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Quantum and classical theory for the phonon bath in atom-surface scattering: Application to the Cu(111) system SHAULI DAON, Weizmann Institute of Science, SALVADOR MIRET-ARTES, Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas, Serrano 123, 28006 Madrid, Spain, ELI POLLAK, Weizmann Institute of Science, ELI POLLAK RESEARCH GROUP AT WEIZMANN INSTITUTE OF SCIENCE TEAM, SALVADOR MIRET ARTES AT SPANISH SCIENTIFIC RESEARCH COUNCIL COLLABORATION — Abstract Inspired by the semiclassical perturbation theory of Hubbard and Miller [J. Chem. Phys.80, 5827 (1984)10.1063/1.446609], we derive explicit expressions for the angular distribution of particles scattered from thermal surfaces. At very low surface temperature, the observed experimental background scattering is proportional to the spectral density of the phonons. The angular distribution is a sum of diffraction peaks and a broad background reflecting the spectral density. The theory is applied to measured angular distributions of Ne, Ar, and Kr scattered from a Cu(111) surface [1]. Abstract The theory is further explored for the study of the effects of the phonon bath in atom-surface scattering. [2] The theory is utilized to derive the angular distribution in three ways. First, we modify the angular width of the incident beam to investigate the effect of beam collimation. [2,3] Second, a continuum limit expression is obtained for a classical phonon bath. Third, numerical discretization is applied to the phonon bath, to solve for all bath modes.

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