

# Computer simulation of deposition behaviour of CdTe films

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A computer program has been developed in Fortran to simulate the voltammetric curves to fix the best conditions for the deposition of n- or p- type CdTe films. It is observed that pH, temperature and  $\text{Cd}^{2+}$  ions and potential variations influence the deposition and nature of the films.

**Key words:** CdTe films, electrodeposition, computer simulation

## INTRODUCTION

**E**lectrodeposition technique involves the optimization of parameters such as pH, temperature, voltage and current density to get stoichiometric CdTe films. As a first hand information, computer simulation will give a near optimized conditions to start with the deposition process. An ingenious and simple kinetic model to simulate electrodeposition of II-VI and III-V compounds which deals extensively with CdTe deposition has been developed [1]. The present study is to develop a program, using this model and the basic data, by which the effect of previously mentioned variables will be predicted to get either n- or p- type CdTe films.

## COMPUTER SIMULATION

The program uses successive iteration technique. It is written in such a way that it satisfies a condition imposed between the current densities observed due to Cd and Te deposition at a particular value of A given as-

$$A = [(2J_{\text{Cd}})/(J_{\text{Te}}) - 1]/2 \quad (1)$$

For different values of  $A = (-0.5 \text{ to } +0.5)$ , the program calculates the current density due to Cd, Te and the sum at different pH(0.1 to 5.0), temperatures (298 to 368K) and potentials (+0.4 to -0.4 vs SHE).

## RESULTS AND DISCUSSION

The influence of Cd and Te current densities on the deposition conditions are studied separately. At pH values less than 1, the contribution to the total current density comes mainly from Te and that from Cd is negligible. This current corresponds to the diffusion limited current density,  $J_{\text{Te}}$  of about  $103 \mu\text{A.cm}^{-2}$ . Figure 1 shows the dependence of pH on  $J_{\text{Te}}$  at 298K for potentials 0.35, 0.1 and 0 - 0.4V. The decrease in pH reduces  $J_{\text{Te}}$ . When potential is 0 and decreased upto -0.4V, it approaches  $J_{\text{Te}}$  where no pH dependence is observed but contribution from Cd starts at -0.2V and increases

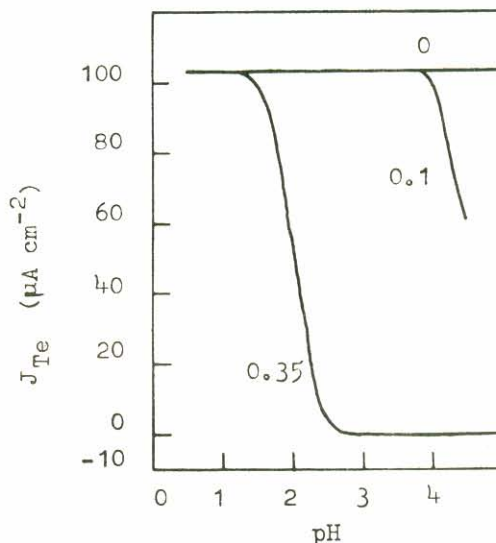


Fig. 1: Dependence of pH on Te current density at 298K

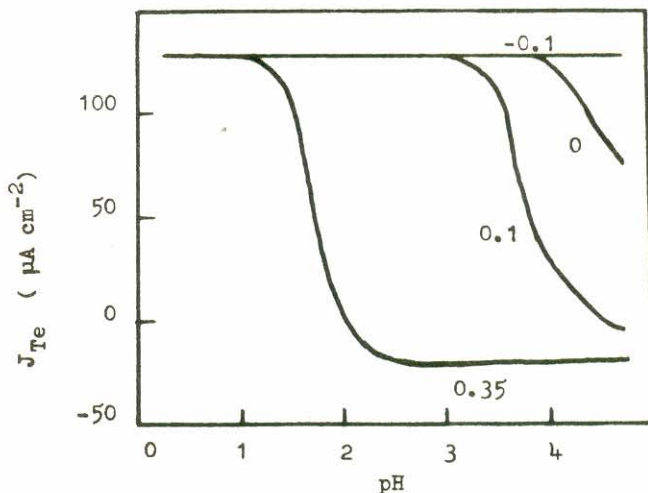


Fig. 2: Dependence of pH on Te current density at 368K

to about  $43 \mu\text{A.cm}^{-2}$  at about -0.4V. When the temperature of the bath is increased to 368K, a similar pH dependence is observed with  $J_{\text{Te}}$  raised to  $127 \mu\text{A.cm}^{-2}$ . A pH independent deposition is observed from -0.1 to -0.4V

as shown in Fig. 2.  $J_{Cd}$  contribution starts at  $-0.15V$  and increases to about  $70 \mu A.cm^{-2}$ .

Since CdTe deposition is intended to be carried out cathodically and  $J_{Te}$  is observed in the pH range 2 - 3 near 0 V, the pH for the deposition may be fixed at 2.5. Polarization curves were simulated keeping pH 2.5 at different temperatures as shown in Fig. 3. A spike at  $-0.30$  and  $-0.25$  V is observed where  $J_{Cd} = J_{Te}$ . This potential of perfect stoichiometry (PPS) is found shifting to positive side when the temperature of deposition is increased. It is evident from the curves, with deposition potentials of about 50 mV to the left of PPS, p-type CdTe may be deposited due to Te contribution which is important for solar cell fabrications. For about 100 mV to the right, n- type CdTe can be deposited where Cd contribution is more.

### CONCLUSION

This simulation program explicitly shows that Te is the rate determining species in CdTe deposition. pH of the bath can be fixed between 2-3. The deposition potential can be kept between  $-0.1$  and  $-0.4$  V. The increased current density and the shift of PPS to positive potentials at high temperatures may lead to thicker film formation with better

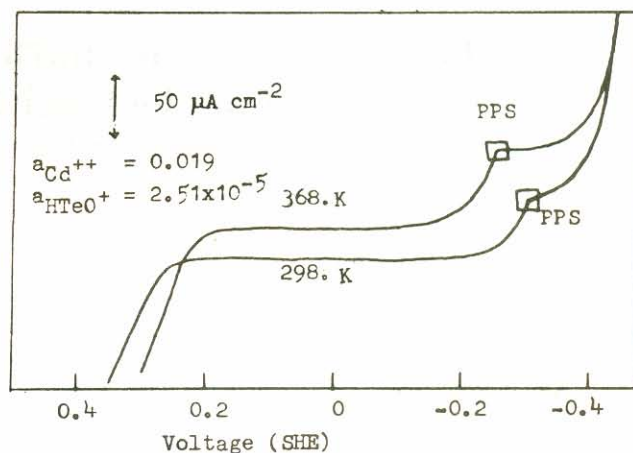


Fig. 3: Simulated voltammograms for CdTe deposition at different temperatures

crystallinity. This suggests the use of nonaqueous baths for deposition.

### REFERENCES

1. R D Engelken and T P Van Doren, *J Electrochem Soc*, **132** (1985) 2904, 2910