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Growth and microstructure of $Cd_{1-x}Zn_xS$ films

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The growth and microstructure of $Cd_{1-x}Zn_xS$ films were studied by depositing the films on to freshly cleaved NaCl, KCl, and LiF substrates at various x values ($0<x<0.27$). Optimum conditions for obtaining films with larger grains and oriented growth are indicated.

1. Introduction

Recent developments in the areas of thin-film photovoltaic solar cells based on $CuInSe_2$ and CdTe with CdS as window layer are noteworthy. Efficiencies between 12 and 14% have already been achieved [1–5] and there are indications that the efficiencies can be further advanced by suitable choice of a window layer having matched lattice parameters and electron affinity [1]. It was further felt that $Cd_{1-x}Zn_xS$ may be an alternative to the CdS layer since the properties of $Cd_{1-x}Zn_xS$ films can be tailored by simply adjusting the zinc content without substantial lowering the band gap. A number of studies [4–9] have been reported on $Cd_{1-x}Zn_xS$ so far, with emphasis on the measurements of electrical and optical properties of the above in thin-film form produced by various techniques. But there seem to be no systematic and motivated studies reported so far on the growth and microstructure of $Cd_{1-x}Zn_xS$ films. As the physical properties depend critically on the microstructure of the films which in turn depend on the deposition parameters, critical and systematic studies on the above will help immensely in a better understanding of the material for its fruitful exploitation as a window layer in photovoltaic technology.

2. Experimental procedure

We report here our studies on the growth and microstructure of $Cd_{1-x}Zn_xS$ ($0 < x < 0.27$) deposited by co-evaporating [10] CdS and ZnS (both 99.999% pure) on to freshly cleaved NaCl, KCl and LiF substrates. The thicknesses of the films were always kept within 70–90 nm and the films were deposited at various substrate temperatures. The films were examined by transmission electron microscopy (TEM) (Hitach H-600) and X-ray diffractron (XRD) (Philips PW 1130). The compositions of the films were analysed by EDX studies.

3. Results and discussion

Micrographs of $Cd_{1-x}Zn_xS$ films deposited on to freshly cleaved NaCl substrates at various deposition temperatures and zinc concentrations are shown in Figs 1–3, while Figs 4–6 show the micrographs for films similarly deposited on to KCl substrates. The thicknesses of the films ranged from 70–90 nm and the evaporation rate was maintained around $0.5\ \mathrm{nm\,s^{-1}}$. Fig. 7 is a graphical representation of the variation of grain size with deposition temperature for the above films as depicted in the micrographs. The curves indicate conventional grain growth with increasing substrate temperature due to increased adatom mobility. The grain growth is quite rapid for films containing more zinc content. It can also be seen that the grain growth in films deposited on to NaCl with $x \sim 0.07$ is quite insignificant compared with that for other films.

Fig. 8 shows representative micrographs for $Cd_{1-x}Zn_xS$ films deposited on to LiF substrates. The grain growth for films deposited on to LiF is also not very sharp (Fig. 7). The micrographs of films deposited on to NaCl (Figs 1–3) indicate that oriented growth leading towards epitaxy is more favoured for films with $x \sim 0.13$. The diffraction patterns indicate a predominantly hexagonal structure. In all cases the pattern is composed of streaks interlinking diffraction spots in a way seemingly similar to the spikes caused by two-dimensional diffraction and refraction effects. It may be mentioned that the diffraction was taken at normal incidence of the electron beam. Also one can observe some satellite spots indicating the presence of stacking faults and possible twin formation.

Fig. 9 shows a typical XRD trace for our $Cd_{1-x}Zn_xS$ films which reveal only a strong $\langle 002 \rangle$ orientation. This implies that the c-axes of the crystallites are perpendicular to the substrate. The sharpness of the peak is an indication of the presence of solid solution without a ZnS gradient along the cross-section of the layer.

The micrographs of films deposited on to KCl substrates (Figs 4–6) are similar in nature excepting that the strength of orientation is much stronger than that for films deposited on to NaCl under identical deposition conditions. One observes more-or-less fully oriented growth at a lower temperature ($\sim 150\,^{\circ}\mathrm{C}$) with substantially larger grains. In contrast with the above, orientation growth was absent for films deposited on to LiF substrates (Fig. 8). It may be pointed out that lattice mismatch between the substrate and

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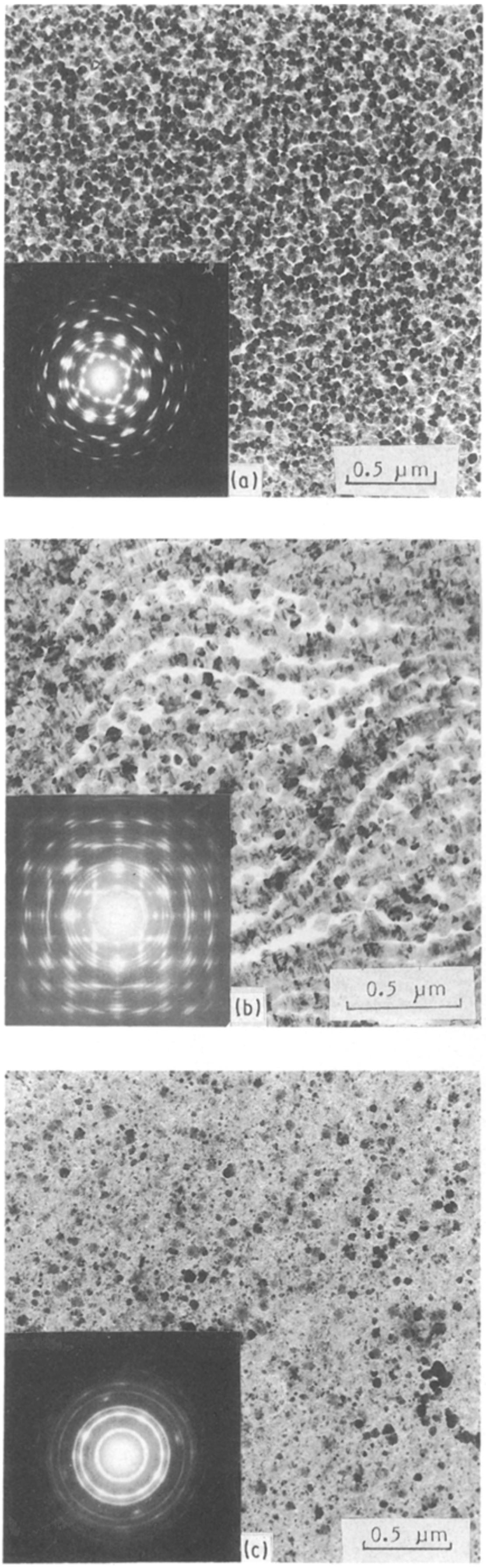


Figure 1 Micrographs of $Cd_{1-x}Zn_xS$ ($x \sim 0.07$) films deposited on to NaCl at different substrate temperatures: (a) 100 °C, (b) 200 °C, (c) 250 °C.

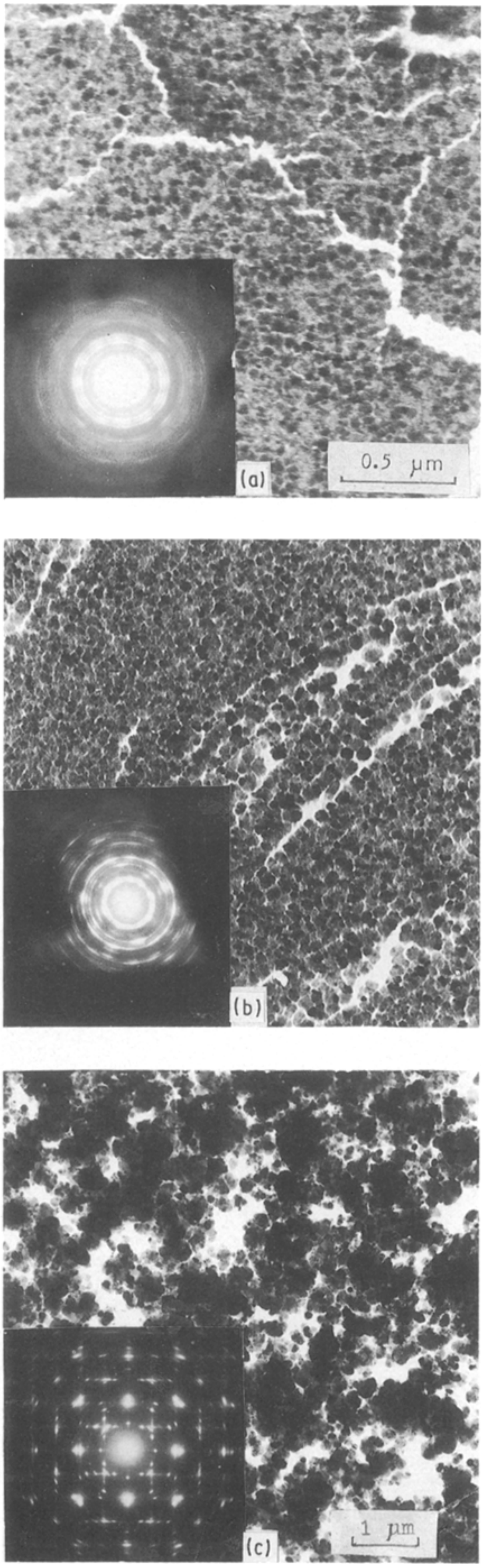


Figure 2 Micrographs of $Cd_{1-x}Zn_xS$ ($x \sim 0.13$) films deposited on to NaCl at (a) 50 °C, (b) 100 °C, (c) 200 °C.

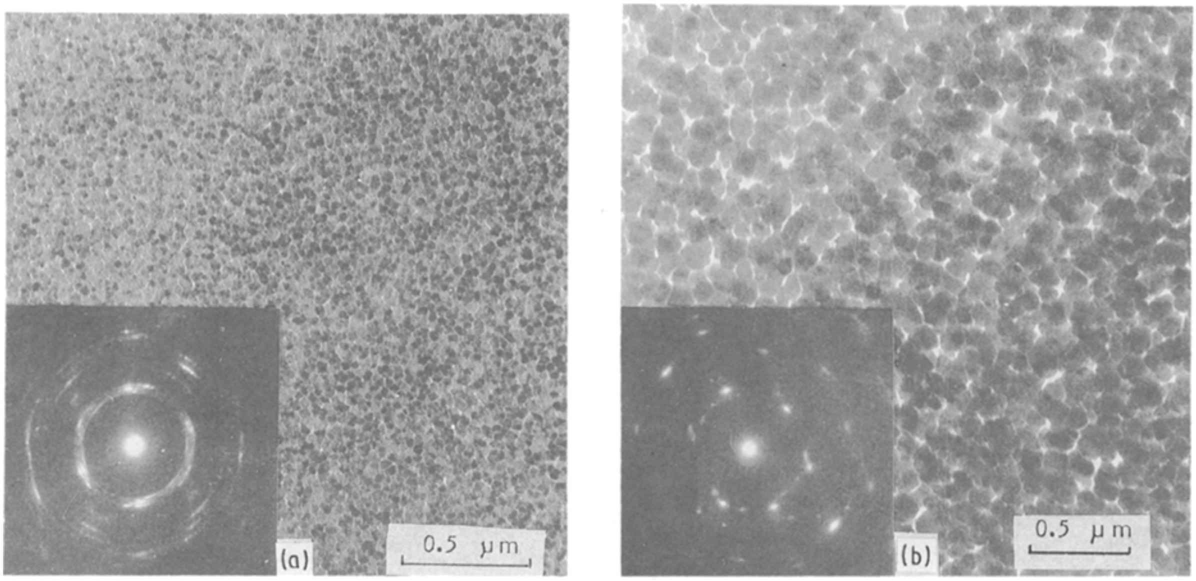
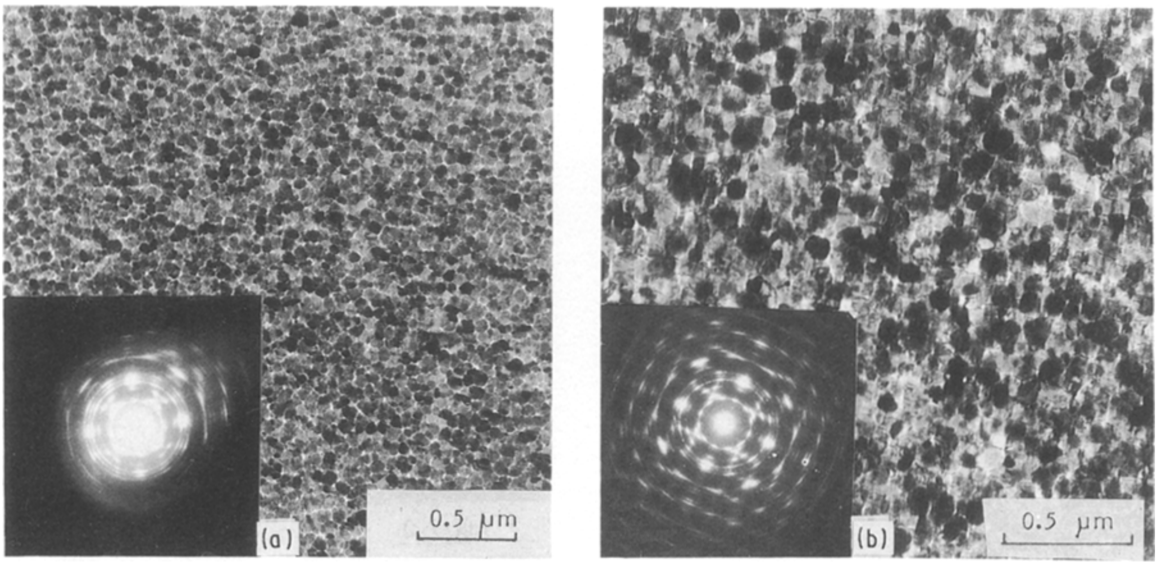


Figure 3 Micrographs of $Cd_{1-x}Zn_xS$ ($x \sim 0.18$) films deposited on to NaCl at (a) 50 °C, (b) 200 °C.



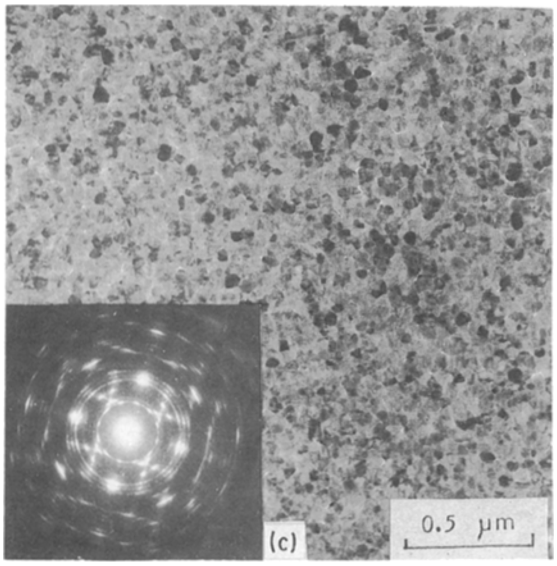


Figure 4 Micrographs of $Cd_{1-x}Zn_xS$ ($x \sim 0.07$) films deposited on to KCl at (a) 100 °C, (b) 140 °C, (c) 170 °C.

the films in this case may be one of the major deciding factors for oriented growth of $Cd_{1-x}Zn_xS$ films. $Cd_{1-x}Zn_xS$ has basically a wurtzite hexagonal structure and the lattice parameter (c) is nearly equal to 0.665 nm for our films. This matches well with the lattice constant of KCl ($\sim$ 0.629 nm) rather than those for NaCl ($\sim$ 0.563 nm) and LiF ($\sim$ 0.414 nm). This result supports the formation of a matched window layer of $Cd_{1-x}Zn_xS$ film on CdTe having lattice constant $\sim$ 0.6477 nm photovoltaic application.

In conclusion, it may be inferred that fully oriented films of $Cd_{1-x}Zn_xS$ with large crystallites can be obtained by depositing the films by co-evaporating CdS and ZnS from co-axial sources on to a lattice-matched substrate.

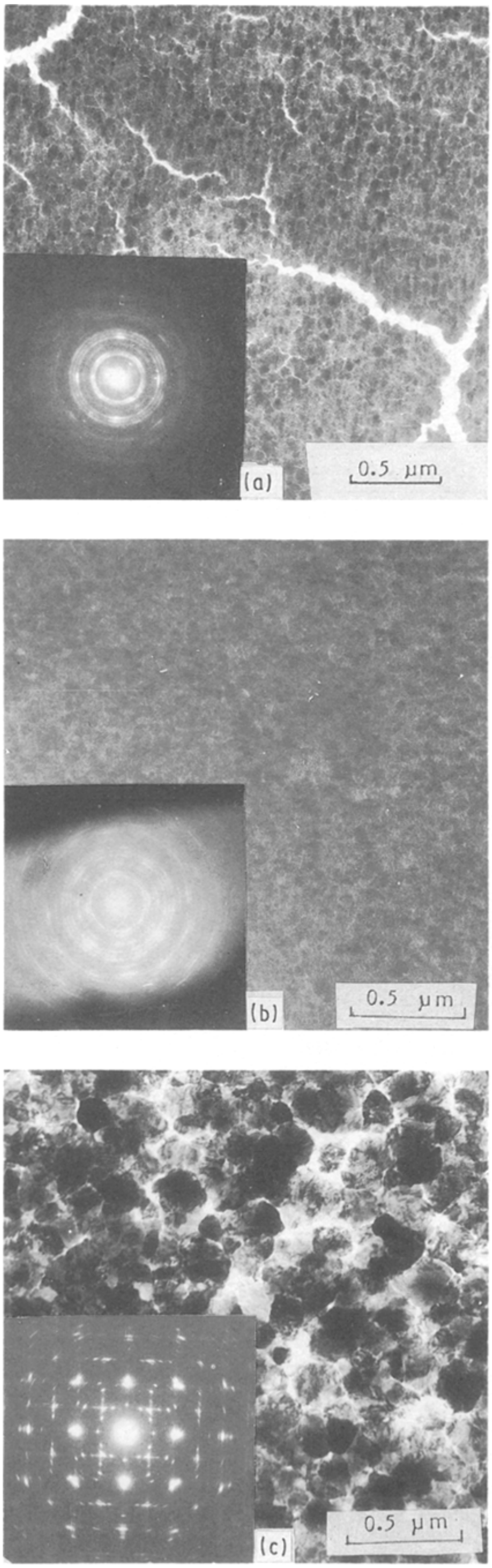


Figure 5 Micrographs of $Cd_{1-x}Zn_xS$ ($x \sim 0.13$) films deposited on to KCl at (a) 50 °C, (b) 100 °C, (c) 170 °C.

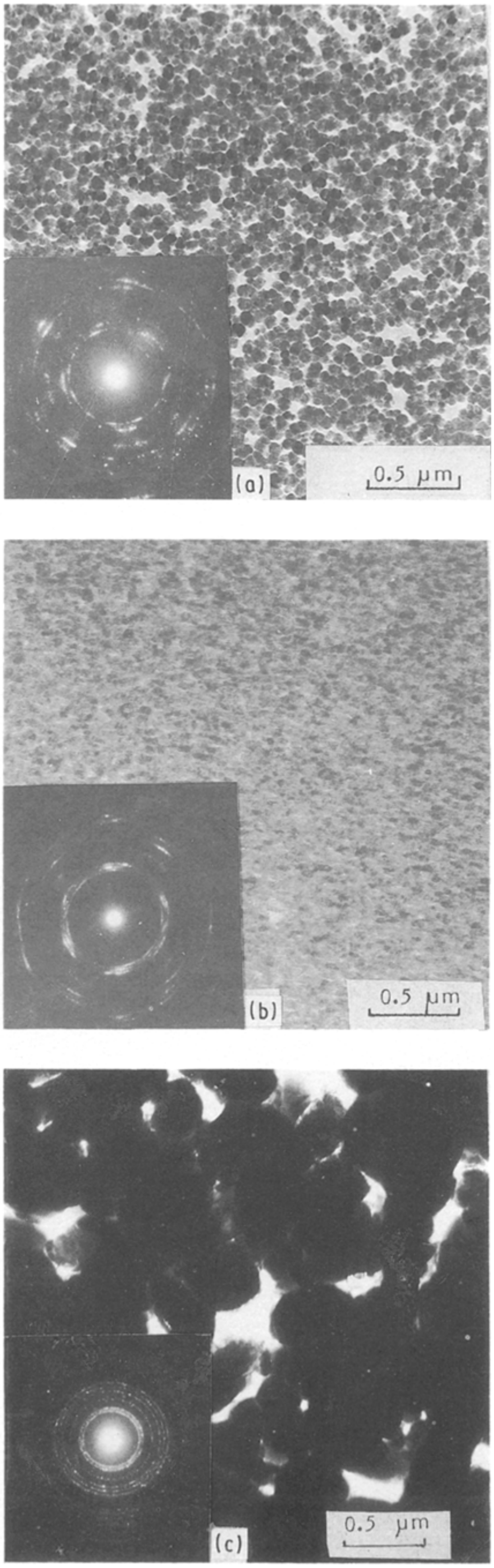


Figure 6 Micrographs of films ($x \sim 0.18$) deposited on to KCl at (a) 50 °C, (b) 150 °C, (c) 200 °C.

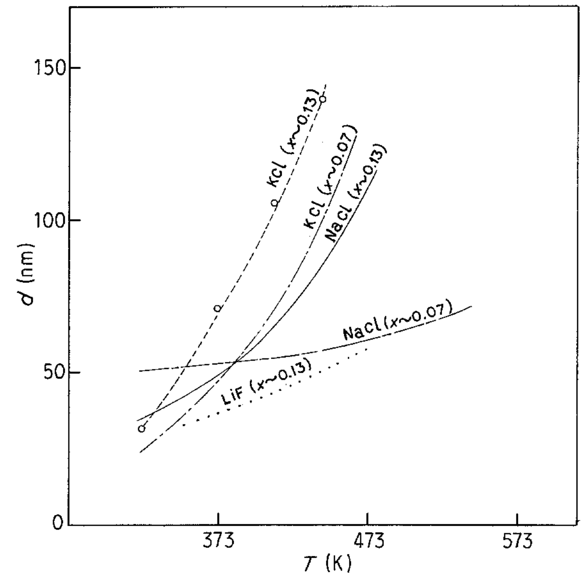


Figure 7 Graphical representation of grain growth of $Cd_{1-x}Zn_xS$ films.

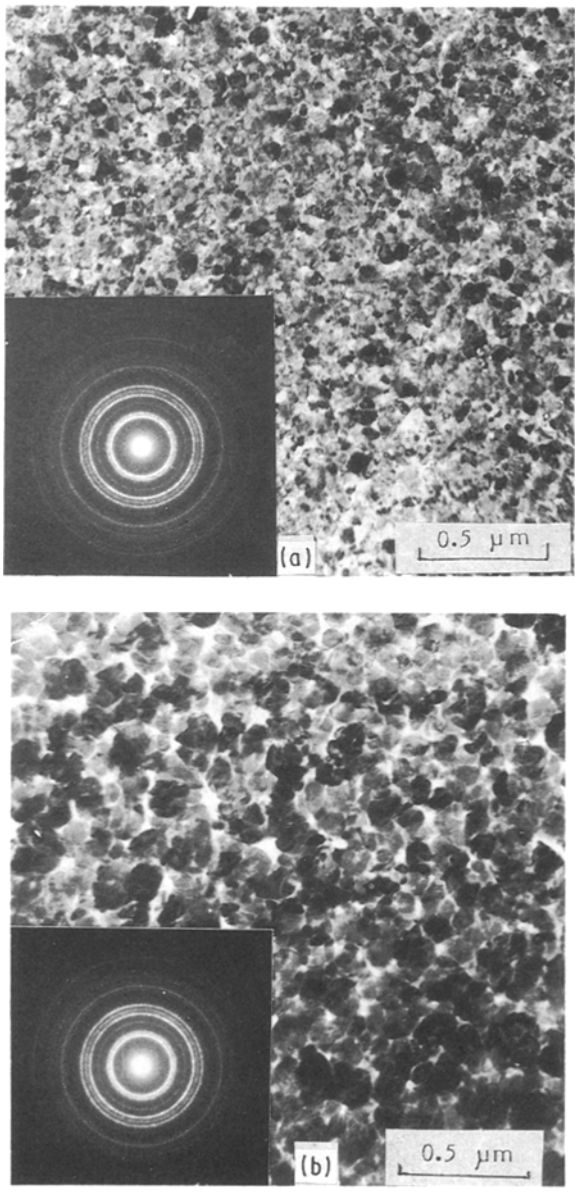


Figure 8 Micrographs of $Cd_{1-x}Zn_xS$ films deposited on to LiF at (a) 170 °C (for $x \sim 0.13$), (b) 200 °C (for $x \sim 0.18$).

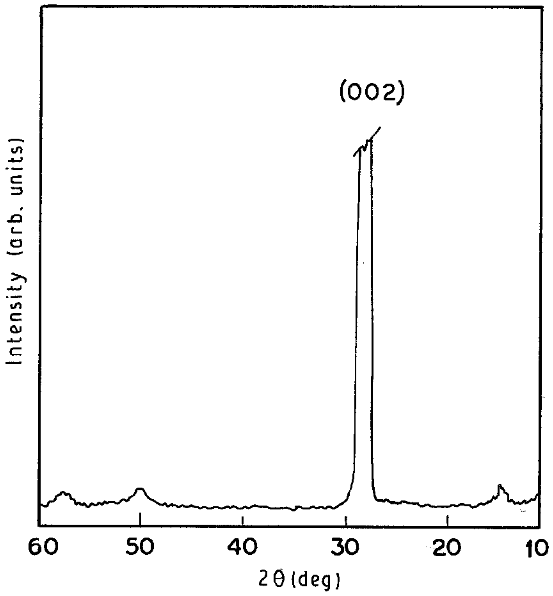


Figure 9 XRD trace for a representative film of $Cd_{1-x}Zn_xS$ ($x \sim 0.13$).

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