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SEMICONDUCTOR STRUCTURES, LOW-DIMENSIONAL SYSTEMS, AND QUANTUM PHENOMENA

Valence-Band Offsets in Strained SiGeSn/Si Layers with Different Tin Contents

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Abstract—Admittance spectroscopy is used to study hole states in $Si_{0.7-y}Ge_{0.3}Sn_y$/Si quantum wells in the tin content range $y = 0.04–0.1$. It is found that the hole binding energy increases with tin content. The hole size-quantization energies in structures containing a pseudomorphic $Si_{0.7-y}Ge_{0.3}Sn_y$ layer in the Si matrix are determined using the 6-band **kp** method. The valence-band offset at the $Si_{0.7-y}Ge_{0.3}Sn_y$ heterointerface is determined by combining the numerical calculation results and experimental data. It is found that the dependence of the experimental values of the valence-band offsets between pseudomorphic $Si_{0.7-y}Ge_{0.3}Sn_y$ layers and Si on the tin content is described by the expression $\Delta E_V^{\text{exp}} = (0.21 \pm 0.01) + (3.35 \pm 7.8 \times 10^{-4})y$ eV.

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1. INTRODUCTION

Silicon is the basic material of micro- and nanoelectronics; however, its application in optoelectronics is limited. This is associated with two features of the material. First, the major minimum of the Si conduction band is shifted with respect to the Brillouin-zone center, which abruptly decreases the efficiency of emitting structures based on Si. Second, the Si band gap is 1.12 eV at room temperature, which makes silicon transparent in the mid- and far infrared (IR) ranges. Therefore, the fact of the implementation of IR photodetectors based on pure silicon causes problems. Much effort is spent overcoming these limitations, and various approaches are used, such as the use of alloys of Group-IV elements and nanostructures on their basis. In different years, it was proposed to consider GeSi heterostructures with quantum dots (QDs) [1–4]. This approach yielded certain results; however, due to the low density of quantum dots, it is impossible to reach a significant quantum yield of light-receiving devices. As an alternative, the use of SiGeSn ternary compound on Si substrates is considered. For GeSn alloy, the change in the fundamental absorption mechanism from indirect-gap to direct-gap at low tin contents was theoretically predicted [5, 6] and experimentally observed [7–9]. The results obtained offer hope for the implementation of light-emitting devices based on a silicon substrate with SiGeSn ternary compound as the active element. Furthermore, since α-Sn is a semiconductor with an inverted band structure, the tin-content variation in alloys provides a significantly larger range of band gaps, which can be used in devices based on SiGeSn alloys, in comparison with SiGe-based devices. At present, there are many experimental studies devoted to the formation of SiGeSn ternary compounds [10–13], measurements of the optical properties of these semiconductors [13–17], and the fabrication of individual device structures using these alloys [18–20]. There are theoretical studies devoted to simulation of the band structures of both strained and relaxed [5, 6] ternary compounds. However, most such studies concern only the problem of the band gap in heterostructures, whereas the problem of determining the band offset at the Si/SiGeSn heterointerface is not considered at all. Sometimes, the Ge and Sn valence-band offset is calculated in the model proposed in [21]. At the same time, the band offset at the Si/SiGeSn interface is very important for forming device structures. In the present work, heterostructures with SiGeSn quantum wells (QW) formed in the Si matrix are studied; the hole localization energies and the valence band offset are determined using admittance spectroscopy.