MECHANISM OF ACCEPTOR IMPURITY INITIATION IN THE TiCoSb INTERMETALLIC SEMICONDUCTOR HEAVILY DOPED WITH A V DONOR IMPURITY. 1. STUDIES OF THE CRYSTAL STRUCTURE AND THE DISTRIBUTION OF THE ELECTRON DENSITY OF STATES

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S u m m a r y

Structural characteristics of the TiCoSb intermetallic semiconductor heavily doped with a donor V impurity (so that the electron concentration $N_D^{\rm V}$ varied from 9.5×10^{19} to 1.9×10^{21} cm^{-3}) have been studied, and the corresponding electron density of states (DOS) has been calculated. Different occupation numbers for the Co and (Ti,V) atomic positions in the $Ti_{1-x}V_xCoSb$ crystal lattices have been revealed, which is equivalent to the introduction of acceptor impurities of two sorts into the semiconductor. The numerical simulation of the investigated physical phenomena has been demonstrated to describe them adequately, if the variable occupation numbers of the atomic lattice sites in the elementary cell of the compound are taken into account while constructing a Wigner–Seitz cell.