Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Self-consistent elastic and inelastic scattering of helium atoms by the monolayer solid Xe/Pt(111) LUDWIG BRUCH, Department of Physics, University of Wisconsin-Madison, FLEMMING HANSEN, Department of Chemistry, Technical University of Denmark — The inelastic scattering of a helium beam by an incommensurate monolayer solid of Xe/Pt(111) for incident energies in the range 2.5 – 50 meV is evaluated in the one-phonon approximation. The calculations treat specific one-phonon excitations and use an extension of our wave packet propagation formulation of helium scattering to treat the elastic and inelastic scattering self-consistently. There is an inelastic (diffuse) background scattering for phonon modes with wavevectors that uniformly sample the Brillouin zone. The fraction of the beam that is scattered elastically into diffraction channels varies from almost 90% to about 15% over this energy range. A low energy case with trapping for more than 200 ps has been simulated. Results of the self-consistent calculations for the inelastic scattering are compared to those of previous calculations that did not include the feedback (coherent phonon annihilation) to the elastic channels.

Ludwig Bruch
Retired

Date submitted: 13 Nov 2013 Electronic form version 1.4