

Ir{100}-c(2x4)-NO/O: A Structure Determination by Quantitative LEED

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We have studied the co-adsorption of nitric oxide and oxygen on the (1x1) phase of Ir{100} using Temperature Programmed Desorption (TPD) and Low Energy Electron Diffraction (LEED). RAIRS¹ and TPD measurements show that NO adsorbs intact on the surface when co-adsorbed with oxygen. This is in contrast to the pure NO layer where NO dissociates and the formation of N₂ is observed. At 360K NO and oxygen form an ordered c(2x4) overlayer. The LEED pattern of this overlayer has missing spots indicating a structure that includes a glide line and a mirror plane. Our LEED-IV structure analysis favours a structural model with a stoichiometry of NO+2O, where the NO molecules and O atoms are both on bridge sites. Substantial buckling (0.09Å) was found for the atoms in the outermost Ir layer, whereas the second layer is essentially bulk-like. IR spectroscopy provides independent support for bridge-site occupation by NO¹, and additional support for this model comes from DFT calculations².

1. S. Khatua, S Pratt, and D.A King; to be published
2. Z-P. Liu, S. Jenkins and D.A King; to be published