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Surface properties of chalcogen passivated GaAs(1 0 0)

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Abstract

Chalcogen atoms like sulphur or selenium are promising candidates for the passivation of GaAs(1 0 0) surfaces. The passivation can be obtained by evaporation of S or Se under ultra-high vacuum (UHV) conditions or by etching in chalcogen containing solutions. In both cases, an additional annealing of the samples leads to Ga-chalcogenide like surface layers showing a 2×1 low energy electron diffraction (LEED) pattern. We have analysed the Se/GaAs(1 0 0)-2×1 geometry in detail by means of density functional theory (DFT) calculations. Comparing with photoemission data and scanning tunnelling microscopy (STM) currents we conclude that this geometry has a single Se atom in the last crystal layer bonded to two Ga atoms of the second layer, and another Se layer replacing the third As layer. While the theoretical calculations show that the band gap of Se-passivated GaAs(1 0 0) surfaces are free from surface states, the experimental data show a band bending that depends on the details of the passivation procedure used.

Author Keywords: Passivation; GaAs; Surfaces; Photoemission spectroscopy; Density functional theory

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