Abstract

Because of its excellent electronic and optical properties GaAs has been accepted as the dominant candidate for high speed and optical devices. Hence, there exists a growing need for high quality substrates and for an improved fabrication method of electrically and optically activ regions in GaAs. In paticular, more efficient dopants are desirable. Moreover, it is of interest to understand in detail the properties of extended defects, surfaces and interfaces. Therefore, in this work the geometry, the stability and the properties of complex structures in GaAs, present during growth, further treatment and doping, are examined theoretically. For these theoretical studies a method is used which is based on density functional theory and therefore guarantees the best accuracy possible. This method is furthermore implemented on parallel computers to allow the examination of extended structures.