

INTERACTION OF MOLECULAR OXYGEN
WITH A SUBMONOLAYER Sb COVERAGE
ON A Si(001) SURFACE

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S u m m a r y

The chemical content of oxides, which appear on a Si(001) surface previously covered with a submonolayer of adsorbed antimony atoms and exposed to molecular oxygen up to 10^8 L (1 L(Langmuir) = 10^{-6} Torr · s), has been studied experimentally by the methods of electron Auger and ionization spectroscopies. It has been shown experimentally for the first time that a submonolayer coverage of antimony on the Si(001) surface at exposures to molecular oxygen more than 10^6 L results in forming both the antimony and silicon oxides, the latter with a stoichiometric content close to that of SiO₂. This feature of Sb distinguishes it from Bi, in the presence of which only silicon oxides appear. This confirms our previous calculations of the adsorption energies of oxygen on the Sb/Si(001) and Bi/Si(001) surfaces. Among the reasons why the exposures that are required for silicon oxides to be formed in the Sb/Si(001) system are noticeably larger as compared with the Bi/Si(001) case, there may be substantially smaller strains and charge transfer between a surfactant and a substrate, which take place in silicon layers when antimony is being adsorbed. The quantum-chemical simulation of antimony oxide phases in submonolayer coverages on silicon showed that the values of the chemical shifts $N_{4,5}$ of the Sb levels are proportional to the variation of the effective charge of Sb atoms.