Physico-chemical nanomaterials science

Adsorption of transition metals (Cr, Mn) and oxygen on the Si(001) surface

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Adsorption of (Mn, Cr, Ti) transition metals on the silicon surface is intensively studied due to possible spintronic applications. Recent studies of the oxidation of the Si(001) surface covered by submonolayer transition metal films had shown significant increasing of the sticking coefficient for the molecular oxygen on such systems compared to the clean Si(001) surface [1].

The Cr, Mn atoms adsorption and co-adsorption with atomic oxygen on Si(001) surface was studied using density functional theory (DFT) method and cluster models. All calculations were carried out by the GAMESS program [2].

The geometric structures and adsorption energies of Cr and Mn atoms adsorbed at different positions on the Si(001) surface were analyzed for the states with different multiplicity. The "*hollow*" site on top of surface dimers row and the "*interstitial*" site under top Si layer of the Si(001) surface were found to be energetically favorable. The most favorable paths - along and across silicon surface dimmers - were obtained. The transitions between the states with different multiplicities can take place during diffusion.

Several metastable structures of an oxygen atom adsorbed on the Cr/Si(001) and Mn/Si(001) surfaces were considered and compared with those on clean Si(001) surface. Oxygen atoms can form metastable structures with transition metal atoms as well with silicon atoms in agreement with recent AES and EELS studies of those systems. Oxygen atoms tend to bind with (Cr, Mn) transition metal atoms adsorbed on the Si(001). The formation of the Cr-O (Mn-O) structures is more favorable the Si-O-Si or Cr-O-Si (Mn-O-Si) bridge structures formation.

1. *I. P. Koval', Yu. A. Len', M. G. Nakhodkin, M. O. Svishevs'kyi, M. Yu. Yakovenko* Interaction of Molecular Oxygen with Si(001) Surface Covered with a Chromium or Titanium Monolayer // Ukrainian Journal of Physics.-2015.-**60**, N 1.-P. 46-51.
2. *Schmidt M. W. et al.* GAMESS, The General Atomic and Molecular Electronic Structure System // J. Comput. Chem.-1993.-**14**.-P. 1347-1358.