



Figure 14.3 (a) CdTe T - x phase diagram (1 atm) [47] and (b) vapor–solid p_{sat} versus $1/T$ diagram for CdTe, CdS, CdCl_2 , Cd, and Te [48]

Cd, $T_m = 321^{\circ}\text{C}$, or Te, $T_m = 450^{\circ}\text{C}$ [49]. A detailed examination of the T - x projection around the CdTe stoichiometric composition indicates a very narrow, $\sim 10^{-6}$ at.%, symmetrical existence region at $T < 500^{\circ}\text{C}$. At higher temperatures, the existence region widens and is asymmetrical on the Cd-rich side up to 700°C and becomes Te-rich at higher temperatures [44]. The existence region and intrinsic defect structure are related by the preparation conditions of the bulk material and have been the subject of intensive investigation from the time since de Nobel [50]. Krüger published a comprehensive review of the defect chemistry in 1977 [51], and recently, theoretical treatments of defect levels in CdTe have extended this basis [52]. A critical topic of study is how the bulk properties transfer to thin-film CdTe.

The solid-state properties of CdTe are derived from the ionic character of the CdTe bond. Among the $\text{II}^{\text{B}}\text{-VI}^{\text{A}}$ compounds, CdTe has the highest value on the Phillips ionicity scale = 0.717, which is below the Phillips' threshold value of 0.785 for octahedral coordination [53]. Geometrical considerations show that tetrahedral coordination is favored in ionic binary compounds having cation/anion radius ratio between 0.225 and 0.732, while octahedral coordination is favored for a ratio greater than 0.732 [54]. In CdTe, the cation/anion radius ratio is $r(\text{Cd}^{2+})/r(\text{Te}^{2-}) = 0.444$, thus favoring tetrahedral coordination.

Tetrahedral atomic coordination, with the four nearest neighbors of the other element and the twelve next-nearest neighbors, leads to diamond structure in monatomic solids and zincblende and wurtzite structures in binary solids. Solid CdTe at atmospheric pressure exists in a face-centered cubic zincblende structure with unit cell dimension of 6.481 Å and CdTe bond length of 2.806 Å. Figure 14.4 depicts two views of the CdTe zincblende structure viewed across the closest-packing (111) plane, with alternating anion and cation planes, and viewed across the (110) plane, with equal numbers of anions and cations in each plane. These are the predominant orientations encountered in CdTe thin films.