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Fast atom diffraction of H and He from a LiF(001) surface: semi-quantum approach

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Synopsis For fast atom diffraction (FAD) from crystal surfaces we introduce a distorted wave method, based on the semi-quantum approach of the quantum evolution operator, in order to improve the description of rainbow effects given by the Surface Eikonal (SE) model. The theory, named Surface Initial Value Representation (SIVR) approximation, is applied to H and He atoms colliding with a LiF(001) surface, using pair-wise additive and DFT–derived potentials. The SIVR approach provides a very good representation of the experimental distributions, even in the angular region around classical rainbow angles where the SE method diverges. In addition, the influence of the incident wave-packet is analyzed.

In spite of the successful performance of the SE approach for the simulation of FAD patterns [1], a weakness of the theory is its deficient description of the rainbow effect, which affects the intensity of the outermost diffraction maxima when these maxima are close to the classical rainbow angles, i.e. the extreme deflection angles of the classical projectile distribution. Such a deficiency is a well-known characteristic of the *classical* representation of the dynamics, which introduces a singularity at rainbow angles. Within a proper *quantum* treatment, these sharp rainbow peaks are replaced by smooth maxima that display an exponentially decaying behavior outside classical rainbow angles, just in the region of classically forbidden transitions.

The goal of this work is to develop a *semi-quantum* approximation for FAD, based on the Initial Value Representation (IVR) method by Miller [2], which can solve the drawback of the SE model without losing the simple description of the interference process in terms of classical scattering trajectories. For this purpose we extend the IVR method by using the corresponding semi-quantum time evolution operator in the frame of a time-dependent distorted-wave formalism. The proposed approach, named Surface-Initial Value Representation (SIVR) approximation [3], is applied to evaluate FAD patterns for H and He atoms grazingly impinging on a LiF(001) surface. The surface potentials were derived from two different ways: accurate density functional theory (DFT) calculations using the "Quantum Espresso" code (Fig. 1) and a pairwise additive model including non local contributions (Fig. 2). Furthermore, the effect of the shape of the incident wave-packet is investigated in the light of Ref. [6].

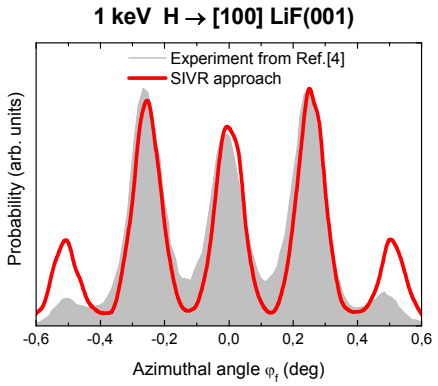

Figure 1. Angular projectile distribution, as a function of φ_f, for H atoms impinging on LiF(001) with the incidence angle θ_i=0.99 deg.

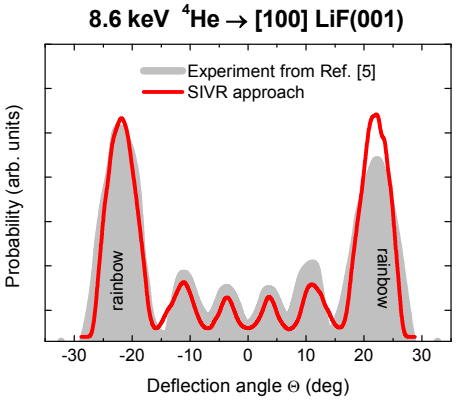

Figure 2. Similar to Fig. 1, as a function of Θ=arctan(φ_f/θ_f), for He projectiles with θ_i=0.71 deg.

References

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