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On the interpretation of ^{57}Fe Mössbauer spectra from CdTe thin films with substitutions of Fe, In, and Sb

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Abstract

^{57}Fe Mössbauer spectra of well characterized CdTe thin films with substitutions of Fe, In and Sb were recorded and interpreted according to the changes in the ionic radii and electronic properties of these substitutions relative to Cd in the CdTe framework. The literature reports of certain correlations among the iron valence, Fe^{2+} or Fe^{3+}, and the crystallinity of the films are critically discussed and an explanation of their origin is provided. The Mössbauer results also allow direct understanding of the effect of In and Sb substitutions on the properties of the films.

Keywords: Semiconductors; Alloys; Sputtering; Mössbauer spectra

1. Introduction

Previous studies on Mössbauer spectra of CdTe thin films, with Fe as impurity, have been reported by Galvao da Silva et al. [1,2] and Sánchez-Sinencio et al. [3,4]. These authors have observed that iron in the studied films is present as high spin Fe^{2+} and Fe^{3+}, and they correlated the amount of Fe^{2+} or Fe^{3+} with the crystallinity of the film. Films with high Fe^{2+} content are amorphous while those where iron is mainly as Fe^{3+} are polycrystalline. Certain correlations of the impurity level and the crystallinity of the film have also been observed for other metals. For instance, $Cd_{1-x}M_xTe$, with M = In, Sb, is polycrystalline for small amounts of the metal M but it becomes amorphous as x increases [5,6]. However, the origin of these correlations has not been discussed in detail. In this contribution, we present the results of ^{57}Fe Mössbauer measurements on four compositions of CdTe thin films with substitutions of Fe, In and Sb. The particularities observed in Mössbauer spectra of these films are explained according to the changes in the ionic radii and electronic properties of these elements (Fe, In and Sb) relative to Cd in the CdTe framework.

2. Experimental

The studied samples have the compositions $Cd_{0.95}Fe_{0.05}Te$, $Cd_{0.90}Fe_{0.10}Te$, $Cd_{0.812}Fe_{0.028}In_{0.16}Te$, and $Cd_{0.90}Fe_{0.05}Sb_{0.05}Te$. These films were grown on 7059 Corning glass substrates at 150°C by r.f. co-sputtering a CdTe target with metallic pieces of ^{57}Fe, In and Sb placed on the top. Their chemical composition was determined by Auger spectroscopy. The samples obtained by this procedure were then characterized according to their crystallinity, morphology, phase compositions and electronic structure. Details of the preparation and characterization methods can be found elsewhere [3,5–8].

Mössbauer spectra were recorded at room temperature with a ^{57}Co in Rh source, using a constant acceleration spectrometer (from Wissel, Germany) operated in the transmission mode. All spectra were fitted using an iterative least-squares minimization algorithm and pseudo-Lorentzian line shapes [9] to obtain the values of isomer shifts (δ), quadrupole splitting (Δ), linewidth (Γ) and relative area (A). The isomer shift values are reported relative to sodium nitroprusside.

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