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MATERIALS CHARACTERIZATION

Characterization of FeS_2-pyrite thin films synthesized by sulphuration of amorphous iron oxide films pre-deposited by spray pyrolysis

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Abstract

FeS_2-thin films with good crystallinity were synthesized by a simple method which consists of sulphuration, under vacuum, of amorphous iron oxide thin films pre-deposited by spray pyrolysis of $FeCl_3 \cdot 6H_2O$ (0.03 M)-based aqueous solution onto glass substrates heated at 350 °C. At optimum sulphuration temperature (450 °C) and duration (6 h), black green layers having granular structure and high absorption coefficient (~5.10^4 cm^{-1}) were obtained. The study of the electrical properties of the as-prepared films vs. the temperature variations showed three temperature domain dependence of the conductivity behaviour. The first one corresponds to the high temperature range (330 K–550 K) for which an Arrhenius plot type was obtained. The activation energy value was estimated at about 61.47 meV. The second domain corresponding to the intermediate temperature range (80 K–330 K) showed a variable activation energy between the grain boundaries. The barrier height, $q\bar{\phi}$ was estimated to 27 ± 0.5 meV, and the standard deviation, $q\sigma_\phi$, was evaluated at about 14 ± 0.5 meV. We found that at lower temperatures (20 K–80 K), the conductivity is governed by two conduction types. The density of localised states, was about 2.45×10^{20} eV^{-1} cm^{-3}.

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1. Introduction

Because of their interesting properties for applications as electro-optical devices, photo-electrochemical solar cells, and battery [1–5], cubic pyrite (FeS_2)

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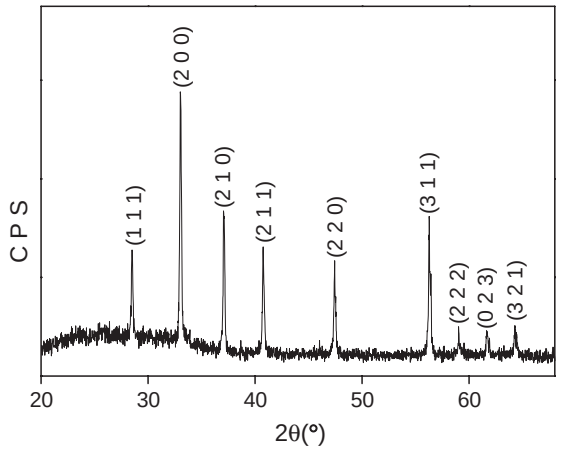

Fig. 1. XRD patterns of FeS_2-pyrite thin films prepared under a vacuum of 10^{-4} Pa for 6 h at 450 °C.

are receiving growing attention by several researchers. Moreover, it is built up by non-toxic and abundant elements, which justifies the pursue of the FeS_2 investigation in spite of the difficulties encountered to obtain reproducible performing films [6,7]. Many techniques of thin film preparation were investigated in order to obtain pyrite films [5,8–14]. It is obvious that preparation processes must play an important part in film behaviour. In the present work, attention was paid to the structural, optical, and electrical characterizations of pyrite films prepared by a simple method consisting of sulphuration under vacuum of amorphous iron oxide thin films pre-deposited by spray pyrolysis. The dependence of the electrical conductivity with temperature is discussed.

2. Experimental results and discussions

The FeS_2-pyrite thin films described in this paper were obtained by sulphuration in vacuum (~10^{-4}Pa) sealed tubes at 450 °C for 6 h, of amorphous iron oxide layers pre-deposited by spray pyrolysis of $FeCl_3 \cdot 6H_2O$ (0.03 M)-based aqueous solution onto glass substrates heated at 350 °C [15].

2.1. X-ray diffractions

The various pyrite phases were determined using X-ray diffraction (XRD) with a Siemens D500 powder diffractometer (CuKα radiation) in the usual θ–2θ geometry. A single pyrite phase was obtained with a good crystallinity (Fig. 1). The peak corresponding to the (200) line is the highest in the tested films. Thus, one may guess that (200) is the preferred orientation of the FeS_2 pyrite crystallites. The XRD patterns show a single pyrite phase and that the as-prepared films crystallised in the expected cubic structure (PDF data 42-1340).

2.2. Scanning electron microscopy

Surface morphology of the sulphured films was investigated by Scanning Electron Microscopy (SEM). Fig. 2(a) shows SEM micrograph surface view of pyrite FeS_2 films annealed at 450 °C under vacuum (~10^{-4} Pa) for 6 h. The surface of the film prepared at 450 °C appears granular but rather homogeneous. The SEM cross-section view (Fig. 2 (b)) shows that the as-prepared pyrite films have a

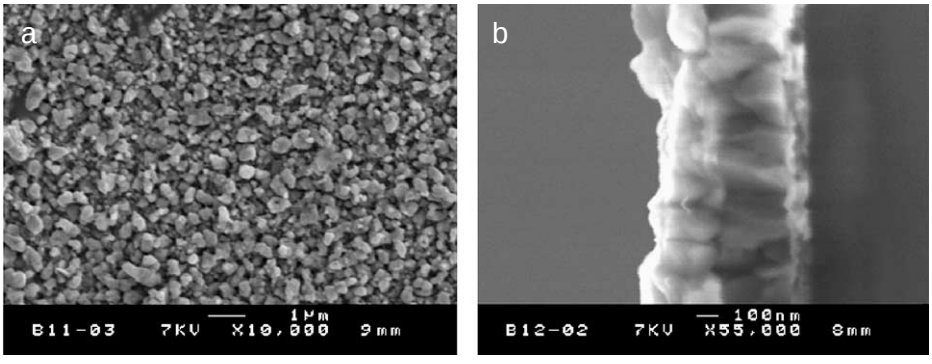

Fig. 2. (a) SEM and (b) cross-section of FeS_2 films sulphurated from iron oxide layers at 450 °C for 6 h under a vacuum of about 10^{-4} Pa.