

# Surface Analysis with Molecular Techniques: fast molecular diffraction from KCl(001) at grazing incidence conditions

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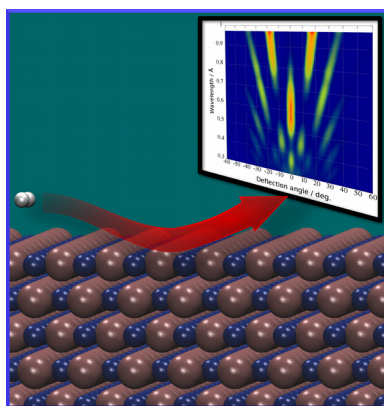
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Following the observation in 2007 of atomic and molecular diffraction by surfaces under fast (0.2-20 keV) grazing (1-3°) incidence conditions [1,2], the potential to characterize surface properties with more accuracy than with traditional atomic diffraction techniques was immediately realized.

One of the main problems in interpreting molecular diffraction under fast grazing incidence (DFGI) experiments is that the initial ro-vibrational state of the molecule is not known. Lack of knowledge on the actual projectile ro-vibrational distributions and the role played by vibrational and rotational excitations in DFGI is therefore the current bottleneck in the field, which prevents experimentalists from exploiting the huge potential of molecular projectiles.

In this context, help from theoretical modeling with real predictive power is crucial to guide experimental research. This modeling requires the evaluation of an accurate potential energy surfaces to describe the molecule - surface interaction and the solution of the time-dependent Schrödinger equation that governs the scattering dynamics in which all the molecular degrees of freedom are taken into account.

We have made a detailed analysis of different molecular projectiles diffracting from a KCl(001) surface, showing the strong dependence on the initial state of the molecule. We also show that these diffraction phenomena are mostly caused by elastic scattering processes, thus greatly simplifying the analysis of the observed spectra. At specific incidence directions, the appearance of high-order diffraction peaks reveals a high degree of rotational excitation in the incident molecular beam, which provides, in the absence of inelastic processes, the ideal scenario for a detailed characterization of the surface.

## References:

[1] A Schüller, S Wethekam and H Winter, *Phys. Rev. Lett.*, **98**, 016103 (2007)

[2] P Rousseau, H Khemliche, A G Borisov and P Roncin, *Phys. Rev. Lett.*, **98**, 016103 (2007)