STRUCTURES OF Cl ADLAYERS ON Ag(111) SURFACE

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S u m m a r y

The lateral interaction between chlorine atoms adsorbed on the Ag(111) surface results in the formation of a $(\sqrt{3}\times\sqrt{3})$R30° structure at the coverage $\theta = 0.33$. This structure is experimentally observed by the methods of low-energy electron diffraction and scanning tunnel microscopy at sufficiently low substrate temperatures. With increase in the temperature, the $(\sqrt{3}\times\sqrt{3})$R30° structure disorders, which results in the vanishing of the characteristic reflexes from the diffraction image at room temperature. The Monte Carlo simulation with parameters of the lateral interaction energy calculated with the help of the density functional theory has elucidated important features of the formation of surface structures and the order–disorder transition taking place with increase in the temperature. In particular, it is shown that the transition is very abrupt, which is due to a sufficient number of free adsorption sites and the substantial repulsive lateral interaction between adatoms.