



**Figure 14.14** CdTe–CdS pseudobinary phase diagram. (Data listed in order from References [73, 140, 145, 148])

The formation of  $\text{CdTe}_{1-x}\text{S}_x$  and  $\text{CdS}_{1-y}\text{Te}_y$  alloys in the absorber layer occurs by interdiffusion between CdS and CdTe during  $\text{CdCl}_2$  treatment in air [135, 204]. Diffusion of CdTe into CdS can reduce the transmissive properties of the window from 500 to 650 nm, but is mitigated by heat treatment of the CdS layer prior to CdTe deposition to increase CdS grain size and density. However, diffusion of CdS into CdTe is a faster process and is more difficult to control, especially for cell structures with ultrathin,  $<100$  nm, CdS films. The progressive diffusion, which creates a distribution of lattice parameters within the film, can be easily detected with X-ray diffraction line-profile analysis (Figure 14.15).

Quantifying the diffusion process for films of a known grain structure showed that the diffusion proceeds via Fickian bulk and grain-boundary diffusion processes having Arrhenius temperature dependence [149] (Figure 14.16). Similar bulk diffusivities were found for CdS/CdTe couples using single-crystal CdTe and thin-film couples in *substrate* and *superstrate* configurations, yielding an activation energy of  $\sim 3.0$  eV, corresponding to Cd self diffusion via Cd interstitials. Likewise, similar grain-boundary diffusivities were obtained for *substrate* and *superstrate* thin-film couples, with an activation energy of  $\sim 2.0$  eV (Figure 14.17). The bulk diffusivity was weakly sensitive to the chemical composition of the treatment ambient, as shown in Figure 14.18. However, the grain-boundary diffusion process is enhanced by the partial pressures of  $\text{CdCl}_2$  and  $\text{O}_2$  during the  $\text{CdCl}_2$  treatment. Finally, it has been demonstrated that grain-boundary diffusion can be retarded by oxidizing grain boundaries prior to exposure to  $\text{CdCl}_2$  species [122] or by deposition of CdTe films in an oxygen-containing ambient.

Thus, alloy formation can be more pronounced in films deposited at low temperature having small grains and high grain-boundary density, such as by electrodeposition. In such films, a high partial pressure or concentration of  $\text{CdCl}_2$  together with  $\text{O}_2$  during  $\text{CdCl}_2$  treatment will result in considerable alloy formation. In addition, alloy formation is dramatically enhanced for cells with CdTe deposited at high temperature in the presence of Cl species during growth, such as spray pyrolysis.