Identification of Defect Sites on MgO(100) Thin Films by Decoration with Pd Atoms and Studying CO Adsorption Properties

Abstract:
CO adsorption on Pd atoms deposited on MgO(100) thin films was studied by thermal desorption (TDS) and FTIR spectroscopies. CO desorbs from the adsorbed Pd atoms at a temp. of about 50 K, which corresponds to a binding energy, \( E_b \), of about 0.7 ± 0.1 eV. FTIR spectra suggest that at satn. 2 different sites for CO adsorption exist on a single Pd atom. The vibrational frequency of the most stable, singly adsorbed CO mol. is 2055 cm\(^{-1}\). D. functional cluster model calcns. were used to model possible defect sites at the MgO surface where the Pd atoms are probably adsorbed. CO/Pd complexes located at regular or low-coordinated O anions of the surface exhibit considerably stronger binding energies, \( E_b = 2\)–2.5 eV, and larger vibrational shifts than were observed in the experiment. CO/Pd complexes located at oxygen vacancies (F or F\(^+\) centers) are characterized by much smaller binding energies, \( E_b = 0.5 \pm 0.2 \) or \( 0.7 \pm 0.2 \) eV, which are in agreement with the experimental value. CO/Pd complexes located at the paramagnetic F\(^+\) centers show vibrational frequencies in closest agreement with the experimental data. These comparisons therefore suggest that the Pd atoms are mainly adsorbed at oxygen vacancies.
F-centers (F+ identification of defect sites on MgO(100) thin films by decoration with Pd atoms and studying CO adsorption properties) Adsorption energy F-centers (identification of defect sites on MgO(100) thin films by decoration with Pd atoms and studying CO adsorption properties) IR spectra (of CO adsorbed on deposited Pd atoms on MgO(100) thin films) Desorption (thermal, temp.-programmed, tpd of CO adsorbed on deposited Pd atoms on MgO(100) thin films) magnesium oxide film defect identification adsorbed palladium carbon monoxide adsorption magnesium oxide film defect identification

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