominal bulk composition of $Al_{70}Pd_{20}Mn_{10}$ and grown by the Bridgman technique was oriented by the X-ray Laue method along a fivefold-symmetry axis and cut by spark erosion perpendicular to this direction [13]. After polishing the sample using diamond pastes with grain sizes down to 0.5 μm, the sample with dimensions of $5 \times 5 \times 1$ mm^3 was mounted on a goniometer and introduced into an ultra-high vacuum chamber with a base pressure in the lower 10^{-10}-mbar range. The sample temperature was measured with a chromel–alumel (K-type) thermocouple pressed onto the front surface and the sample was heated from the backside using a resistance heater. The clean quasicrystalline surface was established by cycles of Ar^+-ion sputtering at 1.5 keV and annealing at 700 K. This preparation procedure leads to a bulk-terminated surface [14]. Low-energy electron diffraction (LEED) was used to investigate the structural order in a near-surface region and Auger-electron spectroscopy (AES) to probe the chemical composition of this region. A three-grid back-view display system with a total opening angle of 100° and operated with a beam current in the low μA range was used for the LEED experiment. Patterns were recorded using a 16-bit charge-coupled device camera and subsequently normalized by the overall response function of the display system in order to eliminate spurious signals. PbTe and CdTe evaporations were performed with non-commercial power-regulated molecular-beam sources, while the sample was kept at constant temperature. After the initial outgassing procedure of the sources, the pressure never exceeded 1×10^{-9} mbar during evaporation. The deposition rates were calibrated in a separate experiment by measuring the 94 eV NOO, the 376 eV $M_5N_{4,5}N_{4,5}$, and 483 eV $M_5N_{4,5}N_{4,5}$ AES signals of Pb, Cd, and Te, respectively, during deposition onto a polycrystalline Cu sample. The deposition rates were found to be for PbTe 1.05 ± 0.05 and for CdTe 1.41 ± 0.05 Å/min. The values of the inelastic mean free paths of the measured electrons, used in the

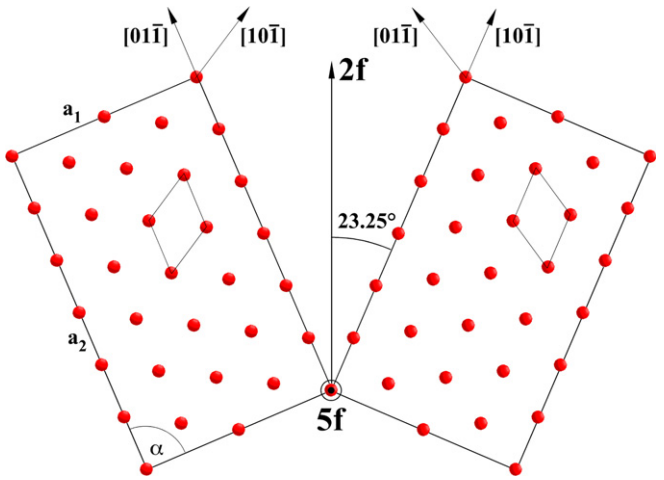

Fig. 1. Orientational relationship between a pair of ℓ-domains and the fivefold-symmetry surface of i-AlPdMn, represented by an in-plane twofold-symmetry axis and the pentagonal direction normal to the sample surface. The unit cell of the oxide layer is spanned by the lattice parameters $a_1 = 10.6$ Å, $a_2 = 17.9$ Å, and $\alpha = 88.7°$. Elementary oxygen cells are symbolized by rhombohedra.