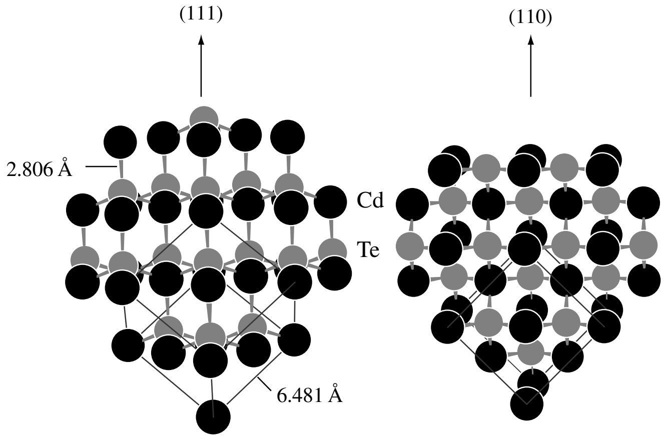

Figure 14.4 Zincblende CdTe crystal structure showing orientation with respect to (111) and (110) planes. The Cd atoms are black and Te atoms are gray. The Cd–Te bonds and F.C.C. unit cells are indicated for each view

CdTe polytypes are also known, depending on the formation pressure [55]. The hexagonal wurtzite structure, typically associated with tetrahedral coordination in predominantly covalent solids, is found in CdTe deposited in vacuum. No pure wurtzite bulk specimens have ever been reported [56]. Octagonal coordination, leading to the halite NaCl structure can be induced in CdTe by subjecting single crystals to high pressure, above 35 kbar. Among II-VI compounds, only CdO, with ionicity = 0.785, occurs with the halite structure at standard pressure and temperature.

The bulk optical and electronic properties of CdTe arise from the electronic-band structure within the periodic lattice near the valence-band maximum (VBM) and the conduction-band minimum (CBM). The VBM and CBM occur at the same momentum position, Γ, within the first Brillouin zone, giving rise to a direct band gap of 1.5 eV at 300 K. The temperature variation of the CdTe band gap is ∼−1.7 meV/K. The band curvature about the extrema represents the effective mass of electrons at the CBM and of holes at the VBM and controls carrier-transport properties and interband density-of-states (see Table 14.1).

Qualitatively, the band structure of CdTe can be understood from its relatively high ionicity, since the parts of the Bloch functions having the same periodicity as the lattice are related to the Cd and Te atomic orbitals. The conduction band arises from the first unoccupied level of the cation, namely, the 5s level of Cd. The uppermost valence band consists of the highest occupied level of the anion, namely, the 5p level of Te. It has been shown that cation d and anion p coupling reduce valence-band offsets in CdTe [57]. Detailed calculations of the E–k band structures in cubic CdTe and other II-VI compounds were originally carried out by the local pseudopotential method in the mid-1960s [58] and more recently using the linearized augmented plane-wave method, considering all electrons and relativistic kinematics [59].

Deviations from perfect single crystals cause profound changes in electronic and optical properties. Imperfections or defects disrupt the periodic structure, producing