THE THERMODESORPTION OF CO FROM THE Mo(110) SURFACE

N.V. Petrova, V.D. Osovskii, D.Yu. Balakin, I.N. Yakovkin, Yu.G. Ptushinskii

Institute of Physics, Nat. Acad. of Sci. of Ukraine
(*46, Prosp. Nauky, Kyiv 03028, Ukraine; e-mail: ptush@iop.kiev.ua*)

S u m m a r y

The problem of the CO adsorption and dissociation on the Mo(110) surface has been studied by means of temperature-programmed desorption (TPD) and density-functional (DFT) calculations. The TPD spectra show a first-order CO desorption, which indicates the desorption from a virgin state, not a recombinative form of desorption. The height of the potential barrier for CO dissociation (2.75 eV), estimated from DFT calculations, substantially exceeds the energy of CO chemisorption on the Mo(110) surface (2.1 eV), which refutes a thermally induced CO dissociation. Monte Carlo simulations of TPD spectra, performed with the use of estimated chemisorption energies, are in good agreement with experiment and demonstrate that the two-peak shape of the spectra can be explained without involving the CO dissociation.