Inelastic diffraction of fast atoms on crystal surfaces a Lamb-Dicke regime in shallow atomic collisions

M. Debiossac, P. Pan and P. Roncin

Institut des Sciences Moléculaires d'Orsay, CNRS, Univ. Paris-Sud, Université Paris-Saclay, Orsay, France

Synopsis Grazing incidence fast atom diffraction (GIFAD) uses keV atoms to investigate properties of crystal surfaces. It exists in two flavors; The elastic diffraction is identified by bright spots sitting on the Laue circle of energy conservation. We will focus on inelastic diffraction with a model where the surface atoms are quantum harmonic oscillators and where the successive collisions of the projectile take place in the Lamb-Dicke regime. The model explains observed lines shapes and predicts a drastic dependence of the energy loss $\Delta E \propto \theta^7$.

GIFAD is a surface sensitive technique providing a rapid characterisation of crystalline surfaces. Not only the atoms do not penetrate below the surface but the grazing incidence is also very sensitive to defects. The large kinetic energy allows efficient detection by imaging detectors collecting at once all the diffracted beams[1] as illustrated on fig.1. So far the main focus was to the elastic signal for which a simple interpretation could be given. Crudely speaking, the analysis of the elastic diffracted intensity is a $|\text{Fourrier}|^2$ transform of the surface were the atoms are bouncing (in blue on fig.1.).

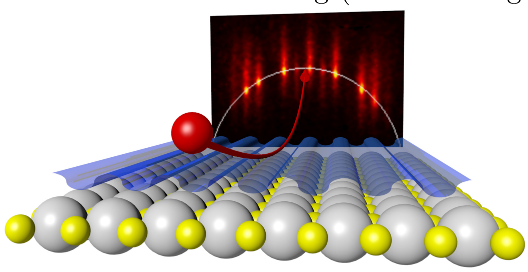

Figure 1. In GIFAD, the elastic intensity is seen as tiny spots on the Laue circle of energy conservation while the inelastic intensity extends beyond.

Inside a molecular beam epitaxy chamber GIFAD was able to to follow in situ and online the growth of the successive layers on a GaAs crystal [2, 4] and to provide a few pm accuracy on the atomic arrangement [3, 5].

The Debye-Waller factor (DWF) describes the amount of decoherence due to the thermal motion of surface atoms; Diffraction will be lost if the amplitude of thermal motion becomes larger than to projectile wavelength. This spatial approach was adapted to GIFAD [6, 7] to account for the fact that the momentum transfer is accumulated in several successive shallow collisions along the grazing projectile trajectory but no prediction could be made on the line-shape.

Taking a momentum approach and simplifying assumptions, we describe [8, 9] these binary encounters as sudden collisions with harmonic oscillators. For each surface atom, the momentum transfer δk to the vibrational wave function Ψ is evaluated. The probability that δk induces a vibrational excitation is $|\langle\Psi|e^{i\delta kz}|\Psi\rangle|^2$ and calculated as $e^{-E_r/\hbar\omega}$ were $\hbar\omega$ is the vibrational energy and $E_r = \delta k^2/2m$ the recoil energy that would be transferred if the atom would be free. In spectroscopy and in the cold atom community, it is known as the Lamb-Dicke probability of Recoil-less emission. The effect of an inelastic collisions would require summing over all initial and final vibrational states, instead we assume a quasi classical behaviour where the position of the surface atom is replaced by its Gaussian probability distribution P(z)=$\langle\Psi|z^2|\Psi\rangle$. Each inelastic collision contributes to a angular broadening taking a log-normal profiles in the polar direction and an associated energy loss equal to the transferred recoil energy E_r (now real). Combining the statistics of successive collisions with the associated probabilities one can reproduce the inelastic line shapes and predict a drastic dependence of the energy loss $\Delta E \propto \theta^7$.

References

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