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Molecular effects in $\text{H}_2$ scattering from metal surfaces at grazing incidence

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Synopsis

Diffraction of fast atoms at grazing incidence has been recently proposed as a promising new tool to determine surface parameters with unprecedented accuracy. We show that using fast light molecular projectiles offers new possibilities, not only because elastic and rotationally inelastic diffraction can provide additional information on the surface characteristics, but also because they can be used to determine sticking probabilities at thermal energies and beyond, from the threshold up to the saturation limit. Therefore, this approach is an ideal complement to traditional sticking experiments at thermal energies to determine sticking curves up to the saturation limit.

Diffraction of atoms from both alkali-halide [1] and metallic [2] surfaces has been recently observed, opening new possibilities to study structural and dynamical properties of surfaces. The physical phenomenon behind these striking experimental results is the strong decoupling between the fast motion along the incidence direction, parallel to the surface, and the slow motion perpendicular to the surface. Along the incidence direction the projectile moves in a periodic potential, which means that the momentum change along this direction is zero. Therefore any momentum transfer comes from the slow motion perpendicular to the surface. This mechanism was proposed by Fariás et al [3] to explain experiments performed at much lower incidence energies, which showed that out-of-plane diffraction becomes dominant as the incidence angle (defined with respect to the surface plane) decreases and the incidence energy increases.

By means of classical dynamics calculations performed with first-principle six-dimensional potential energy surfaces for $\text{H}_2$/NiAl(110) and $\text{H}_2$/Pd(111), we have tried to answer next fundamental questions: i) Does fast light molecules such as $\text{H}_2$ impinging on surfaces at grazing incidence behave as atoms?; ii) Is there any molecular effect that survives at high energies and grazing incidence conditions, and what can one learn from it?

Our results show that molecular diffraction patterns are to some extend more complex than that of atoms, showing extra peaks coming from rotational excitations. But, the most remarkable result we have obtained is that the variation of 1-reflectivity, versus the normal energy for fast grazing incidence look very much like the corresponding sticking curves at thermal energies. As it is shown in Fig. 1, the agreement between normal and grazing results is better for rather open surfaces. We conclude that for open surfaces, like NiAl, measuring the molecular reflectivity in collisions of fast grazing $\text{H}_2$ molecules with surfaces can provide a good estimate of the corresponding sticking curve at thermal energies.

![Fig. 1](image_url)

**Fig. 1.** (Color) 1-Reflectivity, as a function of the collision normal energy for $\text{H}_2$/Pd(111) and $\text{H}_2$/NiAl(110). Black circles, normal incidence results, and red squares, fast grazing incidence along the crystallographic direction [101] and [100]. Blue triangles and green diamonds: fast grazing incidence along the [110] and [111] directions, respectively, for $\text{H}_2(v=0,J=0)/\text{NiAl}(110)$.

References


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