Determination of the optical properties of amorphous selenium films by a classical damped oscillator model

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Amorphous selenium films were produced by vacuum evaporation onto glass and aluminum substrates. The chemical composition of the films and interfaces were studied using scanning Auger electron spectroscopy. To gain some insight into the optical properties of the selenium films, we used the classical oscillator model to fit the transmittance spectrum.

I. Introduction

The purpose of this work is to determine by spectral transmittance the optical properties of amorphous Se films, deposited on glass. In addition Se films deposited on aluminum substrates were chemically analyzed using Auger electron spectroscopy.

As is well known, Se is a material having many uses including electrostatic image processing.[1]

Other workers have determined that Se can be produced in three basic structures: (a) Hexagonal structure, which is the most common and most stable phase showing a high electrical conductivity. (b) Monoclinic structure, which is a relatively high resistivity semiconductor. This structure may be produced by growth from solution and may be transformed into the hexagonal structure by heating. (c) Amorphous structure, which is essentially a supercooled liquid. It may be easily obtained by rapidly cooling from the liquid phase so that crystallites do not form.

A more controlled way of producing amorphous selenium is by vacuum evaporation onto substrates of other materials. In this case, care must be taken so that the substrate temperature is not higher than 70°C.

II. Experiment

Samples were prepared by vacuum ($\sim 10^{-3}$ Pa) evaporation in a standard bell jar system. The substrate temperature was monitored and kept at 60 ± 2°C to prevent crystals from forming. The amorphous character of the films was checked using standard X-ray techniques.

The chemical composition of the film was obtained using a PHI-595 Scanning Auger Microprobe equipped with an argon ion sputtering system. The surface was analyzed using an electron beam of 5 keV and 100-nA beam current. Se films grown on Al substrates were used for this purpose to reduce charging of the surface. Then the films were sputtered with an argon ion beam to obtain composition depth profiles and to study the interface with the substrate. The ion beam used was at 2 keV and 12 μA/cm^2.

To obtain some physical insight into the optical properties of the Se films, transmittance measurements were performed in a Perkin-Elmer model 330 spectrophotometer in the 185–2600 nm range. The thickness of the film was determined by using the interference maxima and minima shown on the transmittance spectrum and the technique reported by Goodman.[2] The curves showed the typical features of amorphous Se films.[3,4]

III. Results

Figure 1 shows the Auger spectrum of the surface of the film where the typical Se Auger peaks may be observed. Figure 2 shows the Auger spectrum of the same sample after sputtering off the Se film with Ar ions. The peaks in the spectrum correspond to the surface of the substrate which in this case is aluminum oxide and showed C, Ca, and Mg residues of the abrasives used for polishing the aluminum surface to a mirror finish. The Auger spectra show that the Se film is clean as regards Auger sensitivity, since no other elements were detected. In addition, by scanning the electron beam on the surface of the film we obtained a secondary electron image (SEM image) of the film,

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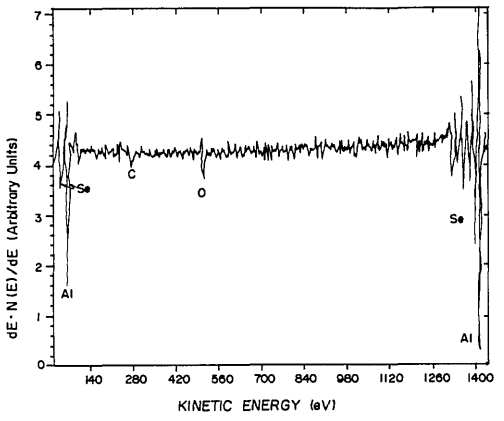

Fig. 1. Auger Spectrum corresponding to a scrap surface of the sample where both the low and high energy selenium and aluminum peaks may be observed.

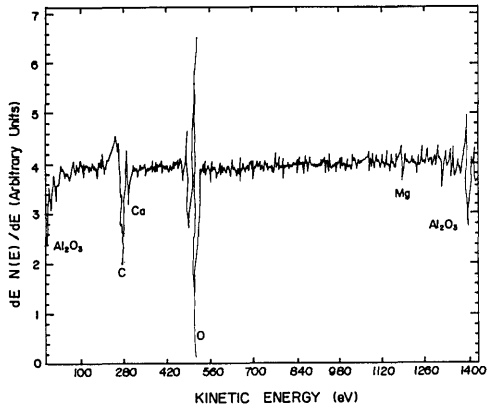

Fig. 2. Auger Spectrum of the sample after sputtering off the Se film with an Ar ion beam. The low and high energy aluminum peaks are shown. These peaks present the typical characteristics associated to aluminum oxide.

showing the formation of Se islands as results of electron beam damage, as can be seen in Fig. 3. A similar effect was also observed[5] with the beam of an electron microscope indicating crystallization of the Se film.

To test that the film is in fact amorphous, we had to rely on x-ray diffraction and the results are shown in Fig. 4. The spectrum shows the typical broad feature which characterize amorphous structures.

Figure 5 shows the transmittance curve. The features in the transmittance spectrum were interpreted following a technique developed by different authors.[6–8] Using this method, the complex dielectric function of the material may be represented by a sum of classical oscillators which may be written as:

$$\epsilon = \epsilon_1 + j\epsilon_2 = \epsilon_\infty + \sum S_i/(1 - (\omega/\omega_i)^2 - j\Gamma_i\omega/\omega_i), \quad (1)$$

where S_i, ω_i and Γ_i represent the oscillator strength, resonance frequency and linewith, respectively. ϵ_∞ is the high frequency contribution to ϵ and $j^2 = -1$. Using Eq. (1) for the dielectric function and a recurrence formula developed by Dupoisot and Morizet[9] a

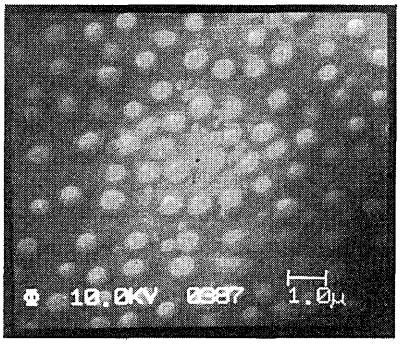

Fig. 3. Secondary electron image (SEM image) of the film showing the formation of Se islands as a result of electron beam damage.

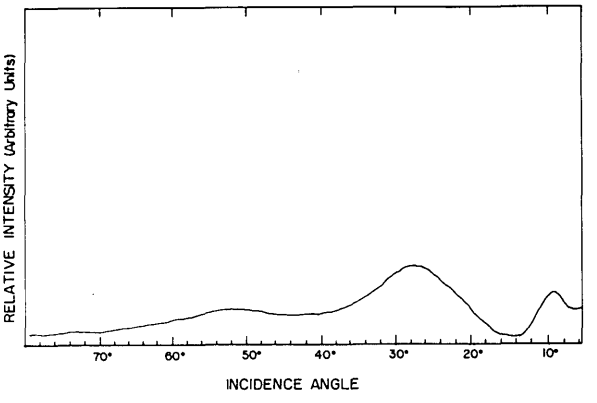

Fig. 4. X-ray diffraction pattern of the Se film.

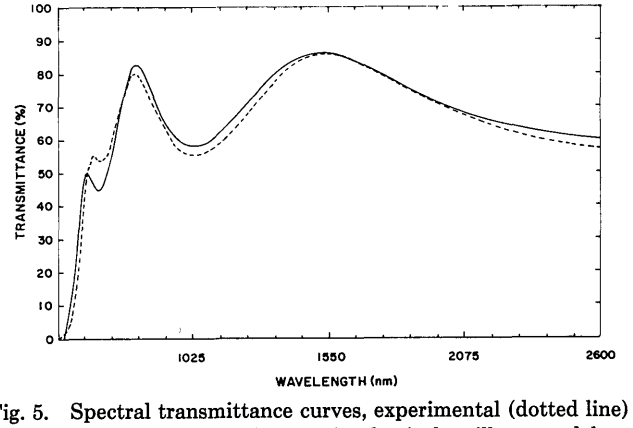

Fig. 5. Spectral transmittance curves, experimental (dotted line) and calculated (solid line) using the classical oscillator model.

very reasonable fit to the experimental data was obtained using two oscillators (discontinuous curve in Fig. 5). The parameters, for these oscillators with a common value of $\epsilon_\infty = 4.8$ are as follows.

$S_1 = 1.20$, $\omega_1 = 2.50$ eV, $\Gamma_1 = 0.05$ eV.

$S_2 = 3.32$, $\omega_2 = 0.23$ eV, $\Gamma_2 = 3.43$ eV.

The deep minimum present in the experimental curve can be attributed to the 2.50-eV oscillator and it

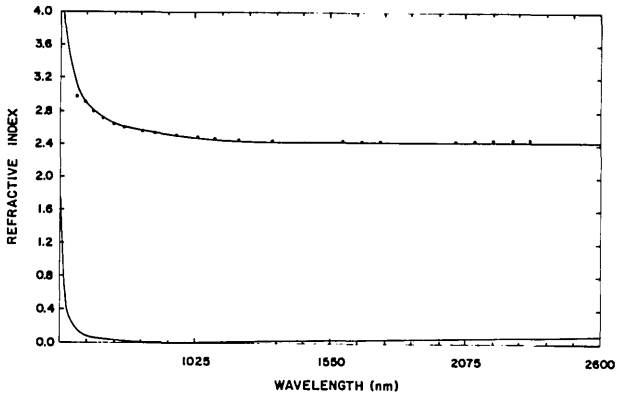

Fig. 6. Plot of the complex refractive index vs λ as obtained from the calculated dielectric function using the classical oscillator model. The dots are experimental values from Ref. 10.

may be associated to a pseudoband gap. Values for this parameter have been reported in the range of 2.13–2.65 eV depending on sample preparation of the amorphous selenium films.[3]

The tendency of the curve towards another minimum in the low energy region of the spectrum can be related to the 0.23-eV oscillator, which in turn may be associated with a plasmon edge of the Se charge carriers, with a density of the order of 10^{-20} cm^{-3}.

To check how good are the values of ϵ obtained from a transmittance spectrum only, we computed the corresponding refractive index from the values of ϵ thus obtained. The results are shown in Fig. 6 where several experimental values (dots) of the $\tilde{n}$ obtained from the literature[10] are included for comparison.

IV. Conclusions

Amorphous Se films were produced by vacuum evaporation on substrates of aluminum and glass. The film structure was verified by x-ray techniques as being amorphous.

Auger electron spectroscopy showed the film to be free of contaminants and that we can induce electron beam damage to the film leading to crystallization.

The dielectric function $\epsilon(\omega)$ was obtained in terms of a sum of two classical damped oscillators. The energy of these oscillators has been associated to the interband transition occurring at the main absorption edge and a low energy plasmon excitation edge.

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