Nuclear Instruments and Methods in Physics Research B 315 (2013) 30–35

Contents lists available at SciVerse ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

# Trajectory dependent energy loss in grazing collisions of keV He atoms from a LiF(001) surface

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A R T I C L E I N F O

*Article history:*
Received 31 October 2012
Accepted 27 February 2013
Available online 22 March 2013

*Keywords:*
Ion scattering
Insulator surface
Electron emission
Rainbow scattering

A B S T R A C T

Angular distributions for scattering of 12 keV He atoms from a LiF(001) surface under a grazing angle of incidence were recorded in coincidence with the projectile energy loss and the number of electrons emitted from the target surface during the collision. For scattering along the low indexed ⟨110⟩ and ⟨100⟩ directions of the crystal surface collisional rainbow peaks were observed. For scattering along a ⟨110⟩ direction the resulting rainbow peaks can be attributed to scattering from strings of anions which form active sites for charge exchange and emission of electrons. The data can be interpreted by trajectory computer simulations where charge transfer takes place from $F^-$ sites.



## 1. Introduction

Collisions of fast atoms and ions with surfaces of ionic crystals show the effect of a more efficient excitation and emission of electrons from the target surface than observed for metals [1–4]. This at first glance surprising feature can be attributed to the formation of negative ions during the collision process where the energy defect in the collision is mediated by the Madelung potential which leads to the confluence of electronic levels of valence band and transient negative ions [5]. Charge transfer under these conditions is so efficient that for reactive ions large negative ion fractions can be found. As a prominent example we mention the grazing scattering of F atoms from a KI(001) surface where in the range from some keV to several 10 keV $F^-$ fractions close to 100% were observed [6]. In detailed experimental and theoretical studies it was shown that the efficient mechanism for electronic excitation and charge transfer proceeds via the formation of transient negative ions [7]. These ions are formed in near-resonant capture of an electron from an $F^-$ ion embedded in the crystal lattice (“active site”) where electron transfer for the remaining energy defect in the collision is kinematically assisted. In studies on the projectile energy loss after scattering of fast atoms from surfaces of ionic crystals this mechanism has been studied in detail. For metal surfaces this process is absent and energy transfer to conduction electrons proceeds in terms of binary collision with the atomic projectiles giving rise to a threshold behaviour [8,9]. At low projectile energies/velocities this excitation mechanism is less efficient than the transient formation of negative ions in front of insulator surfaces and explains the lower electronic excitation mechanisms at metal surfaces compared to insulators.

In the work presented here we have extended studies on this topic by following specific trajectories during the collision of fast atoms with an insulator surface under axial surface channeling conditions, i.e. the grazing scattering of projectiles along low indexed directions in the surface plane of an ionic crystal. In this regime of (classical) atom surface collisions an azimuthal scattering out of the initial scattering plane containing the surface normal and the direction of the incident beam is observed owing to the corrugation of the interaction potential across the axial channels formed by strings of surface atoms. At the extreme of azimuthal angular deflection so called “rainbow peaks” are observed in accordance with basic concepts of classical scattering theory [10,11].

In contrast to scattering under a random azimuthal angle of incidence where scattering proceeds in the regime of “planar channeling” with very similar trajectories resulting in a defined single peak in the angular distributions, for scattering in the regime of axial surface channeling different types of trajectories can be identified [12]. By recording angular distributions of scattered projectiles for axial surface channeling in coincidence with the projectile energy loss, it is possible to relate specific electronic excitation and emission processes to defined trajectories for the collision with the surface. We will show that for different trajectories substantially different probabilities for electronic excitations can be found.

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http://dx.doi.org/10.1016/j.nimb.2013.02.055

On the basis of a detailed analysis of data in term of computer trajectory simulations we demonstrate that the observed effects are in good accord with the established models for the interaction mechanisms. In this respect our work provides further independent support for the interaction scenario between fast atoms and insulator surfaces based on the transient formation of negative ions.

## 2. Experiment and results

In our experiments we have scattered 12 keV He atoms from a flat and clean LiF(001) surface under a grazing angle of incidence $\Phi_{in} = 1.4\,°$. The azimuthal orientation of the target surface was arranged in a way that the direction of the incident beam was along ⟨100⟩ or ⟨110⟩. Then scattering from the surface proceeds in the regime of axial surface channeling where the axial channels are formed by strings of alternating $F^-$ and $Li^+$ ions for the ⟨100⟩ direction and by strings formed by $F^-$ or $Li^+$ ions only for the ⟨110⟩ direction. For scattering under channeling conditions the interaction with the solid can be separated in a regime of fast motion parallel with respect to surface plane which proceeds with about the total projectile energy $E$ according to $E_{\parallel} = E\cos^2\Phi_{in} \approx E$ and amounts to about 12 keV here [12,13]. The energy of motion normal to the surface and axial strings formed by surface atoms is $E_{\perp} = E\sin^2\Phi_{in}$ and amounts for 12 keV atoms and $\Phi_{in} = 1.4\,°$ to $E_{\perp} = 7.2$ eV.

$He^+$ ions were produced in a hollow cathode ion source, chopped by a pair of electric field plates, and neutralized in a He gas target via resonant charge transfer with negligible change in energy and energy spread of the incident beam. The gas target and the beam line is separated from the UHV target chamber via two differential pumping stages where slits of 0.2 mm width serve for the collimation of the incident beam to a divergence of less than 0.03 °. The target surface was prepared by cycles of sputtering with 100 keV $Ar^+$ ions under a grazing angle of incidence $\Phi_{in} \approx 2\,°$ and subsequent annealing at 400 °C for about 30 min. After the preparation over several weeks a well defined target surface was achieved, widely free of defects as manifested by angular distributions of scattered projectiles [12,14].

Scattered projectiles were recorded by means of a position sensitive micro-channelplate (MCP) detector positioned 80 cm behind the target. The position of atoms impinging on the active surface of the MCP was obtained via the timing information from a delay line array [15]. The so derived position was stored in a list-mode file together with the information on the arrival (start) time for the time-of-flight (TOF) setup. Analysis of this file allowed us to derive the angular distributions in coincidence with the flight time of the projectiles. Thus the angular distributions could be related to the energy loss of projectiles during the collision with the surface.

Electrons emitted during the collision of He atoms with the surface were recorded by means of a surface barrier detector biased to a high voltage of about 20 kV [16,17]. Since the pulse height of the detector output is proportional to the number of electron-hole pairs created by the accelerated electrons, the pulse height reflects the number of electrons emitted during the impact of single atoms on the surface and the pulse height distribution the number distribution of emitted electrons [18]. First studies on the coincident detection of scattered projectiles with the number of emitted electron have been reported by Lemell et al. for grazing scattering of $Ar^{8+}$ from an Au(111) surface [19].

In Fig. 1 we show in the upper panel a 2D-plot of the total angular distribution for 12 keV He atoms scattered from a LiF(001) surface under $\Phi_{in} = 1.4\,°$ along the ⟨110⟩ azimuth. The data reveals a circularly shaped distribution owing to the cylindrical symmetry of the scattering potential for axial channeling conditions. Striking features are the rainbow peaks at the extreme of azimuthal angular deflection and an intensive peak in the centre primarily caused by double scattering within the middle of the corrugated interaction potential across the axial channels. The angular positions of the rainbow peaks allow one to obtain information on the interaction potential as it has been demonstrated in a fair number of studies over the recent years [11,20].

In the middle and lower panels of Fig. 1 we show for the same case the angular distributions related to the energy loss of the

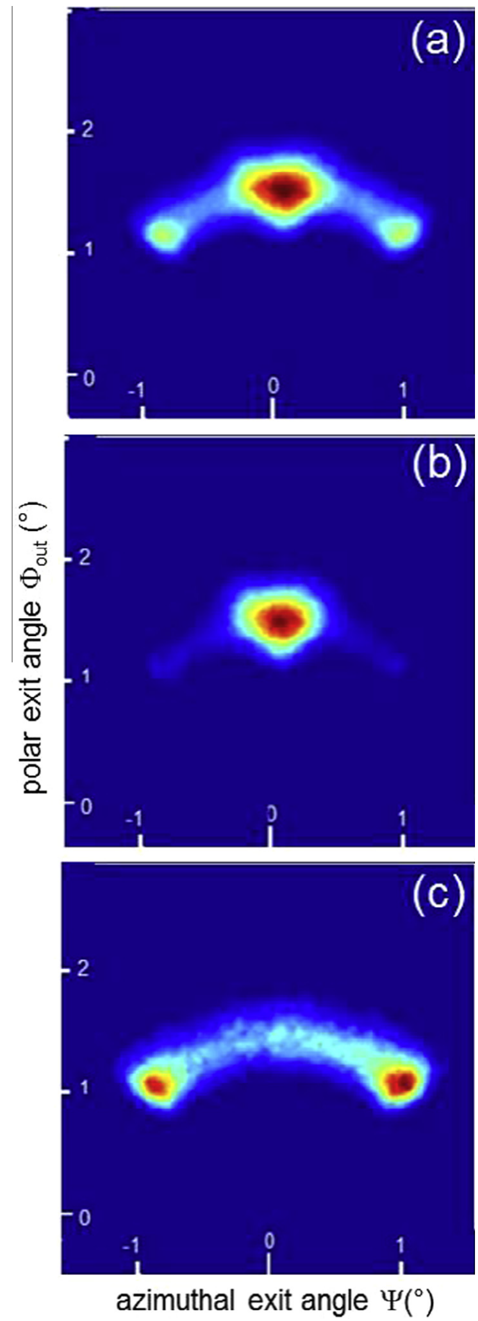


**Fig. 1.** Two-dimensional angular distributions recorded with position sensitive micro-channel plate (MCP) detector for scattering of 12 keV He atoms from LiF(001) under $\Phi_{in} = 1.4\,°$ along ⟨110⟩. (a) Total intensity, (b) intensity coincident with elastic scattering of projectiles, (c) intensity coincident with inelastic scattering of projectiles. Color code: red = high intensity, blue = low intensity. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)