Nanostructured surfaces

Computer simulation of diffusion in submonolayer coadsorbed films on atomic anisotropic faces

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Surface diffusion is one of the most interesting processes in adsorbed particles dynamics. Many modern technologies are directly related to adatom and molecule transport on surfaces of solids. It is known that phenomena of self-assembly of adsorbed atoms strongly electropositive to adsorbent are observed on furrowed, atomically smooth and stepped monocrystal faces of transition metals and semiconductors. We consider the cases of formation of adatom linear chains with structure p(1×n). Earlier, we investigated experimentally the surface diffusion of lithium coadsorbed with some number of strontium atoms in submonolayer film on (112) tungsten face [1]. It was shown that strontium strongly bound with substrate depressed the lithium diffusion. It was hypothesized that the effect arose because of phase state change of lithium adsorbed film with coverage degree increasing due to strong interaction with strontium atoms. The aim of our research now is investigation of the surface diffusion in phase-inhomogeneous coadsorbed submonolayer films with repulsive lateral interaction of adatoms.

It is known that chain structures p(1×n) oriented perpendicularly to atomic furrows of substrate form in submonolayer films of alkaline lithium and alkaline-earth strontium at corresponding temperatures on (112) faces of tungsten or molybdenum. However, the temperatures of existence of lithium linear structures are lower than strontium ones. We showed that if two adsorbates had tendency towards formation of linear superstructures with different periods then the tendency remained in coadsorbed film with domination of properties of component which more strongly bound with substrate. Lithium adatoms easy build into strontium chains. Our results demonstrate the complex character of effects in coadsorbed systems. Slow-moving strontium adsorbed atoms strongly affect the diffusion kinetics of lithium. The affection is caused by interplay between coadsorbed particles and collective mechanisms of surface diffusion.

1. *Loburets A.T., Zaika S.A., Naumovets A.G.* Influence of coadsorbed strontium atoms on surface diffusion in lithium submonolayer films on tungsten (112) face // Ukr. J. Phys. – 2012. – **57**, N 6. – P. 661 – 669.