Structure determination of Co(0001)-(r3xr3)-Ga surface by LEED Patterson inversion

HIU LUNG LI, HAN DONG LI, HUA SHENG WU, MAO HAI XIE, Department of Physics, The University of Hong Kong — A low-energy electron diffraction Patterson function (PF) with multiple incident angles was used to determine the structure of the Co(0001)-(r3xr3)-Ga surface. The experimental LEED I-V data were first inverted as Patterson function map which gives the inter-atomic distances between all atomic pairs in the structure. By comparing the experimentally obtained PF map and the simulated PF map of all proposed atomic structure models, impossible atomic structure models were effectively eliminated. Finally, the true atomic structure and detailed atomic positions on surface were deduced from tensor-LEED I-V curve fitting. Our result shows that Ga adatoms situate on T4 sites above the bulk surface of Cobalt.

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