

Chapter 7

SCHOTTKY BARRIER HEIGHT EXPLAINED WITH BULK CHARGE DENSITY

The explanation of the formation mechanism of the SBH at MS interfaces has occupied the attention of scientists for decades. Analyses of band alignment problem in general, including discussions in Chapter 4, tie the magnitude of the SBH to the charge distribution of the interface. Accordingly, the SBH at any MS interface is predictable if its charge distribution can be approximately modeled. Thanks to the nearsightedness principle of electron density, this is actually feasible, which forms the main topic of this chapter. Even though the vast majority of MS interfaces employed in actual devices are polycrystalline and the development of traditional theories on SBH formation was based almost exclusively on results from polycrystalline interfaces, it is not practical to delve directly into the charge distribution at polycrystalline interfaces. A more efficient way to understand SBH formation is still through studies of epitaxial MS interfaces. The uniqueness in the atomic structure of the epitaxial interface avoids the problem of electrical inhomogeneity at polycrystalline MS interfaces and allows the experimentally measured SBH to be directly compared with the atomic structure. With each interface studied in isolation, a comparison of results from different epitaxial interfaces most readily reveals the dependence of the SBH on the specifics of the interface. Epitaxial interfaces are also important for the reason that theoretical investigations can reveal not only the magnitude of their SBHs but also the energetic and spatial distributions of their electronic states. These details, essential for a complete understanding of the SBH problem, are available only from epitaxial MS interfaces. Furthermore, the charge density modeling planned for this chapter can be demonstrated explicitly only with epitaxial interfaces of known atomic structures. Therefore, this chapter relies heavily on epitaxial MS interfaces to illustrate how SBH