On the description of the quantum surface diffusion: Non-markovian effects vs. jump dynamics

V. Ignatyuk

Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 1 Svientsitskii Str., 79011 Lviv, Ukraine, E–mail: ignat@icmp.lviv.ua

A description of diffusion processes of light particles adsorbed on metallic surfaces is a topical problem of surface physics and of a high interest both for experimentalists and theorists. Even in the case of a tracer diffusion, the memory effects can be present, if the substrate has no time to relax during the adparticle motion. In our studies we focus on the situation when the memory effects play an important role and can not be excluded from consideration.

We consider surface diffusion of a single particle, which performs site-to-site under-barrier hopping, fulfils intrasite motion between the ground and the first excited states within a quantum well and interacts with surface phonons. We obtain a chain of quantum kinetic equations for one-particle distribution functions and non-equilibrium hopping probabilities. The generalized (time-dependent) diffusion coefficients are derived, and the generic non-Markovian diffusion equation is presented both for an infinite lattice model and in a continuous media limit. In the latter case a one-particle distribution function obeys a Telegrapher's equation that could give us a non-monotonic behaviour of the intermediate distribution function at the large values of a wave vector. In a weak coupling limit, when the energy exchange between the adparticle and the substrate (which plays a role of the thermal bath) is very slow, the relaxation times of the generalized diffusion coefficients exceed an inverse Debye frequency by two orders of magnitude. If the vibrational energy is comparable with temperature, there are also pronounced oscillations of the generalized diffusion coefficients. In our studies we also touch upon the recrossing/multiple crossing phenomena, a problem of the long tails of the generalized diffusion coefficients as well as a possibility of long jumps of the adparticle.