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A two-layer model to explain the thickness dependence of conductivity and thermoelectric power of semiconductor thin films and application of the model to PbTe thin films

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A two-layer model to explain the thickness dependence of conductivity and thermoelectric power of semiconducting thin films has been developed assuming that the film is a parallel combination of resistances of the three layers: The first is the interior "grain-boundary" layer, and the other two, outer layers on opposite sides, whose conductivities are altered by the band bending (and is also affected by surface-gas interactions). The equations obtained in this model lead to an inverse thickness dependence of both the conductivity and thermoelectric power of thin films. The model is applied to analyze the conductivity and thermoelectric variation with thickness of PbTe thin films and the parameters U_g, the energy dependence of the "grain-boundary" mean free path l_g, and σ_g the surface conductivity, have been evaluated.

I. INTRODUCTION

The theories put forward by Fuchs and Sondheimer and later by Mayadas and Tellier, Tosser, Boutrit and Pichard, do not take into account the surface band bending in their calculations, because they were essentially obtained for metallic thin films. Hence, strictly speaking, the above theories cannot be used for semiconductors. However, since an adequate theory for the thickness dependence of various electrical properties in semiconductors is not available, workers still use Fuchs–Sondhemier, Tellier, and other models for their calculations.

A two-layer model to explain the size effect in semiconductor thin films can be obtained on the basis of simple assumptions as described below. In this model, the film is considered to be made up of two layers, a high/low resistive surface layer of thickness t_s on both sides of the film, and a normal bulk layer (having the same microstructure as that of the film) of thickness t_g. This is in view of a considerable difference in conductivity at the surfaces of the semiconductors due to surface band bending because of the surface and interface states.

II. THE TWO-LAYER MODEL

In the two layer model, the following assumptions are made. (i) The thickness t_s of the surface layers on both sides of the film is constant for all films of various thicknesses and is approximated to be equal to the Debye length

$$\lambda = \left[\frac{\epsilon kT}{4\pi^2 e^2 n}\right]^{1/2}$$

of the material. ϵ is the dielectric constant, n is the carrier concentration, e is the electronic charge, T is the absolute temperature, and k is the Boltzmann's constant. The thickness of this modified layer is chosen to be equal to the Debye screening length, because only up to a depth equal to the Debye length from the surface the band bending occurs by the definition of the Debye length. (ii) $t_g = t - 2t_s$ is the thickenss of the middle layer of the film. This layer is assumed to have all properties of a bulk which has the same grain structure as that of the thin film. It may be noted that the conductivity of this interior of the film will not be that of a bulk material, but lower because the film grain sizes will be smaller.

Considering that the thickness of the surface layer t_s and the surface layer resistivity ρ_s are constants for all the films of a given material because of the Debye length λ, giving the length to which the surface effects and hence the layer extends, depends on the material. The resistance of the film can be written as a parallel combination of the resistances of the surface and the interior layers. Then we have

$$\frac{1}{R_F} = \frac{1}{R_s} + \frac{1}{R_g} + \frac{1}{R_s},$$

where R_F is the film resistence, R_s is the resistance of the surface layer, and R_g is the resistance of the interior layer. The subscript g refers to the grain structure of the interior layer which is that of the film.

As

$$\frac{1}{R_F} = \frac{R_s + 2R_g}{R_s R_g},$$

we get

$$\frac{1}{R_F} = \left(\frac{b}{l}\right)\left(\frac{2t_s}{s} + \frac{t_g}{g}\right),$$

where l and b are the length and breadth of the film sample.

But

$$\sigma_F = \left(\frac{1}{bt}\right)\frac{1}{R_F}.$$

Substituting for $1/R_F$ from the above equation, we have

$$\sigma_F = \frac{1}{\rho_g}\left(\frac{t_g}{t}\right) + \frac{1}{\rho_s}\left(\frac{2t_s}{t}\right).$$

But since $t_g = t - 2t_s$ we have,

$$\sigma_F = \frac{1}{\rho_g}\,\frac{t - 2t_s}{t} + \frac{1}{\rho_s}\,\frac{2t_s}{t}$$

$$= \frac{1}{\rho_g} - \frac{2t_s}{t}\left(\frac{1}{\rho_g} - \frac{1}{\rho_s}\right),$$

or

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$$\sigma_F = \sigma_g \left[1 - \frac{2t_s}{t}\left(1 - \frac{\rho_g}{\rho_s}\right)\right] \quad \text{for } \sigma_g = \frac{1}{\rho_g}.$$

From the above equation, we find that σ_F varies linearly with the inverse of thickness as t_s, σ_g, and s are constants. If we plot a graph of σ_F against $1/t$, we will get a straight line with intercept equat to σ_g and slope equal to

$$-2t_s\sigma_g[1-(\rho_g/\rho_s)] = -2t_s[\sigma_g - \sigma_s].$$

Assuming t_s to be equal to the Debye length of the material, and knowing σ_g from the intercept, we can calculate the surface layer conductivity σ_s.

We can use the above result to obtain an expression for the thickenss dependence of the thermoelectric power also. We have, from the rigid band model, the thermoelectric power of a thin film as[1]

$$S_F = +S_B\left[1 + \left(\frac{\partial \ln l_g}{\partial \ln E}\right)\left(\frac{\beta_F}{\beta_g}\right)\right].$$

Since[2]

$$(B_F/\beta_g) = (\sigma_F/\sigma_g),$$

we have, by substituting for β_F/β_g from the equation for σ_F,

$$S_F = S_B\{1 + U_g + U_g(2t_s/t)[\rho_g/\rho_s) - 1]\}$$

where $U_g = (\delta \ln l_g)/(\delta \ln E)E = E_F$.

Here also, we find that S_F varies linearly with the inverse of thickness, according to this model. The intercept value equal to $S_B(1+U_g)$ gives the grain boundary thermoelectric power S_g.

The slope of the S_F vs $1/t$ plot is equal to

$$S_B U_g 2t_s[(\rho_g/\rho_s) - 1].$$

Knowing the value of S_g and S_B, we can calculate U_g from the intercept.

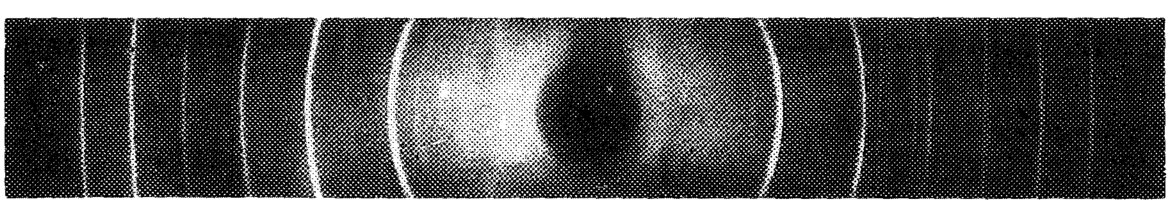
Knowing U_g, S_B, t_s, and ρ_g, we can calculate ρ_s, the surface layer resistivity of the sample.

III. EXPERIMENT

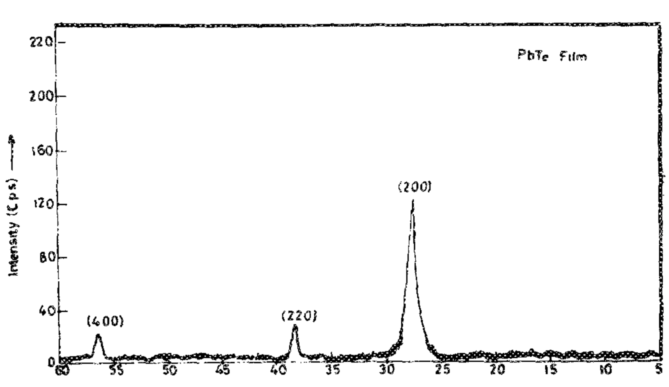
PbTe thin films of various thickness between 300 and 2500 Å were prepared by vacuum deposition of the bulk PbTe alloy in a vacuum of 5×10^{-5} Torr on cleaned glass substrates held at room temperature directly above the source. The source to substrate distance was 25 cm and the film lateral dimensions were 6 and 1 cm for the conductivity measurements, and 6 and 0.5 cm for the thermoelectric power measurements. The deposition of different thickness films was made in separate evaporations for both the measurements, and each time a given quantity of the alloy was taken in the boat and was completely evaporated at a fast rate to avoid fractionation of the alloy in the boat in successive evaporations. The thermoelectric power was measured on air-exposed PbTe thin films as they had to be mounted on the measurements setup after the film formation; and the chamber was re-evacuated to 5×10^{-5} Torr before measurement. The thermoelectric power was measured by the integral method. The conductivity measurements were made on as-grown (unexposed) specimens immediately after the formation of the films using an *in situ* conductivity setup with the help of predeposited, thick silver contact films. Experimental setups for both the measurements have already been described in earlier papers[3,4] and hence need not be described here again.

IV. RESULTS

Figures 1(a) and 1(b) show the typical x-ray powder photograph of the bulk PbTe alloy and the x-ray diffractograms of the PbTe film. The *d* values of the peaks in the x-ray diffractogram of Fig. 1(b) matched with the *d* values of the area of the diffraction pattern of Fig. 1(a) thereby confirming that the thin films formed were those of PbTe alloy. The table comparing the two diffraction patterns has been given earlier[3] and hence is not repeated here.



(a)



(b)

FIG. 1. (a) X-ray powder photograph of the bulk, PbTe alloy. (b) X-ray diffractogram of the typical PbTe film.

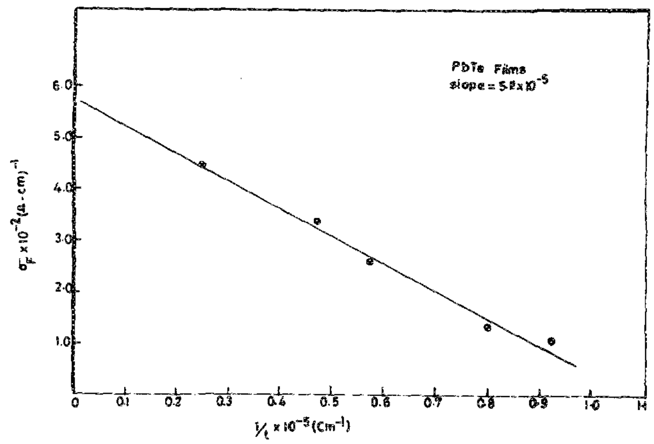


FIG. 2. PbTe film conductivity vs reciprocal thickness plot showing linearity.

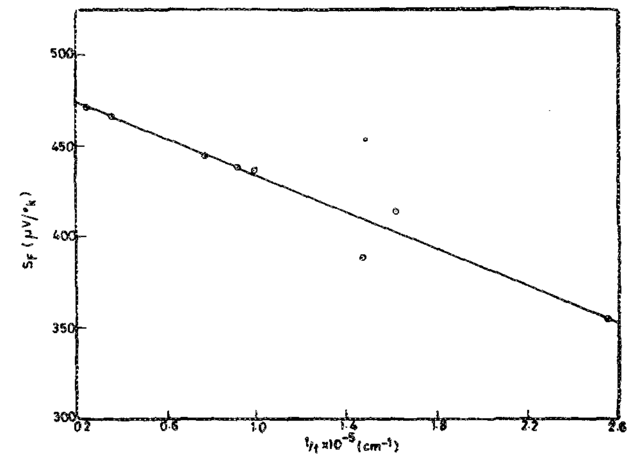


FIG. 3. PbTe film thermoelectric power vs reciprocal thickness plot showing linearity.

Figure 2 shows the plot of film conductivity as a function of inverse film thickness while Fig. 3 shows the plot of film thermoelectric power against inverse thickness. It can be seen from the two figures that the experimental points fit a straight-line plot very well, thus establishing a linear inverse thickness dependence of the conductivity of PbTe thin films. This linear dependence was earlier[3,4] explained by the Tellier[5] model of the effective mean free path. In this paper, we explain the linear inverse thickness dependencies of these by our two-layer model and evaluate the parameters σ_s, the surface conductivity, and the energy dependence of the grain-boundary mean free path U_g.

V. APPLICATION OF THE TWO-LAYER MODEL AND DISCUSSION

We have the expressions for conductivity and thermoelectric power as a function of thickness according to the two-layer model (from Sec. II) as

$$\sigma_F = \sigma_g\{[1-(2t_s/t)][1-(\rho_g/\rho_s)]\}$$

and

$$S_F = S_B\{(1+U_g) + V_g(2ts/t)[(\rho_g/\rho_s)-1]\}.$$

Clearly, both the expressions show inverse thickness dependence of conductivity and thermoelectric power, respectively.

The value of the intercept of the σ_F vs $1/t$ plot in Fig. 2 is $\sigma_g = 5.75\times10^2$ $(\Omega\text{ cm})^{-1}$ and the slope is -5.11×10^{-5} Ω^{-1}. The slope of the σ_F vs $1/t$ plot according to the two-layer model will be slope $= -2t_s(\sigma_g-\sigma_s)$. We get

$$\sigma_s = 5.7\times10^2(\Omega\text{ cm})^{-1}.$$

The intercept of the S_F vs $1/t$ plot in Fig. 3 is $S_g = 487$ μV/K and hence the energy dependence of the mean free path U_g is derived from the relation $S_B(1+U_g) = S_g$ if we take the value of $S_g = 300$ μV/K from the literature,[6] as $U_g = 0.62$.

The slope of the S_F vs $1/t$ plot is -5.4×10^{-10} μV K^{-1} cm. Therefore, substituting for ρ_B, U_g, $\rho_g = 1/\sigma_g$, and t_s in the expression

$$\text{slope} = 2S_B U_g t_s[(\rho_g/\rho_s)-1],$$

we can calculate the surface layer resistivity ρ_s as 0.25×10^{-2} Ω cm, or σ_s the surface layer conductivity as 3.9×10^2 $(\Omega\text{ cm})^{-1}$.

It is seen that there is a difference in the surface conductivity values obtained from the slopes of the σ_F vs $1/t$ and S_F vs $1/t$ plots. This is certainly due to the fact that the conductivity measurements were made on unexposed, as-grown PbTe thin films, whereas Seebeck coefficient measurements were made on air-exposed PbTe films. It is worth mentioning that PbTe thin films are very sensitive to atmospheric exposure due to adsorption of gases, principally oxygen, as has been shown by us previously[3,7] and by others.[8–14] As the thermoelectric measurements were made on air-exposed films while the conductivity measurements were made on unexposed films, the surface layer conductivities of the films are naturally different in the two cases, as the gas adsorption modifies the properties of the films. We are planning to carry out Seeback coefficient measurements *in situ* on unexposed PbTe thin films the results of which when reported are expected to substantiate the above fact of the gas-interaction effect modifying the properties of PbTe thin films, as has already been shown by us regarding conductivity changes in PbTe films earlier.[3,7]

VI. CONCLUSIONS

A two-layer model has been developed to explain the size effect on conductivity and thermoelectric power of semiconducting thin films. The model leads to an inverse thickness dependence of the two quantities. The model has been applied to explain the inverse thickness dependence observed of both thermoelectric power and electrical conductivity of PbTe thin films. The calculations show that the surface layer conductivity σ_s calculated from conductivity studies is different from that calculated from thermoelectric studies. This has been explained by the fact that PbTe is a material very susceptible to atmosphere, and hence the surface layer conductivity is different in the two cases as the thermoelectric power was measured on air-exposed films, while the conductivity was measured on unexposed films.

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