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Channeling regimes in ion surface scattering

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Abstract

We report on surface channeling experiments of singly charged ions on single crystal surfaces of Pt(1 1 0) and Pd(1 1 0). Using a time-of-flight system installed in forward direction we analyze the energy distribution of the scattered projectiles. By variation of the primary energy and the angle of incidence we investigate effects of the perpendicular energy on the channeling features. The perpendicular energy is defined as $E_\perp = E_0\sin^2\psi$ with ψ the angle of incidence. In combination with precise azimuthal rotations of the crystal, we are sensitive to axial channeling and obtain information about the limits of axial surface channeling. From a comparison with detailed trajectory calculations we find that axial channeling effects are most pronounced for a perpendicular energy between 5 and 20 eV. As a result, we obtain an exemplary channeling map for the interaction of nitrogen ions with the (1×2) reconstructed Pt(1 1 0) surface identifying different channeling regimes.

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1. Introduction

Channeling is a well-known crystalline property, firstly reported from particle trajectory calculations in the sixties by Robinson and Oen [1]. Many bulk experiments were performed giving evidence that channeling effects influence the outgoing energy and charge state distribution of the scattered particles, e.g. in case of planar channeling multi-peak structures are observed in the measured energy spectra [2,3]. These structures have been explained by transverse oscillations of the ions as a consequence of multiple interactions with the planar potential walls. Datz and co-workers could show that it is possible from the oscillatory behavior of the trajectories in combination with

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the structures found in the energy loss spectra to map the stopping power inside the planar channel [2].

In case of surface channeling, one ensures a planar geometry by choosing properly small angles of incidence according to the critical angles e.g. given by Lindhard [4]. Due to the broken symmetry, however only one hemisphere acts to guide the ions, why the range of impact parameters is not limited as in case of bulk channeling. Therefore, the oscillatory behavior cannot be observed in planar surface channeling and a mapping of the stopping power depending on the surface distance is difficult since both, the surface electron density and the ion trajectory are not well known. By choosing the geometry in such a way that scattering takes place along surface channels, one deals with symmetric potential walls comparable to planar channeling in bulk material. The interaction of the ions with the side walls of the surface channels is known as axial surface channeling, which is from the point of trajectories characterized by the appearance of three independent groups of trajectories: *on-top*, *in-row* and *zigzag* channeled particles [5,6]. Axial channeling is found to be an interesting surface tool having the ability to characterize the electronic surface of a crystalline target [7]. In earlier work we showed by comparing the spectral features with the characteristics of the ion trajectories that it is possible to identify the different trajectory classes as single contributions in the energy spectrum [6,8]. The trajectories were calculated using the PSD computer code [9] by applying a ZBL potential [10]. This finding allows us now to track the intensities with which the different trajectory classes contribute to the energy spectrum in dependence of the geometry or the primary energy.

In the presented work we aim to investigate the *strength* of axial effects when changing experimental conditions like the primary energy E_0 or the angle of incidence ψ obtaining a kind of surface channeling map; the *strength* of axial effects is investigated by means of two different methods by changing the perpendicular energy $E_\perp$: (i) by analyzing the change in mean energy loss for axial and planar surface channeling and (ii) by analyzing the change in the intensity ratio between *in-row* and *on-top* channeled particles. The perpendicular energy is defined as $E_\perp = E_0 \sin^2\psi$. We evaluate data for two projectile–target systems, nitrogen on Pt(1 1 0) and He on Pd(1 1 0), respectively. Both crystals have a face-centered cubic (fcc) structure. Since axial surface channeling originates from the guiding forces of the atomic strings in the first surface layers, the presented technique is very sensitive to surface modifications [11,12]. Therefore, the experimental challenge is to deal with well-prepared, i.e. clean and atomically flat surfaces.

2. Experiment

The experiments are performed at the Surface Science Department of the University of Osnabrück using two similar ultra-high vacuum (UHV) setups. The N–Pt measurements were done at the LLOKI lab, the He-Pd experiments at the JUSO lab. The typical base pressure in both setups is in the 10^{-10} mbar range. Both targets are cleaned by sequent cycles of Ar-sputtering and annealing. Chemical target cleanness is controlled by low-energy ion scattering (LEIS). In case of Pt, we use low-energy electron diffraction (LEED) to ensure the (1×2) *missing-row* surface reconstruction [13]. Precise crystalline orientation is obtained using axial surface channeling, i.e. performing azimuthal scans and measuring the intensity of projectiles scattered in forward direction (see e.g. [5,14]). The accuracy of this technique is found to be better than 0.2°. Further experimental details can be found in [15].

The UHV systems are equipped with a plasma ion source, a sector field magnet for mass over charge separation and different lens and slit systems to define the primary ion beam. A pulsed ion beam is available allowing time-of-flight (TOF) analysis of neutral and ionic scattered projectiles. Both contributions can be separated by post-acceleration of the ionic part, however the ionic percentage is found to be rather small, of the order of a few percent. The energy divergence of the primary beam is of the order of $5\times10^{-3}E_0$ and the divergence in space defined by several slits is approximately 0.3°. A multi-channel-plate (MCP) configuration with 32 mm (LLOKI) and 25 mm (JUSO) diameter is used as particle detector, mounted 1558 mm (LLOKI) respectively 1246 mm (JUSO) downstream from the target resulting in an acceptance angle of approximately 1.2° in both cases. The overall energy resolution E/E_0 of the detection system is estimated to be in the range of 10^{-3}, basically limited by our pulsing and calibration system.

3. Results and discussion

Typical energy loss spectra are presented in Fig. 1. Parts (a) and (b) show spectra varying the primary energy in order to change the perpendicular velocity component. The ions scatter along the $[1\bar{1}0]$ direction of Pt and Pd, respectively. The abscissa is normalized to the primary energy. The effect of rotating the crystal's scattering axis with respect to the beam is shown in Fig. 1(c). Primary energy and angle of incidence are fixed, the significant change in the multi-peak structure is only caused by slight changes of the azimuthal direction. Strongest spectral changes are observed between 2° and 3°.

For both investigated systems we observe two main contributions, one with a low energy loss of approximately 2.5% which does not significantly change when varying E_0, the other having a pronounced energy loss between 5% and 10%, depending on the scattering conditions. In earlier publications we could show that the first contribution belongs to *on-top* scattered particles interacting weakly with the ridge atoms, the second one is attributed to projectiles penetrating the surface channels, a super-composition of *zigzag* and *in-rows* scattered particles [5,6]. It is straightforward that the latter contribution is more pronounced in case of interacting with a reconstructed Pt(1 1 0) surface since the *missing-row* structure results in wide and deep surface channels easing the penetration of the projectiles. In the following we will discuss the strength of the axial channeling contribution using two different methods.

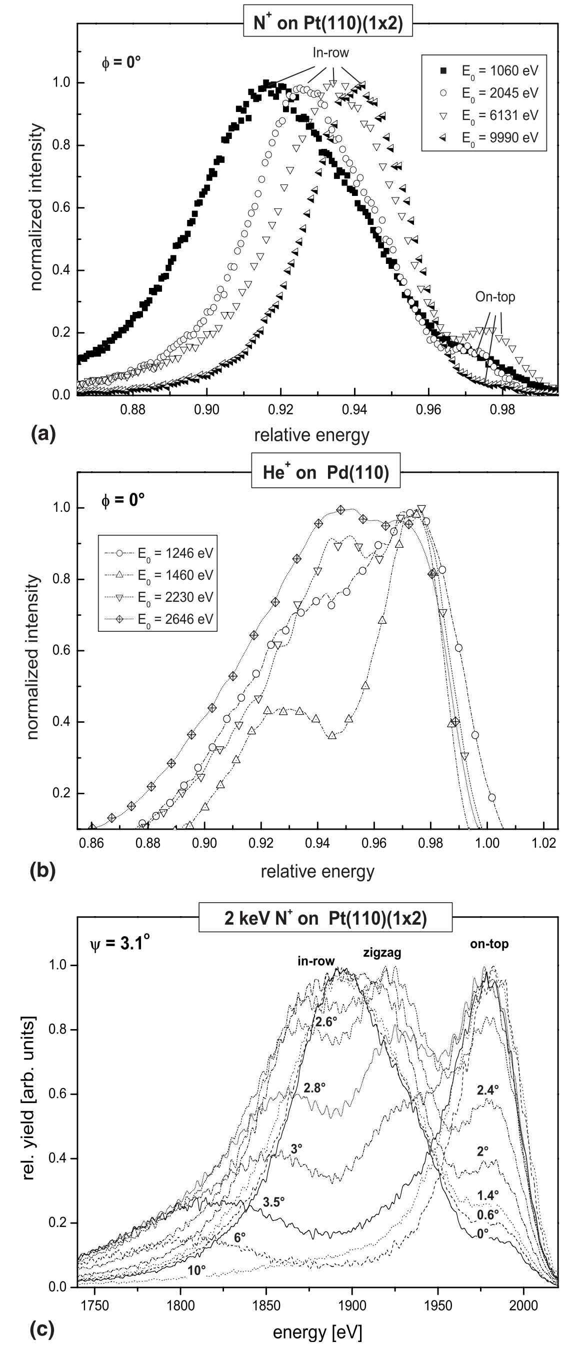

Fig. 1. Experimental energy loss spectra along the $[1\bar{1}0]$ surface channel for different primary ion energies: (a) N^+ on Pt(1 1 0)(1 × 2), (b) He^+ on Pd(1 1 0). Part (c) shows a sequence of nitrogen ions scattering of Pt(1 1 0) with constant primary energy, varying in small steps the azimuthal angle close the $[1\bar{1}0]$ surface channel.

3.1. Energy loss ratio

Axial channeling effects in surface scattering have been mostly studied in terms of changing the azimuthal axis of the surface direction with respect to the incoming beam and tracing the evolution of the spectral features [6,7]. For the analysis of the obtained energy spectra, detailed trajectory calculations have been performed [5]. Comparing the suffered energy losses one observes remarkable differences in case of axial and planar surface channeling [8]. Conclusively, to characterize the strength of axial channeling one can compare the obtained mean energy losses with the case of planar channeling – i.e. choosing a geometry ideally without any guiding forces from the surface channels – introducing the energy loss ratio $\Delta E^{\text{axial}}/\Delta E^{\text{planar}}$. It is found for nitrogen ions scattering off Pt(1 1 0) that the mean planar energy losses are almost identical to the losses suffered by the *on-top* contribution shown in the spectra of Fig. 1(a).

From Fig. 1(a) and (b) it can be seen that the maximum position of the *in-row* contribution varies when changing the primary energy. This is due to different stopping power values sampled along the trajectories during the interaction, i.e. depending on the perpendicular velocity component different electron density regimes are probed. To measure the strength of axial channeling we analyze the ratio between the mean energy loss suffered by the planar-channeled ions (the *on-tops*) and the axial channeled particles (the *in-rows* and *zigzags*).

For the slow ions under consideration we find the axial losses exceeding the planar energy losses significantly, even by more than a factor of two, i.e. the effect is clearly stronger than in case of MeV nitrogen ions interacting with Pt(1 1 0) [16]. For MeV ions in the Bohr velocity regime the axial losses are found to exceed the planar losses by roughly 20% only. In both velocity regimes we find a maximum in the energy loss ratio $\Delta E^{\text{axial}}/\Delta E^{\text{planar}}$ at a certain perpendicular energy $E_\perp$ which indicates the regime of *strongest* influence of axial channeling.

The graphs presented in Fig. 2 prove this behavior. They show the percentage which the mean en-

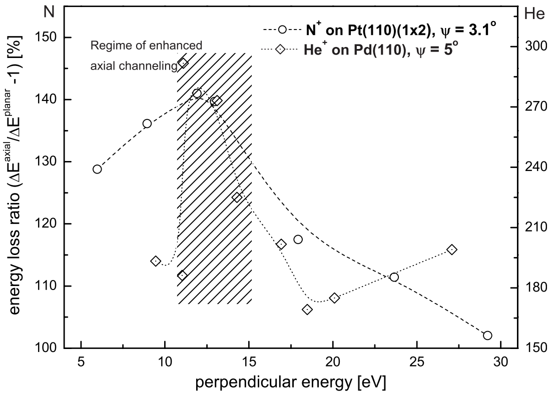

Fig. 2. Experimentally obtained energy loss ratio comparing the energy loss under axial and planar channeling conditions when varying the perpendicular energy. Lines are drawn to guide the eye. The angle of incidence is kept constant. Similar behavior is found for MeV nitrogen ions [16].

ergy loss for axial channeling exceeds the mean losses for planar channeling, indicating a maximum around $E_\perp = 13$ eV for both systems under investigation. In case of He on Pd we find another maximum at a smaller perpendicular component of $\simeq 7$ eV (spectra not included in Fig. 1(b)). The main reason is the fact that the energy loss of the *planar* scattered ions comes close to zero, whereas the *in-row* scattered particles experience already a significant stopping power. Furthermore, a different geometry representing the planar case might cause this difference to the N–Pt data. For He on Pd we have chosen an azimuthal angle of $\phi = 45°$ to evaluate the energy loss in case of planar channeling.

A similar behavior of the energy loss ratio is found when varying the angle of incidence instead of the primary energy: a clear intensity shift from the low-energy loss peak to the high-energy loss is observed [15]. However, for 4.5 keV nitrogen ions scattering under small angles like $\psi < 2°$ the *in-row* contribution becomes very small, therefore an evaluation of the mean energy for this contribution becomes rather uncertain. Due to this problem we cannot evaluate a graph like given in Fig. 2 for the ψ-series. But we clearly observe the two contributions coming closer when increasing the angle of incidence up to $\psi = 6°$. It is noted here that all spectra discussed within this work are measured under specular scattering conditions, i.e. $\theta = 2\psi$ holds.

3.2. Trajectory intensity ratio

To analyze the dependency of axial channeling on the angle of incidence we evaluate the relative intensity ratio between *in-row* and *on-top* channeled particles. These can be obtained from Monte Carlo trajectory calculations using the computer code PSD [9]. The results for N on Pt(1 1 0)(1 × 2) are given in Fig. 3. They lead to a maximum of the intensity ratio at perpendicular energies between 20 and 25 eV. In comparison to the results obtained for the series with varying primary energy, the maximum is shifted to a larger perpendicular energy. This is also seen from the experimental maximum obtained for the intensity ratios when varying the primary energy. Here, the maximum is between 15 and 20 eV which is closer to the value obtained from comparing the mean axial and planar energy losses.

It is now interesting to compare the regime of strongest axial effects with the minimum surface distance, z_0, of the ions. Exemplary, we have analyzed z_0 for the system N on Pt for a fixed incident angle of $\psi = 3.1°$ using axial channeling conditions

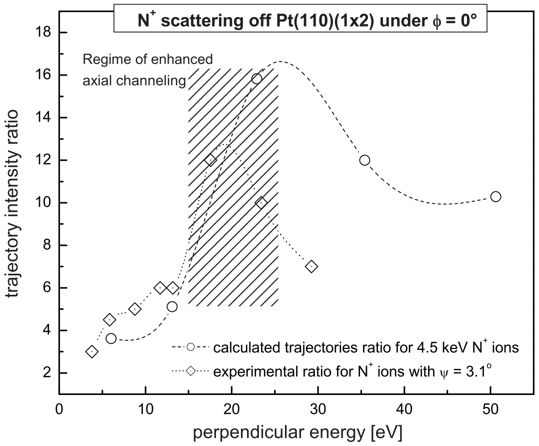

Fig. 3. Intensity ratio of particles scattered *on-top* and *in-row* the surface channels. The ratio indicates the strength of *axial channeling*. Experimental and calculated intensities are compared when varying the perpendicular energy of the primary ions. Lines are drawn to guide the eye.

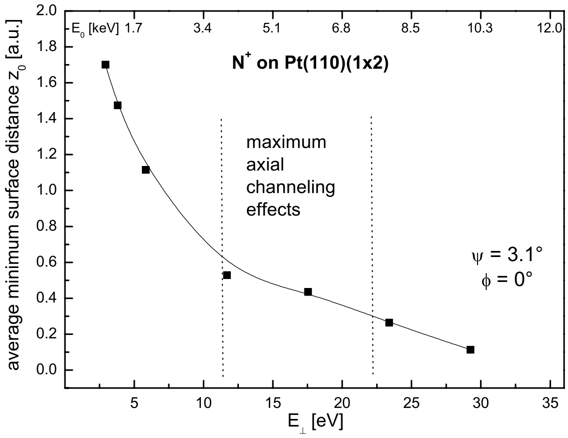

Fig. 4. Average minimum surface distance depending on the perpendicular energy for nitrogen atoms scattering along the [1 $\bar{1}$ 0]-surface channel of Pt(1 1 0). Values are obtained from Monte Carlo trajectory calculations [5,9].

($\phi = 0°$). From Fig. 4 one sees that the regime of strongest axial effects corresponds to minimum surface distances of about 0.5 a.u., i.e. the ions enter the electronic surface far enough to experience the corrugation of the electron density perpendicular to the surface channels. If z_0 is outside the region where the electronic surface corrugation is probed, surface channeling is not sensitive to this effect. In case of N on Pt the average minimum surface distance for $E_\perp \simeq 5$ eV is approximately 1.5 a.u. for scattering along the [1 $\bar{1}$ 0]-direction. Therefore, the projectiles do not completely enter the surface channels, but stay *on-top* the surface during the interaction. In this case, a planar description is a good approximation for the scattering process.

As essential result of this work we find that in ion-surface scattering one deals with different surface channeling regimes which depend strongly on the perpendicular component $E_\perp$ of the incident ions. This is summarized in Fig. 5 as a kind of surface channeling ‘road-map’. We find less axial effects in surface channeling for $E_\perp < 5$ eV. In this regime, ion-surface scattering is found to be *planar* in a good approximation. Hereby, it does not matter if experiments are performed varying the angle of incidence or the primary energy in order to change $E_\perp$. For large $E_\perp$ exceeding 35 eV the

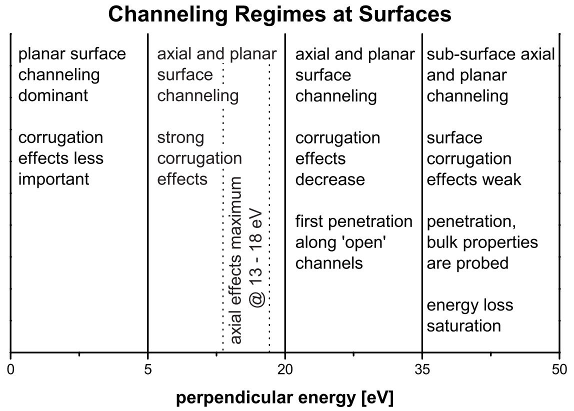

Fig. 5. Road-map of surface channeling regimes depending on the perpendicular energy obtained from the two scattering systems under consideration.

scattering becomes more and more bulk-like, i.e. many projectiles penetrate the first layers, and axial surface channeling effects vanish again. In-between, we observe the strongest influence of axial surface channeling: from the energy loss ratio this happens between 10 and 15 eV, using the intensity ratio as indicator the maximum effects occur at approximately 20 eV. Between 20 and 35 eV axial effects are still significant but decrease. Especially when choosing 'open' channels, e.g. the [1 1 2] channel, one observes strong penetration phenomena in this regime [14].

4. Conclusions

In conclusion, we analyzed the effect of axial surface channeling on the energy spectrum of scattered ions. With the methods presented within this work we obtain an experimental maximum of axial channeling effects between 10 and 20 eV. Axial effects strongly decrease for $E_\perp < 5$ eV, where channeling can be described as planar within good approximation. We find similar tendencies for both investigated projectile–target systems as well as for both experimental parameters varied in order to change the perpendicular velocity component of the ions – so the perpendicular component $E_\perp$ is the relevant parameter to characterize the surface channeling behavior. The tendencies found for the primary energy series are more straightforward than for the series varying the incident angle. Also, the maxima found for the influence of axial channeling are sharper for the primary energy series. Two methods have been presented to characterize the axial channeling effects in the energy loss spectra in dependence of the perpendicular energy. Both techniques are proven to be applicable and lead to similar results. For the case of ψ-variation we compare the experimental results with calculated trajectory intensity ratios resulting in a reasonable agreement. In general, trajectory calculations are found to be a useful tool to help understanding the details of the ion-surface interaction in the case of axial channeling.

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