Scattering of Thermal Energy Atoms and Molecules from Cold Copper Surfaces

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ABSTRACT

Slow heavy atoms scattering from cold surfaces excite many phonons, but still have a finite elastic scattering fraction. Usually, coherent quantum scattering of atoms and molecules from surfaces is associated with light species like helium or hydrogen, which are known to exhibit a considerable amount of elastic scattering from metal surfaces. Results in this Thesis show that at sufficiently low substrate temperatures around 10 K, quantum phenomena like diffraction is observed also for heavier, thermal-energy particles like Ar, Kr and N_2 scattering from a Cu(111) surface. At the low temperatures these particles stick permanently to the surface – pulsed laser desorption enables us to keep the surface clean also in this extreme temperature regime. The probability for elastic scattering of heavy particles is very sensitive to the influence of lattice vibrations and the observed elastic intensities are significantly attenuated at elevated surface temperatures in a Debye-Waller like manner. From a simple semiclassical model treating the case of slow, heavy atom scattering, the exponent $2W$ of the Debye-Waller factor, e^{-2W}, is predicted to show simple mass dependencies. At zero substrate temperature, $2W$ is independent of m, while $2W \propto m^{1/2}$ at elevated temperatures. Experiments for Ne, Ar and Kr scattering from a 10 K Cu(111) surface confirm these qualitative predictions. Improved calculations using accurate atom-surface potentials and phonon densities-of-state yield also good quantitative agreement with experiments for Ne, Ar and Kr. The comparison also illustrates that useful information about physisorption potentials and surface phonons can be extracted from experiments in this regime. The comparatively light particles He, H_2 and D_2 show clear deviations from the semiclassical predictions.

Molecules, unlike atoms, also exhibit rotationally inelastic scattering. Sharp coherent quantum scattering features are observable in angular distributions of N_2, O_2 and CH_4 scattering from Cu(111) at low substrate temperatures. Compared to atoms of similar mass, rotational transitions reduce the elastic scattering probability for these molecules by about an order of magnitude. At low incident energy this effect is negligible for D_2. Scattering calculations for N_2 and D_2 confirm that the observed large difference in the probability for rotationally inelastic scattering can be explained by the difference in rotational constants of the two molecules.

Resonance phenomena in gas-surface scattering provide a powerful experimental method to explore details of the interaction potential. Due to occurring large elastic intensities, selective adsorption measurements have been primarily used for investigations of light particles and shallow interaction potentials. We demonstrate, for the Ne- and Ar-Cu(110) systems, that at low substrate temperature the method can provide relevant information about the physisorption potentials also for heavier atoms and deeper potential wells.

Keywords: surface, physisorption, potential, atoms, molecules, Debye-Waller factor, copper, diffraction, rotational excitations, resonances, semiclassical model, molecular beam, laser induced thermal desorption