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Residual strain in cadmium telluride/gallium arsenide (001) heterostructures as a function of temperature

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ABSTRACT

Optical studies of residual strain in cadmium telluride (CdTe) films grown using molecular beam epitaxy on gallium arsenide (GaAs) substrate have been performed using photoreflectance techniques. Measurements have been conducted to determine the fundamental transition energy, heavy-hole and light-hole transition energy critical-point parameters in a range of temperatures between 12 and 300 K. There are problems inherent in the fabrication of optoelectronic devices using high-quality CdTe films, due to strain effects resulting from both the lattice mismatch (CdTe: 14.6%) and the thermal expansion coefficient difference. The CdTe film exhibits compressive stress causing valence-band splitting for light and heavy holes. We have used different models to fit the obtained experimental data and, although the critical thickness for the CdTe has been surpassed, the strain due to the lattice mismatch is still significant. However, the strain due to the thermal expansion is dominant. We have found that the fundamental transition energy, E_0, is affected by the compressive strain and the characteristic values are smaller than those reported. In addition, the total strain is compressive for the full measured range, since the strain due to the lattice mismatch is one order of magnitude higher than that calculated from the thermal expansion.

1. Introduction

Technological advances in the fabrication of thin films have enabled the increased commercialization of solar cells, which are used to generate electricity. This increase is due to a reduction in production cost, along with the fact that solar cells represent an attractive renewable energy source, with the potential to solve the critical energy crisis if higher efficiency can be achieved. Among them, thin-film semiconductors based on binary oxides are of increasing importance, including cadmium telluride (CdTe), which has become the world leader in solar cell module production because of its high photon absorption coefficient and optimal band gap. The use of new and improved growth techniques has led to the production of high-efficiency cells at lower cost. Currently, the record laboratory efficiency of CdTe solar cells is approximately 19.6% [1,2]; however, this value is significantly behind that of the theoretical maximum. The most likely limiting factors are defects such as grain boundaries (GB) and intragrain dislocations, which produce charge-trapping centers and increased power dissipation in optoelectronic devices [3], as well as decreasing the average minority carrier lifetime. The high efficiency of the cells depends on the crystalline quality of the films (among other factors), which is decreased by the presence of structural defects [4], some of which are generated by residual strain [5–8].

II–VI semiconducting compounds have become particularly attractive due to their considerable potential applications in engineering optoelectronic devices [9]. Again, CdTe is one of the most important materials in terms of

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technological applicability, since it has been used in the development of semi-insulating crystals for gamma-ray detectors and also in electro-optical and acousto-optical designs [10] in solar cells (because its band gap is 1.5 eV, 300 K). It is also used in liquid-crystal optical imaging devices and infrared optics [11]. In addition, CdTe is important for the implementation of non-linear materials with high commutation speeds, such as optical interrupters, signal amplifiers, or solar-energy converters, due to its electro-optical factor, which is approximately three times higher than that of the corresponding III–V semiconductors.

Nevertheless, the epitaxial growth of CdTe on gallium arsenide substrates (CdTe/GaAs) exhibits strain effects and misfit dislocations due to the large lattice mismatch (14.6%, 300 K) [12,13]. CdTe films can be grown using different techniques, such as molecular beam epitaxy, metalorganic chemical vapor deposition, and pulsed laser deposition [14], while thin films can be epitaxially grown on lattice-matched substrates with similar crystal structure (see Fig. 1). Thin films are extensively used in wafer fabrication and layers, and have the advantage that they can grow high quality crystalline films compared with the bulk crystal. For the CdTe/GaAs heterostructure, the critical thickness is only a small number of atomic monolayers (6–7 Å) [15]. The CdTe films (a=6.482 Å, $\alpha=5.6\times10^{-6}$/K, 300 K) on GaAs substrates (a=5.431 Å, $\alpha=5.2\times10^{-6}$/K, 300 K) have differences in lattice parameters as well as in thermal expansion coefficients; therefore, the first CdTe layers are deposited under compressive stress. As a result of these differences, the strain in the heterostructures is not only induced by the lattice mismatch but also the difference between the thermal expansion coefficients.

CdTe is a semiconductor that has a direct energy gap located at the Γ point of the Brillouin zone and its temperature dependency is of interest to many researchers. The temperature dependence of the band-gap energy is attributed to the electron–phonon interaction and the lattice thermal expansion; the first process is the main contributor while the second contributes between 2% and 20% of the temperature dependence at room temperature in most semiconductor materials [16–18]. Despite the contribution to the temperature dependence in the exciton transition energy, the thermal expansion mechanism is not taken into account in some reports. The negative thermal expansion at low temperature does not have monotonic dependence, and this behavior is attributed to the negative Grüneissen parameters of the transversal acoustical phonon branches near the limit of the Brillouin zone [19,20]. The regions in the band diagram where an abrupt change in the absorption coefficient occurs (and hence in the joint density of states), are linked to the points where the electronic transitions occur (the critical points (CPs)). The band gap, E_0, is a critical point within the electronic band structure of semiconductors, and these critical points are dependent on temperature. This has been reported in theoretical calculations, which take both the effects of thermal expansion and electron–phonon interaction into account [21].

One optical spectroscopic technique that can be used to determine the critical points is photoreflectance (PR). Several researchers have measured both photoreflectance (PR) and photoluminescence (PL) spectra in the optical gap region for CdTe, in order to characterize CdTe/GaAs heterostructures [22] as functions of the chemical scrubbing of the substrate as well as the film thickness [23]. The measured PR spectra provide information on the GaAs fundamental transition as well as two additional transitions corresponding to the valence-band splitting in the light-hole (LH) and heavy-hole (HH) bands of the CdTe film due to the compressive strain (see Fig. 2). The thermal expansion effects on the exciton transitions for other heterostructures have also been reported in the literature. In one study, the competition between the negative thermal expansion and the electron–phonon interaction in the low temperature range was demonstrated [24]. In addition, several analytical models used to describe the temperature dependence of the band-gap energy have been developed in recent decades [25–28]. In this paper, we conduct optical studies of residual strain on a CdTe/GaAs (001) heterostructure to determine the fundamental transition energy, E_0, the heavy-hole transition energy, E_0 (HH), and the light-hole transition energy, E_0 (LH), CP parameters. We report PR results for wavelengths around the critical point, E_0, of CdTe at temperatures between 12 and 300 K and analyze the spectra using Aspnes' third derivative functional form.

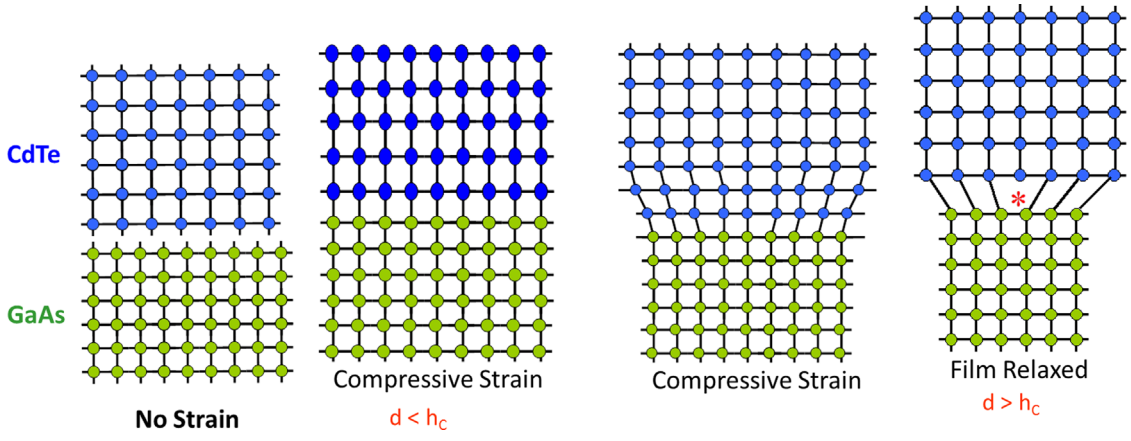

Fig. 1. Epitaxial growth of CdTe on GaAs substrate when the film thickness exceeds the critical value, *hc*.