On a relation between the temperature dependence of the T-mode of adsorbate and the nature of the "adsorbate-substrate" interaction

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A temperature behavior of the frustrated translational mode (T-mode) of a light particle, coupled by different regimes of ohmicity to the surface, is studied within a formalism of the generalized diffusion coefficients [1]. The memory effects of the adsorbate motion are considered to be the main reason of the T-mode origin. Numerical calculations yield a thermally induced shift and broadening of the T-mode, which is found to be linear in temperature for Ohmic and super-Ohmic systems and nonlinear for strongly sub-Ohmic ones. We obtain analytical expressions for the T-mode shift and width at weak coupling for the systems with integer "ohmicity" indexes $n = 0 \div 2$ in zero temperature and high temperature limits. We provide [2] an explanation of the experimentally observed *blue*- or *red*-shifts of the T-mode [3, 4] on the basis of a comparative analysis of two typical times of the system evolution: a time of decay of the "velocity–velocity" autocorrelation function, and a correlation time of the thermal bath random forces. A relation of the T-mode to the multiple jumps of the adsorbate is discussed, and generalization of conditions of the multiple hopping to the case of quantum surface diffusion is performed.

References

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