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Contribution of Vibrational Dynamics to Adatom Diffusion on Metal Surfaces[1] HANDAN YILDIRIM, SONDAN DURUKANOGLU, Department of Physics, Istanbul Technical University, ABDELKADER KARA, TALAT S. RAHMAN, Department of Physics, Kansas State University — We have calculated the vibrational dynamics and thermodynamics for a series of scenarios where an adatom is adsorbed of flat and stepped surfaces for both cases of hollow site and saddle-point adsorption. We have used the embedded atom method for the interatomic potential for Cu. The local vibrational densities of states were calculated using real space Green's function formalism and the thermodynamical functions were evaluated using the harmonic approximation. Activation energies for the static systems show a strong anisotropy for Cu(110) and near a step. For Cu(110), for example, we find activation energies of 0.230 and 1.146 eV for diffusion along and perpendicular to the open channel respectively. The change in the vibrational free energy for these two cases was found to be about 50 meV which represents about 20% for the first case and less than 5% for the second. Trends extracted from our detailed study on the contribution of the vibrational dynamics to the diffusion prefactors will be presented and comparisons with experimental data will be made when available.

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Abdelkader Kara
Department of Physics, Kansas State University

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