- As mentioned above, material grown under compression is usually more stable to relaxation than material under tension, allowing one to err more toward negative values of $\Delta\theta$.
- Because of dynamical scattering effects, the measured $\Delta\theta$ for a thin ($\leq$0.1 μm) epilayer will be less than that of a thicker layer with the same composition and lattice mismatch [39].
- The value of $\Delta\theta$ for epilayers grown on nonsingular (100) substrates is not unique, but depends on the orientation of the substrate with respect to the X-ray beam. The effective $\Delta\theta$ is the average of two measurements of $\Delta\theta$. The first measurement is made in the conventional manner; the second measurement is made with the sample rotated by 180° [40]. For vicinal substrates close to (100), this effect is small, usually ∼10% at misorientation of 6°; however, for {511} substrates, the effect is closer to 50%.

9.6.3.2 Optical properties of GaInP

9.6.3.2.1 Ordering in GaInP

Prior to 1986, it was generally assumed that the band gap of a III-V ternary alloy semiconductor such as $Ga_xIn_{1-x}P$ was a unique function of the composition, and most publications showed $Ga_xIn_{1-x}P$, lattice matched to GaAs, as having a band gap of 1.9 eV. However, in 1986 Gomyo *et al.* [42] reported that the band gap of $Ga_xIn_{1-x}P$ grown by MOCVD was usually less than 1.9 eV and depended on the growth conditions. In a subsequent paper [43], they showed that the band gap shift was correlated with the ordering of Ga and In on the Group III sublattice. The ordered structure is CuPt-like, with alternating {111} planes of $Ga_{0.5+\eta/2}In_{0.5-\eta/2}P$ and $Ga_{0.5-\eta/2}In_{0.5+\eta/2}P$, where η is the long-range order parameter. Perfectly ordered GaInP ($\eta = 1$) would be composed of alternating {111} planes of GaP and InP. The first theoretical treatments of ordering in $Ga_xIn_{1-x}P$ were put forward by Kondow and coworkers [44] using the tight binding theory, and by Kurimoto and Hamada [45] using the "first-principles" Linearized Augmented Plane Wave (LAPW) theory.

The functional relationship between the band gap's change, ΔE_g, and the order parameter for GaInP was first published by Capaz and Koiller [46]:

$$\Delta E_g = -130\eta^2 + 30\eta^4 \text{ (in meV)} \tag{9.20}$$

A more recent result [47] suggests that

$$\Delta E_g = -484.5\eta^2 + 435.4\eta^4 - 174.4\eta^6 \text{ (in meV)} \tag{9.21}$$

The effects of various growth parameters on the ordering and the band gap of $Ga_xIn_{1-x}P$ have been studied extensively. The band gap of $Ga_xIn_{1-x}P$ is a function not only of the growth temperature, T_g, but also of the growth rate, R_g, the phosphine partial pressure, P_{PH3}, substrate misorientation from (100), and the doping level. Some of these effects are illustrated in Figure 9.14. Although the behavior is very complicated, there are a few characteristics that stand out. For example, for substrates that are closely oriented to within a few degrees of (100), the band gap of GaInP, using typical values for T_g, R_g, and