Making channeling visible: keV noble gas ion trails on Pt(111)

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Abstract. The impact of argon and xenon noble gas ions on Pt(111) in grazing incidence geometry are studied through direct comparison of scanning tunneling microscopy images and molecular dynamics simulations. The energy range investigated is 1–15 keV and the angles of incidence with respect to the surface normal are between 78.5° and 88°. The focus of the paper is on events where ions gently enter the crystal at steps and are guided in channels between the topmost layers of the crystal. The trajectories of the subsurface channeled ions are visible as trails of surface damage. The mechanism of trail formation is analyzed using simulations and analytical theory. Significant differences between Xe\textsuperscript{+} and Ar\textsuperscript{+} projectiles in damage, in the onset energy of subsurface channeling as well as in ion energy dependence of trail length and appearance are traced back to the projectile and ion energy dependence of the stopping force. The asymmetry of damage production with respect to the ion trajectory direction is explained through the details of the channel shape and subchannel structure as calculated from the continuum approximation of the channel potential. Measured and simulated channel switching in directions normal and parallel to the surface as well as an increase of ions entering into channels from the perfect surface with increasing angles of incidence are discussed.

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1. Introduction

The investigation of damage production induced by charged energetic particles in a solid target is an important tool for understanding the physics of the ion–solid interaction. Analyzing the damage allows one to gain insights into the mechanisms of energy transfer, particle ejection and ion-induced defect formation.

Swift ions with energies in the MeV to GeV range are subject to electronic stopping. For them nuclear energy losses are marginal. In a narrow cylinder centered around the ion trajectory, electrons are efficiently removed, resulting in a large number of positively charged ions. Due to Coulomb interaction these ions repel each other and eventually produce damage \[1\]. By means of chemical etching the resulting damage cylinder, denoted as the ion track, can be removed and well-defined hole diameters on the nanometer scale are produced. These tracks can be observed by electron microscopy \[2, 3\]. Applications range from porous membranes over particle counters to radiation dosimetry \[4–6\]. The entrance spot of a swift heavy ion may be visualized by atomic force microscopy as a hillock or crater \[7–9\]. Chains of dots due to a grazing incidence swift heavy ion passing through SrTiO\(_3\) were reported in \[10\].

In contrast, heavy ions with energies of a few keV have large nuclear, but negligible electronic stopping. The ion ranges are small (\(<100\,\text{Å}\)) and tracks of individual particles in the solid are not observable. The collective bulk damage of keV ions can be analyzed by transmission electron microscopy (TEM) \[11\]. The surface damage of individual ions may be observed by scanning tunneling microscopy (STM) or atomic force microscopy. Such data yield insights into adatom production, sputtering and thermal spike formation \[12–14\] and complement molecular dynamics (MD) simulations of the interaction of keV ions with solids \[15–18\].
Figure 1. STM topograph of Pt(111) after an exposure to $6 \times 10^{16}$ ions m${}^{-2}$ 2.5 keV Ar$^+$ at 62 K. The ion beam direction is indicated by the arrow. The polar angle of incidence of the ion beam is $\vartheta = 86^\circ$ with respect to the surface normal. The labeled impact patterns are discussed in the text. The image size is 1280 × 1280 Å.

In order to make entire trails (‘trails’ instead of ‘tracks’ for distinction from damage originating from electronic stopping) of keV ions visible, we image the surface of Pt(111) by STM after a low fluence of grazing incidence ions at low temperatures. A typical STM image after an ion exposure experiment is shown in figure 1. Firstly, by sputtering at 750 K large hexagonal vacancy islands were formed, which are bounded by well-defined monatomic steps. Subsequently, the Pt(111) surface was subjected to an additional very low ion fluence of 2.5 keV at 62 K, where surface diffusion is absent on Pt(111). The ion angle of incidence $\vartheta$ with respect to the surface normal was set to $\vartheta = 86^\circ$. Under the conditions used, on average only 1 out of 250 surface atoms has been hit by an ion. Ion impacts on the flat terrace cause no damage and are reflected from the surface [19]; this process has been termed ‘surface channeling’. The damage resulting from step edge impacts depends strongly on the precise impact positions and shows a large variety. In figure 1, it is present at and behind the ascending step edges if viewed in the ion beam direction. Three events that can unambiguously be attributed to single ion impacts are highlighted. Event (1) in figure 1 shows a piece of step edge nibbled off and surrounded by a massive adatom island. This direct hit event is characteristic of localized energy deposition with a subsequent thermal spike [17]. Event (2) in figure 1 shows a chain of adatom clusters extending over a distance of about 220 Å from the step edge away in the ion beam direction. Here an ion entered the crystal at the step bottom and was steered in a channel formed through chains of atoms of the two top most layers in the $\langle 1\bar{1}0 \rangle$ direction until it presumably left the crystal again. The stopping force (energy loss per unit length) is greatly reduced compared to direct hit events and proceeds only by small angle collisions. Surface layer atoms become adatoms when they are gently hit from below by the moving ion. Such well-channeled events with extended damage patterns are the focus of this paper. Event (3) in figure 1 shows a smaller ensemble of adatom clusters elongated in the ion beam direction and extending over a distance
of about 80 Å behind the step. Close to the end of the adatom cluster ensemble a small vacancy crater is visible. Apparently, at the end of the channeled trajectory a large angle scattering event took place, causing the breakdown of channeling (dechanneling). The significant energy transfer at the dechanneling location forms the crater and the accumulation of adatom clusters around the crater. In figure 1 and similar topographs, other damage patterns are visible. Most of them can be attributed with little ambiguity to single ion impacts, but for some it is uncertain whether the damage of several impacts overlaps. Also a few lonely adatoms are seen which may originate from the formation of an adatom–vacancy pair created in a terrace impact (although with small probability) or by the long-distance displacement of an adatom of an existing step edge impact damage pattern through a hit by a subsequently impinging ion.

Subsurface channeling of grazing incidence ions has already been discussed for high-energy ions [20, 21], highly charged ions [22] and keV ions [23]. Subsurface channeling of grazing incidence keV ions improves the regularity of ripple patterns forming under prolonged ion exposure at the surface [24, 25]. As was reported in a recent paper by us [26], by performing single-ion impacts with Ar⁺ and Xe⁺ at low temperature, it is now possible to make the full trajectory of channeled ions visible at the surface. Here, we extend this work by reporting on the stopping force, damage production mechanisms and trajectories of subsurface channeled particles as well as the dependence of subsurface channeling on ion energy, ion species and ion incidence angle.

2. Experimental

The experiments have been performed in a variable temperature STM apparatus with a base pressure in the low 10⁻¹¹ mbar range [27]. The sample is a Pt(111) single crystal aligned in the [110] direction with respect to the ion beam. The sample is cleaned by sputtering at room temperature and flash annealing to 1273 K. The differentially pumped ion source is equipped with a Wien filter for mass selection. The ion energy is varied between 1 and 15 keV and the polar angle of incidence θ varies from 78.5° to 88°. The ion flux is measured with a Faraday cup prior to and after ion exposure.

The experimental sequence is the following: firstly, the crystal is sputtered with an ion dose of 0.75 monolayer equivalents (MLE) at 750 K resulting in well-separated hexagonal vacancy islands (cf figure 1) bounded by monatomic steps. One MLE is the fluence equal to the areal density of the surface atoms on Pt(111) (1.504 × 10¹⁹ ions m⁻²). Subsequently, cooling traps are filled with liquid nitrogen. A large trap is used to reduce the overall system pressure to below 1 × 10⁻¹¹ mbar, while a smaller one surrounding the sample and STM prevents adsorption of residual gas molecules on the sample in the STM imaging position. Then the sample itself is cooled down by an evaporator cryostat. Just before ion exposure starts, the sample is briefly flashed to 750 K in order to desorb molecules that might have adsorbed meanwhile. The sample temperature returns quickly to the low temperature needed for ion exposure. The temperature of ion exposure is chosen as low as possible to prevent annealing of the ion-induced surface defects by diffusion but high enough to rule out adsorption of the noble gas species used for ion exposure. For Ar⁺ the surface temperature was set to 62 K, which is well below the onset temperature of single Pt adatom diffusion [28, 29]. For Xe⁺, 115 K is used since Xe starts to adsorb at about 110 K on flat terraces [30]. At 115 K diffusion of single adatoms is unavoidable on a time scale of seconds, but dimers and all larger clusters are still frozen on the experimental time scale [29, 31]. Once the desired temperature is stabilized, ion exposure is started with a
low fluence of $1.3 \times 10^{-3}$ MLE, if not otherwise indicated. After ion exposure the sample is quenched to 20 K for Ar$^+$ and to 105 K for Xe$^+$, respectively. At and below the temperature of ion exposure, surface vacancy diffusion is frozen [32].

A comment regarding STM image interpretation is necessary here. The finite STM tip size strongly affects imaging of adatoms (or small adatom clusters) and surface vacancies (or small clusters of them), but in opposite directions for the two species. Due to tip surface convolution, adatoms and adatom clusters are greatly exaggerated in size (the more, the blunter the tip) and even single adatoms are always visible in the STM images. For the same reason, single surface vacancies are typically invisible to the STM. Additionally, with the nearby adatoms resulting from the ion impacts the tunneling resistance (i.e. the tip surface distance) cannot be chosen too small to prevent imaging instabilities. As the corrugation of the local density of states decays with the tip distance from the surface under these conditions, even a sharp tip does not measure a detectable corrugation above a surface vacancy. Only larger or laterally more extended vacancy clusters give a faint height signal of the order of 0.1 Å; the more pronounced, the sharper the STM tip. To make vacancy structures visible in the topographs wherever information is encoded, the image contrast is greatly exaggerated in the images shown here, and also edge enhancing filters were used.

Based on our MD simulations we know (see below) that for Ar$^+$ the surface vacancy clusters are usually only of monatomic width and consist only of a few vacancies, accompanied by correspondingly small adatom structures. For Xe$^+$ the surface vacancy clusters are considerably larger, form often continuous strings of more than monatomic width and are accompanied by larger, more sparse adatom clusters (also a result of the higher sample temperature during ion exposure not preventing single adatom diffusion). Therefore, on STM topographs after Ar$^+$ ion exposure, usually vacancy clusters are invisible, while after Xe$^+$ exposure, at least a good part of the created vacancy clusters and vacancy strings are visible as faint depressions.

3. The molecular dynamics (MD) procedure

In the MD procedure, the ions are incident along the [110] azimuth. We employ a many-body interaction potential [15] to describe the Pt interatomic interaction, which is splined at the high-energy regime to the Ziegler–Biersack–Littmark (ZBL) repulsive potential [33]. The interaction between the ions and the target atoms is modeled to be purely repulsive according to the ZBL potential. All simulations are performed at 0 K.

The target crystallite has a size of 298 Å along the ion direction and is 86 Å wide, consisting of 18 Pt(111) layers. An ascending step is positioned 120 Å from the crystallite edge; behind the step the crystal extends for 178 Å. In the simulation, we let 5 keV Ar$^+$ and Xe$^+$ ions impinge in front of a kinked step at glancing incidence of 86° (compare with figure 2(a)). A total of 625 ion trajectories were simulated, which varied in the location of the ion impact point with respect to the step edge. The impact area extends up to 75 Å in front of the step, but only 5 Å behind the step. For the defect analysis, we follow the atom trajectories up to 25 ps.

To observe the entrance of an ion into a subsurface channel from the flat Pt(111) terrace, we vary the incidence angle $\vartheta$ of 5 keV ions, and evaluate the trajectories. We identify a trajectory as channeled if the ion stays at least a length of $x_c/2 = d_{111} \tan \vartheta$ inside the crystal. Here, $d_{111}$ denotes the distance between Pt(111) layers. The other trajectories are identified as being reflected or implanted according to the final position of the ion. In this simulation, we use a
Figure 2. (a) Sketch of the simulation geometry for bulk and subsurface channeling (see text). (b) Side view of the trajectory of a \(5\text{ keV} \text{ Ar}^+\) ion performing bulk channeling in the [110] channel. The dashed lines (gray) denote the positions of the (111) planes and the full red line the ion trajectory.

nine-layer target crystallite of length 416 Å in the flight direction of the ion, and of width 86 Å. The impact point of the projectile is varied over a unit cell of the surface mesh to gather sufficient statistics. For each angle, 100 trajectories were simulated. As in this simulation we are interested only in the propagation of the ion, the trajectories are followed only for 1 ps.

Frequently, we specify the stopping force \(dE/dx\) of the primary ion. The stopping force is approximated by the energy loss \(\Delta E\) of the noble gas ion during its trajectory of length \(\Delta x\) inside a channel within our simulation crystallite. For subsurface channeling, we consider only ions that stay in the channel until the end of the simulation crystallite. We evaluate the energy loss of the channeled ions in a length interval of 20 unit cells; our evaluation only starts after a distance of 10 unit cells behind the step. In order to compare the stopping force in subsurface channeling to the one in bulk channeling we simulate the latter process as well. To this end we let ions impinge in the normal direction onto a Pt crystallite with a (\(\bar{1}10\)) surface (compare with figure 2(a)). Of these ions, the so-called channeling fraction will be caught in the axial [1\(\bar{1}0\)] channel. We evaluate the energy loss of the channeled ions in length intervals of 20 unit cells; our evaluation only starts at a depth of 12.5 Å behind the surface to exclude phenomena accompanying the capture of the ion into the channel. In this series of simulations, we use 500 impact events in order to gather sufficient statistical data.

Our simulations do not take into account electronic losses. Neglect of electronic losses (e.g. emission of secondary electrons or electronic coupling to the heat bath) does not change the surface damage formed to any significance. The main effect of this neglect is on the length distribution of the channeled projectiles. However, as well-channeled particles mostly leave our simulation cell, the effect of electronic losses is insignificant compared to the limitations imposed by the size of our simulation cell.

4. Bulk versus subsurface and \(\text{Ar}^+\) versus \(\text{Xe}^+\) channeling

As a reference for the discussion of subsurface channeling, we start our analysis by presenting MD simulations of keV bulk channeling, a phenomenon known since the early 1960s [34, 35] for swift heavy ions and well described by analytical theory [36]. As shown in figure 2(a), we simulate bulk channeling by injecting a particle parallel to the surface plane in a deeper layer.
Figure 3. (a) STM topograph of damage patterns of 5 keV Ar$^+$ incident at $\vartheta = 86^\circ$. The marked chain of adatom clusters decorates a long trajectory. (b) Corresponding MD simulation in top view. (c) Corresponding MD simulation in side view. (d) STM topograph of damage patterns of 5 keV Xe$^+$ incident at $\vartheta = 86^\circ$. (e) Corresponding MD simulation in top view. (f) Corresponding MD simulation in side view. The open dots above the top most crystal layer in (c) and (f) represent the adatoms created. They are located at the $x$-position of their creation. The open blue triangles in (f) represent the additionally sputtered atoms at the $x$-position of their creation. STM image size in (a) and (d) is 580 × 580 Å.

Data taken from [26].

of the crystal along the [1 1 0] direction. By changing the entrance layer depth of the projectile we can monitor the difference between bulk channeling and subsurface channeling. Figure 2(b) displays a 5 keV Ar$^+$ trajectory. The ion moves 12 layers underneath the surface. No damage is created along the ion trajectory and its mean oscillation period is 23 Å. The stopping force of the ion along the trajectory is 1.3 eV Å$^{-1}$.

In figure 3(a), the damage of a subsurface channelled Ar$^+$ ion incident on Pt(111) at $\vartheta = 86^\circ$ is highlighted. Adatoms and clusters thereof decorate the ion trail (for this specific case, we estimate that $\approx 40$ adatoms have been created assuming that the smallest visible ‘clusters’ are single adatoms). The ion trail extends over a length of 320 Å. The damage pattern resulting
from an MD simulation of a comparable event is shown in figure 3(b) as a top view. Similar to what is observed in experiment, a chain of adatom clusters forms along the ion trail. The corresponding surface vacancies next to the adatom clusters are not seen in experiment (compare with the discussion in section 2). The side view of the MD simulation in figure 3(c) displays irregular oscillations of the ion between the two topmost layers with an average period of 33 Å. It is apparent from figure 3(c) that adatoms are created whenever the ion hits the top layer atoms from below. Each adatom created is represented in figure 3(c) by an open dot at the $x$-position of its creation. No damage is formed in deeper layers. For this particular MD event $dE/dx = 1$ eV Å$^{-1}$.

Finally, in figure 3(d) characteristic damage patterns of single 5 keV Xe$^+$ ion impacts are visible. The highlighted damage pattern consists of adatom clusters—similar to 5 keV Ar$^+$—and a continuous groove of surface vacancies aligned along the [110]. In addition to the highlighted long channeling event, also one with a short vacancy groove and two direct step hit events are visible. The adatom clusters after Xe$^+$ ion exposure are more sparse and larger than for the case of Ar$^+$ shown in figure 3(a). Due to the higher sample temperature during ion exposure for the Xe$^+$ case, single adatoms are absent and only clusters of at least two adatoms are imaged. The highlighted Xe$^+$ trail is slightly shorter than the Ar$^+$ trail, indicating a larger stopping force. In agreement with the experiment, the top view of the comparable MD damage pattern shown in figure 3(e) displays a continuous vacancy groove as well. Such vacancy grooves are never observed for Ar$^+$ impacts, neither in experiment nor in MD simulations, while such events are frequent for Xe$^+$ impacts, both in experiment and in simulation. The side view of the MD simulation event in figure 3(f) exhibits a strongly reduced oscillation amplitude and period of the ion trajectory. In addition to the enhanced number of adatoms created (open dots above the surface layer in figure 3(f)), sputtering also takes place (indicated by open blue triangles above the surface layer in figure 3(f)). During the passage through the simulation cell about 30 atoms were sputtered. Close inspection of figure 3(f) reveals that atoms are preferentially sputtered whenever the ion hits the top layer atoms from below (for Ar$^+$ at these locations only adatoms were formed). Adatoms are formed even when the Xe$^+$ ion trajectory in the channel is most distant from the surface (for Ar$^+$ at these locations no damage was created). For this specific event of a well-channeled Xe$^+$ trajectory, we measure $dE/dx = 7.6$ eV Å$^{-1}$.

We performed MD simulations to analyze systematically the stopping force as a function of ion species, depth underneath the surface and also ion energy (the latter will be discussed in section 6) for ions moving in the [110] channel. Figure 4 displays the resulting stopping force data. It is evident that the particular stopping forces for the 5 keV MD events of figure 3 are close to the ensemble averages of 0.76 and 11.1 eV Å$^{-1}$. These averages are very similar to those obtained in our simulations for well-channeled trajectories in the bulk, which are 0.9 and 9.1 eV Å$^{-1}$ for 5 keV Ar$^+$ and 5 keV Xe$^+$, respectively. Xe$^+$ ions suffer an energy loss, which is about one order of magnitude larger than Ar$^+$ ions. This is due to the larger repulsion felt by the Xe$^+$ ions as a consequence of their higher nuclear charge $Z$.

The decrease of nuclear stopping with increasing ion energy exhibited in figure 4 is intriguing since in a random medium the energy loss will increase with ion energy. There exists very little previous published knowledge on the nuclear energy loss of low-energy channeled ions. We are only aware of the work by Andersen and Sigmund [37], who calculated the nuclear energy loss of well-channeled low-energy (sub-keV) ions by considering the simultaneous multiple collision of the ion with the ‘ring’ of atoms bounding the channel. Their results show that the stopping force is maximum at energies of 14 and 100 eV for Ar (Xe) traveling in the
Figure 4. Stopping force of well-channeled Xe\(^+\) and Ar\(^+\) ions as a function of ion energy. The ions fly in a [1\(\bar{1}\)0] channel deep inside the crystal. Black symbols: stopping force of Xe\(^+\) ions which enter a subsurface channel via a step edge at 86° to the surface normal. Unless plotted, error bars are smaller than the symbol size. Data partly from [26]. Lines to guide the eye.

Pt [1\(\bar{1}\)0] channel and then decreases as 1/\(E^2\) with ion energy \(E\). Our results, figure 4, are for considerably higher energies; a power-law fit to our data yields an exponent of 0.8 ± 0.05 for both ions, demonstrating that the agreement with [37] is only qualitative. For high-energy ions (>100 keV, say) Lindhard predicts also the nuclear energy loss of channeled ions to increase [36]; this prediction is based on evaluating individual collisions of the channeled ion with atoms bounding the channel. In our regime of low-energy (i.e. keV) channeling, the main effect of an increased ion energy is an increase in the channel width (cf figure 6(a)); this increases the wavelength of channeled ions in the channel and reduces the number of ion–wall collisions.

While the stopping force and oscillation period of the channeled particles in bulk and just underneath the surface are similar, their damage is not. While damage is absent in Ar\(^+\) and marginal in Xe\(^+\) bulk channeling, damage consisting of adatoms and surface vacancies becomes significant with the channeling trajectory just a few atomic layers under the surface, being strongest for channeling underneath the surface layer. These differences can be traced back to different bonding of surface and bulk atoms. Surface atoms are marginally stabilized against motion normal to the surface if energized from below: there are no atoms above exerting restoring forces. As a consequence the ‘surface displacement threshold’ is similar to the work needed for adatom creation of \(\approx 2.4\) eV in Pt [15]. In contrast, the bulk displacement threshold is \(\approx 37\) eV and thus more than an order of magnitude larger [38]. In consequence, the damage during channeling and dechanneling depends on the depth of the channel inside the crystal.

The marked difference in the damage patterns of 5 keV Ar\(^+\) and 5 keV Xe\(^+\) impacts is apparently due to the Xe\(^+\) stopping force being larger by more than a factor of 10 compared to Ar\(^+\). The more efficient stopping of the 5 keV Xe\(^+\) supplies sufficient energy to individual surface atoms to overcome the sputtering threshold, which is of the order of the cohesive energy for Pt(111) of 5.8 eV atom\(^{-1}\) and thus considerably larger than the threshold for surface vacancy.
adatom pair production of about 2.4 eV. The smaller oscillation amplitude of the channeled Xe\(^+\) ion and the fact that adatoms are formed even at locations where the Xe\(^+\) ion is most distant from the surface appears to indicate that—loosely speaking—the Xe\(^+\) is ‘too big’ for the channel (or the channel is too narrow). Apparently, even if the Xe\(^+\) is most distant from the surface atom in the channel its impact parameter is large enough to transfer more than the 2.4 eV necessary for surface vacancy adatom pair production to surface atoms.

This idea can be visualized and quantified analytically using the shadow cone concept\,[36]. A shadow cone represents the ensemble of trajectories from a binary collision for varying impact parameters. Figure 5 shows the calculated shadow cone for an Xe\(^+\) projectile hitting a Pt atom at rest. A ZBL interaction potential was used to calculate the trajectories. To characterize the size of the shadow cone we specify in figure 5 its radius \(R_{sc}\) at the Pt nearest neighbor distance \(d = 2.78\) Å behind the scattering target atom. A quick estimate of the shadow cone radius can be performed by assuming an unscreened Coulomb potential\,[36]. Here, the radius of the cone \(R_{sc}(d)\) at a distance \(d\) behind the shadowing atom is given by

\[
R_{sc}(d) \approx \frac{2}{\sqrt{4\pi \varepsilon_0 E}} d, \tag{1}
\]

where \(Z_1\) and \(Z_2\) are the atomic numbers of the colliding atoms and \(E\) is the ion energy. It is evident that a high-\(Z\) ion produces a larger scattering shadow cone around the target atom than a low-\(Z\) atom. Our calculations based on a ZBL interaction potential are consistent with this picture and result in \(R_{sc} = 1.45\) Å for 5 keV Xe\(^+\) and \(R_{sc} = 1.23\) Å for 5 keV Ar\(^+\). Consequently, the Xe\(^+\) ion sees a smaller channel and thereby the amplitude of its channeling oscillation is strongly reduced compared to Ar\(^+\). Moreover, the Xe\(^+\) ion moving in the channel will hit the shadow cone of each individual ion at a larger angle, which corresponds to larger momentum and energy transfer.

Figure 5. The shadow cone around a Pt atom (full circle) resulting from scattering of a 5 keV Xe\(^+\) ion. The open circle denotes the position of the next Pt atom in the [1\(\bar{1}\)0] direction, at a distance of \(d = 2.78\) Å. The shadow cone radius at this position measures \(R_{sc} = 1.45\) Å. For a 5 keV Ar\(^+\) ion, the shadow cone is of similar shape, but narrower with \(R_{sc} = 1.23\) Å.
Figure 6. Potential of a 5 keV Xe\(^+\) ion in a channel along the [1\,\overline{1}0] direction calculated within the continuum approximation (see text). (a) Equipotential contour lines. The positions of the atomic strings bounding the channel are indicated by black dots connected by thin grey lines; the lateral axis on which two subchannels form is displayed as a thick gray line. Green, red and black double arrows are discussed in section 5.2. (b) Projection of the continuum potential onto the lateral axis. The two subchannels form at the same positions for Ar\(^+\) and Xe\(^+\) ions, but the energy of the saddle point strongly depends on the ion species.

In the shadow cone picture, a channel is built of strings of overlapping shadow cones one fixed at each atom. In the continuum approximation introduced by Lindhard [36], the scattering from a row of individual atoms is substituted by a continuous potential field. Figure 6(a) shows the result of such a calculation for an Xe\(^+\) ion using the ZBL potential, where equipotential lines are shown. A channeled ion moves almost perpendicular through this cut with a low kinetic energy of motion in the figure plane. This in-plane kinetic energy amounts to

\[ E_\perp = E \cos^2 \vartheta, \]

where \( E \) is the total kinetic energy of the projectile and the angle \( \vartheta \) measures the deviation from the figure plane. An ion impinging at 86\(^\circ\) with an energy \( E = 5000 \text{ eV} \) has therefore an initial \( E_\perp = 24 \text{ eV} \), which corresponds to the inner dumbbell-shaped curve in figure 6(a). On its travels the ion therefore moves in the open space defined by the equipotential curve.

The overall shape of the channel for Ar\(^+\) and Xe\(^+\) is similar, but the width of the channel for an Ar\(^+\) ion with the same \( E_\perp \) is larger. This is visible in figure 6(b), which displays the projection of the continuum potential onto the line connecting the top-right and bottom-left atom strings of a channel, as shown in figure 6(a) with a gray line, the lateral channel axis. Besides the saddle point at the center of the channel axis—its significance for channeling will be discussed in the next section—it is obvious that a 5 keV Xe\(^+\) experiences a much narrower channel than a 5 keV Ar\(^+\), as both are confined to the space bounded by a net potential of 24 eV.

In conclusion, we find that subsurface channeling and bulk channeling are very similar in view of the ion motion through the crystal. However, the damage left behind by the ion differs markedly: while for bulk channeling, damage is usually absent, subsurface channeling leaves a trail of damage on the surface, making keV ion trajectories visible. The nuclear stopping
force of a channeling ion increases dramatically with the projectile nuclear charge and thus has a strong influence on damage and ion trail: for 5 keV Xe\(^+\), large sputtering yields and the formation of continuous vacancy grooves are observed, while both features are absent for 5 keV Ar\(^+\) projectiles.

5. Asymmetric damage, unstable channeling and channeling length

Figure 7(a) shows a damage event with a surface trench and adatom clusters produced by a 5 keV Xe\(^+\) single-ion impact. The corresponding sketch shown in figure 7(b) highlights the surface trench and the position of the adatom clusters. Two interesting observations can be made: (i) the distribution of adatom clusters on both sides of the surface trench is asymmetric. (ii) The surface trench is not straight but displays kinks where apparently the ion switches between different axial channels in a plane parallel to the surface. The same features are found in the MD simulation of a corresponding event represented by figures 7(c) and (d).

5.1. Asymmetry of damage production

We first discuss observation (i), the apparent asymmetry of adatom production. In the STM topograph of figure 7(b), we find seven adatom clusters to the left of the ion trail and five adatom clusters to the right, if viewed in the ion beam direction. A similar event with stronger asymmetry is present in figure 3(d), where nine adatom clusters are on the left and three are on the right-hand side of the vacancy groove. In order to quantify the asymmetry in adatom
production, we analyzed 5 keV Xe$^+$ events displaying a vacancy trench, since for these events the distinction between left and right of the ion trail is unambiguous. Figure 8 visualizes the adatom asymmetry

$$A = \frac{A_{\text{right}} - A_{\text{left}}}{A_{\text{right}} + A_{\text{left}}},$$

where $A_{\text{left}}$ denotes the number of adatom clusters on the left of the trench and $A_{\text{right}}$ denotes that on the right of the trench. As it is experimentally impossible to measure the number of adatoms in a cluster, we refer, for the experimental distribution, to the number of adatom clusters. Adatoms are not present after 5 keV Xe$^+$ impacts as they are mobile at the sample temperature of ion exposure. If adatom clusters showed on average no asymmetry and we had good statistics, the distribution in figure 8 would be a binomial centered at $A = 0$. However, our experimental data show an average asymmetry of $\bar{A}_{\text{ex}} = -0.15$. Using MD events resulting in vacancy trenches our simulations give $A_{\text{MD}} = -0.36 \pm 0.04$; this is in reasonable agreement with experiment when considering the different evaluation procedures. The simulations also provide us with data on the damage asymmetry produced by Ar$^+$ ions. Figure 8 shows a higher asymmetry than for Xe$^+$. The average asymmetry for Ar$^+$ amounts to $A_{\text{MD}} = -0.40 \pm 0.05$.

The asymmetry of adatom creation can be traced back to the asymmetric shape of the $\langle 110 \rangle$ channel as shown in figure 6(a). The asymmetric channel shape implies an asymmetry of the ion trajectories with respect to the atomic rows bounding the channel towards the surface. Our MD simulations even show that, depending on the impact position at the step edge, the ion primarily uses different regions of the dumbbell channel. Figure 9 shows exemplary Xe$^+$ trajectories (a) propagating in the lower subchannel, (b) moving back and forth between two subchannels and (c) propagating in the upper subchannel. The manner in which an ion propagates in a subsurface channel correlates with the form of the damage created on the surface. In case (a), the ion effectively interacts only with surface atoms in the upper left row (compare with figure 6(a)). This will cause the formation of a single-row surface vacancy trench and adatom deposition to
Figure 9. Exemplary trajectories of Xe$^+$ ions propagating inside the [110] subsurface channel. The three cases selected exhibit motion in the (a) lower subchannel, (b) both subchannels and (c) upper subchannel. In each case, we display a cross-sectional view as in figure 6(a) (the ion moves into the paper plane), a top view showing the damage produced at the surface (the ion moves from right to left) and a side view (red: ion trajectory; gray: (111) lattice planes; dashed: saddle-point plane separating subchannels). For these cases the asymmetry amounts to (a) $A = -1$, (b) $-0.3$ and (c) $+0.24$.

the left of the trench resulting in an asymmetry $A = -1$. In case (c), the ion propagates in the upper subchannel between two surface atomic rows. Accordingly, a trench with double-row width and less anisotropic adatom distribution is created. More adatoms are found on the right-hand side resulting in $A = +0.24$. In case (b), when the ion is moving in both subchannels an intermediate asymmetry of $A = -0.3$ results.

To obtain a deeper insight into the subchannel motion, we focus now on the continuum potential along the lateral channel axis as shown in figure 6(b). A saddle point is located in
Figure 10. Exemplary trajectories of Ar$^+$ ions propagating inside the [1$\bar{1}$0] channel. Analogous presentation to figure 9; however, due to the low saddle-point barrier, trajectories are never confined to one subchannel only. (a) The ion slowly switches between the lower and the upper subchannel. In the lower subchannel, it creates no damage; after switching to the upper subchannel adatoms are created only on the left-hand side. (b) The ion oscillates more quickly between the two subchannels. In this case, adatoms are produced also on the right-hand side; this occurs when the ion moves in the upper subchannel close to the saddle-point plane.

The middle of the channel, forming a barrier of around 10 eV in the case of Xe$^+$. In the energy range under consideration, an ion can easily overcome this barrier whenever the polarization of the oscillatory motion is nearly parallel to the axis. In order to maintain its motion inside a subchannel, the ion must constrain the polarization perpendicular to the axis and keep the projection of its kinetic energy below the barrier. As a consequence, it experiences almost central collisions with atoms in the top-left string. Consequently, surface atoms on the left-hand side of the channel are knocked out resulting in a left-biased adatom distribution. This mechanism operates both in the lower and upper subchannels. However, in the upper subchannel an ion may also interact with top-right atoms (cases (b) and (c) in figure 9), which makes the adatom distribution more slightly asymmetric to the right. This situation applies particularly to the heavy ion (Xe$^+$).

For the lighter Ar$^+$ ion the barrier is lower, as can be seen in figure 6(b). The Ar$^+$ ion can move more freely inside the channel, switching between subchannels frequently. This situation makes it difficult to confine an Ar$^+$ ion within only one subchannel for a long propagation distance, cf figure 10. Nevertheless, the influence of the ion’s polarization is analogous to that
discussed for the Xe\textsuperscript{+} ion above. Figure 10 shows exemplary trajectories of Ar\textsuperscript{+} ions, together with the created damage and a side view of the trajectories. In figure 10(a), the ion oscillation has a strong polarization perpendicular to the lateral channel axis, and hence adatoms are created on the left-hand side (negative asymmetry). Figure 10(b) gives an example of an ion with a rather high polarization along the lateral channel axis; in consequence, adatoms are produced on both sides, with a slightly positive asymmetry in the present case.

5.2. Hyperchanneling and unstable channeling

We will now focus on observation (ii), the switching of ions between different channels while moving. Already in their early computer simulations Robinson \textit{et al} \cite{35} observed channeling events where the ion switches between different atomic strings without violating the channeling condition. We therefore make a distinction between hyperchanneling (also called proper channeling) where the ion motion is confined to a single channel, and unstable channeling in which the ion switches the channel in one layer or between channels of different layers. The reason for the possibility of channel switching is that the potential at the saddle point between the atomic strings is smaller than the critical value of the potential for ‘normal’ axial channeling. We note that the saddle points for channel switching (arrows in figure 6(a)) amount to about 350 eV for Xe and 150 eV for Ar. In figure 6(a), double arrows indicate three different options for channel switching of a subsurface ion in the [1\bar{1}0] channel: (1) The ion switches the channel in plane and remains underneath the first atomic layer, as observed in figure 7(a) and indicated by black double arrows; (2) the ion moves between channels underneath the first and the second atomic layer as indicated by a red double arrow; (3) the ion moves between the subsurface channel and the surface as indicated by the green arrow.

In this section, we discuss cases (1) and (2), while case (3) is analyzed in section 7.

In experiment, we find the absence of lateral channel switching (case (1)) for 30\% of the channeling trajectories; this was assessed by confirming that the vacancy trenches showed no kinks. In order to compare to the MD simulations, we analyze the well-channeled Xe\textsuperscript{+} trajectories, i.e. those which remained channeled throughout our simulation crystallite. Among these we find that 89\% are hyperchanneled, i.e. they do not switch channel.

Although lateral channeling switching is observed in experiment and simulation, the quantitative discrepancy between the two needs some discussion. An experimental uncertainty is the identification of a kink in a vacancy groove with a channel switch. Subchannel switches also give rise to small kinks in vacancy grooves, which could be misinterpreted in the experimental data analysis as channel switch events. Moreover, hyperchanneling is sensitive to the azimuthal orientation of the crystal with respect to the ion beam. The accuracy of the azimuthal orientation in experiment is only $\pm 3^{\circ}$. This is already of the magnitude where Fang \textit{et al} \cite{39} observe changes in the hyperchanneling probabilities for 4 keV Ne ions in Pt.

The theoretical criterion for hyperchanneling relies on the absence of channel switching within the channeling length of 178 Å within the cell. As more than 60\% of the ions escape the simulation cell this criterion therefore considerably underestimates channel switching. Moreover, typically the ions leave the simulation cell with more than 3 keV kinetic energy. It may well be that channel switching becomes more likely towards the end of the ion trajectory, when the ion has already slowed down considerably. Channel switching is sensitive to thermal vibrations \cite{39} and the simulations neglect quantum mechanical zero point vibrations and are performed at 0 K instead of 115 K.
Figure 11. (a) STM topography of 5 keV Ar\textsuperscript{+} single-ion impact. (b) Sketch highlighting the adatom clusters; the dashed line indicates the trajectory of the ion. Image size: 640 × 260 Å. (c) Top view of the corresponding MD simulation. The adatoms are distributed rather sporadically around the ion trajectory; this is typical if the ion penetrates deeper into the crystal. (d) Side view of the ion trajectory. The ion is penetrating down to the third layer below the surface.

Now case (2) is analyzed, the switching of ions between channels underneath the surface at different depths. Figure 11(a) shows the damage pattern of a 5 keV Ar\textsuperscript{+} ion impact. Figure 11(b) gives a schematic representation of the damage pattern. The image shows the ion trail starting at the ascending step edge in the lower left corner of figure 11(a). After a distance of 250 Å the trail crosses a descending step edge of a hexagonal vacancy island. If subsurface channeling would be confined between the first and the second layer the adatom production should stop here, as the ion would escape from the crystal at this place. However, adatom and adatom clusters continue to be present in the line of the initial trail within the vacancy island and even on the terrace behind the vacancy island. From the damage distribution it is evident that the ion has entered a channel at least two layers underneath the surface prior to arriving at the descending step edge.

The same phenomenon is also observed in the MD simulations as visualized through the damage pattern and the ion trajectory of the event of figures 11(c) and (d). Whereas in the surface view of figure 11(c) adatoms and surface vacancies are visible, the side view of the crystal (figure 11(d)) with the ion trajectory displays its switching between layers without violating the channeling condition. For 5 keV Ar\textsuperscript{+}, we observed some trajectories to move down to the 10th layer, while 5 keV Xe\textsuperscript{+} ions only arrive down to the fourth layer. The larger channel for Ar\textsuperscript{+} implies a smaller potential at the saddle point between different channels and thus a smaller \(E_{\perp}\) is sufficient for Ar\textsuperscript{+} projectiles to change the channel.

5.3. Channeling length

Since ion trails display a large diversity as a function of the ion impact position at the step edge, they also exhibit a broad distribution in trail length. Figure 12 shows the experimental and
Figure 12. Ion trail length distribution of 5 keV Xe\(^+\) with \(\vartheta = 86^\circ\) from experiment (gray bars) and from MD simulation (red bars). The probability \(P(x)\Delta x\) to find a channeling length \(x\) in a bin of width \(\Delta x = 10\ \text{Å}\) is plotted. In the simulation, only trails exceeding a length of 27 Å have been recorded.

simulated trail length distributions of 5 keV Xe\(^+\) with \(\vartheta = 86^\circ\). In experiment, most impacts have a short trail with a most probable length between 30 and 40 Å. The experimental distribution in figure 12 spreads far out to long distances of up to 400 Å corresponding to well-channeled projectiles. Our MD simulations reproduce the experimental distribution qualitatively up to trail lengths of 170 Å. The artificial peak representing events with trail lengths between 170 and 180 Å contains all events that have left the simulation cell after a channeling length of 178 Å.

We note that in experiment the probability for short trail lengths is systematically higher than in the simulation. The neglect of electronic stopping in the MD simulations as well as the presence of thermal vibrations in the experiment at 115 K—the substrate temperature of ion exposure—tends to diminish the experimental compared to the simulated trail length. Also experimental limitations in the precision of the azimuthal crystal orientation, crystal impurities and adsorbates will all tend to diminish the experimental channeling length.

6. Energy dependence of subsurface channeling

We now discuss the energy dependence of subsurface channeling for the case of Xe\(^+\) impinging with \(\vartheta = 86^\circ\). Figure 13 shows the evolution of the damage for ions with energies ranging from 1 to 15 keV. For 1 keV ions, the induced damage is located exclusively at the step edge as shown in figure 13(a). Not a single vacancy trench is observed. For 2.5 and 5 keV Xe\(^+\) ions, well-developed vacancy trenches are present as shown in figures 13(b) and (c). For 10 and 15 keV Xe\(^+\), the ion trails increase in length as shown in figures 13(d) and (e) (note the smaller magnification of figure 13(e)), but the vacancy grooves are not as well developed at the beginning of the trajectory as for 2.5 and 5 keV. This is particularly visible in figure 13(f), which displays the end of the ion trail of figure 13(e) in a magnified view. Apparently the
Figure 13. STM topographs after low fluence Xe$^+$ ion exposure at $\vartheta = 86^\circ$ at different ion energies of (a) 1 keV, (b) 2.5 keV, (c) 5 keV, (d) 10 keV and (e) 15 keV. Topograph (f) is a zoom-in of (e). Image sizes are, for (a)–(d) and (f), 580 × 580 Å and, for (e), 1300 × 1300 Å. Inset in (a): 1.25 keV Ar$^+$, image size: 310 × 180 Å.

damage pattern changes along the trail as the ion energy decreases: surface vacancy production evolves from separated surface vacancy clusters at the beginning to continuous vacancy trenches at the end of the trajectory. We note that in figure 13(e) two trajectories are visible, which cross a descending step edge. This indicates that deeper layer channeling becomes more probable for higher ion energies.

The energy-dependent damage evolution for Ar$^+$ is quite similar, with ion trail lengths increasing with ion energy. However, while channeling is absent for 1.0 keV Xe$^+$ ions (figure 13(a)), the inset of figure 13(a) shows that even for the lowest ion energy of 1.25 keV used for Ar$^+$, we still observe well-developed ion trails. This demonstrates that channeling still takes place for Ar$^+$ ions at our lowest energy.

To understand the breakdown of subsurface channeling at low energies for Xe$^+$, we will recall key results of the Onderdelinden theory of bulk channeling [40]. According to the theory the ion beam hitting the surface (usually at non-grazing angles) along a low index direction can be divided into the channeling and the non-channeling fraction resulting from the random distribution of the ion impact parameters. The channeling fraction will penetrate the surface layer and will be steered deep into the crystal along an axial channel formed by atomic rows. This fraction is lost for sputtering. Sputtering is due to the non-channeled fraction,
Figure 14. Channeling fraction $\eta$ as a function of the ion energy $E$ for Xe$^+$ and Ar$^+$ ions impinging under an angle $\alpha = 4^\circ$ with respect to a [110] direction. Symbols: simulation results for Xe$^+$ impact. Lines: Onderdelinden theory (A.5).

which undergoes large angle scattering processes with the surface atoms. As the shadow cone diameter of a single atom increases with decreasing ion energy (see (1)), the channeling fraction decreases. Based on the calculations in the appendix (see (A.5)) figure 14 shows the dependence of the channeling fraction $\eta(Z_2, E, \alpha)$ on ion energy $E$ along the [110] direction in Pt for Ar$^+$ and Xe$^+$ ions. For the calculation, we assumed an angle of incidence $\alpha = 4^\circ$ with respect to the atomic strings forming the channel corresponding to our experimental $\vartheta = 86^\circ$. We note that the results for $\alpha = 0^\circ$ and $4^\circ$ are almost indistinguishable on the scale of figure 14.

The channeling fraction decreases from $\eta = 0.7$ for 15 keV Xe$^+$ to $\eta = 0$ for 1.1 keV Xe$^+$. This result is in good agreement with our experimental observation that channeling for Xe$^+$ ceases between 1.0 and 2.5 keV. Due to the smaller nuclear charge of Ar$^+$, at a given energy the channels are wider for this projectile and channeling vanishes only at 500 eV. Again this finding is consistent with our observation of channeling Ar$^+$ ion trails at ion energies as low as 1.25 keV.

Our simulations of bulk channeling, in which ions impinge in the normal direction onto a ($\bar{1}10$) Pt crystal, allow us to obtain data on the channeling fraction. In figure 14, we compare our simulation data for Xe$^+$ and Ar$^+$ impacts with (A.5). It is seen that the analytical result predicts the main trend and the order of magnitude of the channeling fraction correctly. The simulations also corroborate our experimental finding on the absence of channeling for 1 keV Xe$^+$. While the above results apply to bulk channeling, we find that 1 keV Xe$^+$ ions are also unable to enter the crystal via a step edge. The reason for this is as follows. The 1 keV Xe$^+$ incident with $\vartheta = 86^\circ$ is reflected at a rather great height (minimum approach distance is roughly 2.3 Å) through repulsive interaction with the surface. Accordingly, the ion is just focused on the step atoms of the upper terrace, but does not approach close enough to be able to reach the channel between the upper and lower terraces at the step. In consequence, we observe only typical step erosion damage as in figure 13(a).

To discuss trends of the damage pattern evolution with ion energy semi-quantitatively, we analyzed for each ion energy the five events with the longest ion trails within our limited
Figure 15. Full squares and left ordinate axis: trail length $l_{\text{trail}}$ as a function of Xe$^+$ ion energy. Open triangles and the right ordinate axis: density of adatoms and adatom clusters per unit trail length $\rho_{\text{Ad}}$ as a function of Xe$^+$ ion energy $E$. All quantities are averages over the five longest trails for each $E$ out of the respective experimental data sets. The lines are a guide to the eye.

set of data. This circumvents difficulties related to the broadness of the channeling length distribution (compare figure 12) and ambiguities in the identification of events. The result is shown in figure 15 where the average trail length of these events $l_{\text{trail}}$ is plotted versus the ion energy $E$ (full square symbols). The data confirm the increase of trail length with increasing ion energy, as already visible in the STM topographs of figure 13. Up to 10 keV the trail length increases more strongly than linearly with ion energy, which is indicative of a decrease of $dE/dx$ (cf also section 4 and figure 4). For 15 keV ion energy, the trail length exceeds the average initial terrace width of our sample, which may have partly suppressed the presence of long trails (note, however, the 15 keV event in figure 13(e) with a length of 1300 Å passing over two terraces). The assumption of a decrease of $dE/dx$ with ion energy is supported by the analysis of the density of adatoms and adatom clusters per unit trail length, $\rho_{\text{Ad}}$, as plotted in figure 15. For an energy-independent stopping force $dE/dx$ we would expect a constant $\rho_{\text{Ad}}$. The decrease of $\rho_{\text{Ad}}$ with ion energy in figure 15 thus supports the assumption of a decrease of $dE/dx$ with increasing $E$. The sharp drop from 1 to 2.5 keV visualizes the transition from step edge impacts to subsurface channeling.

We note that the trail length $l_{\text{trail}}$ averaged over the five longest events from our data sets is 330 Å for 2.5 keV Ar$^+$ and only 120 Å for 2.5 keV Xe$^+$. The ratio three in trail length of the two ion species reflects the strong difference in stopping force for Ar$^+$ and Xe$^+$. An extension of this analysis for higher Ar$^+$ ion energies is subject to large errors as the trails become extended over too large a distance to unambiguously identify their length.

As is apparent in figure 4—the MD simulation results for the stopping force—the stopping force substantially decreases with ion energy up to ion energies of about 10 keV and then appears to saturate. The stopping force $dE/dx$ of Xe$^+$ particles entering from the step edge and channelled within the entire simulation cell decreases from 11 eV Å$^{-1}$ at 5 keV via 4.6 eV Å$^{-1}$ at 10 keV to 3.7 eV Å$^{-1}$ at 15 keV consistent with our qualitative observations.
Figure 16. MD damage patterns after (a) 10 keV and (b) 15 keV Xe\(^+\) impact. The excess of surface vacancies over adatoms is due to sputtering.

In the discussion of figures 13(d)–(f), it was noted that for 10 and 15 keV Xe\(^+\) the vacancy groove is not developed at the beginning of the trajectory and only becomes continuous towards its end. In our MD simulations for 10 keV projectiles, we do not find any double-row trenches and for 15 keV Xe\(^+\) even the continuous single-row trenches have disappeared. Two characteristic MD damage patterns at these ion energies are shown in figure 16. The strong reduction in energy loss by increasing the ion energy from 5 to 10 keV and above is the reason for the reduced damage production. As the ion energy decreases along the trails below 5 keV, the energy loss increases and the continuous vacancy trench at the end of the 15 keV Xe\(^+\) trails shown in figure 13(e) and magnified in figure 13(f) results.

The apparent increase in deeper layer channeling and channel switching is a simple consequence of an increase of \(E_\perp\) with ion energy, giving the projectile a higher probability to transit the saddle point between different axial channels. Increasing the Xe\(^+\) projectile energy from 5 to 15 keV increases \(E_\perp\) from 24 to 73 eV. From our MD simulations, we also find the fraction of trajectories with channel switching to increase with ion energy. In the next section, it will be shown that increasing \(E_\perp\) for 5 keV Xe\(^+\) by decreasing \(\vartheta\) may have an even more dramatic effect on channel switching.

7. Angular dependence of subsurface channeling

The angular dependence of subsurface channeling is investigated for 5 keV Xe\(^+\) from \(\vartheta = 88^\circ\) to \(\vartheta = 78.5^\circ\). Figure 17(a) shows experimental results for \(\vartheta = 83^\circ\), figure 17(b) and (c) for \(\vartheta = 80^\circ\) and figure 17(d) for \(\vartheta = 78.5^\circ\). It is apparent that with decreasing \(\vartheta\) the damage on terraces not related to step edge impacts increases. Specifically for \(\vartheta = 80^\circ\) and even more pronounced for \(\vartheta = 78.5^\circ\), a large number of adatoms is visible, which can only be attributed to terrace impacts. Due to the increase of \(E_\perp\) from 24 eV for \(\vartheta = 86^\circ\) to 199 eV for \(\vartheta = 78.5^\circ\) adatom production by terrace impacts becomes significant. This is consistent with our previous MD simulations related to the \(\vartheta\)-dependence of terrace damage [18].

More striking is the presence of vacancy trenches in figures 17(c) and (d) for \(\vartheta = 80^\circ\) and \(\vartheta = 78.5^\circ\), which start on the terrace and are unrelated to ascending step edges. For \(\vartheta = 80^\circ\) their number is still very limited, but for \(\vartheta = 78.5^\circ\) most visible trenches start on the flat terrace as visualized by figure 17(d).
For decreasing $\vartheta$, surface channeling loses its hyperchanneling property and a ‘channel switch’ from the surface to an axial [110] channel below the surface becomes possible. This is case (3) of channel switching and indicated in figure 6 by a green double arrow. The ion moves from the surface at the potential saddle point between two atomic strings to a subsurface channel. This behavior is well known from previous surface channeling experiments [19, 41]. From computer calculations, Danailov et al [19] deduced the total reflection from Pt(111) along the [110] direction to break down for $\vartheta \approx 79^\circ$ in reasonable agreement with our experiments.

In order to corroborate our experimental finding, we analyzed the damage on the flat terrace by MD simulations. Figure 17(e) displays the simulated damage pattern of a 5 keV Xe$^+$ impact for $\vartheta = 78.5^\circ$. The ion penetrated the crystal surface smoothly and then channeled underneath the surface layer, thereby creating a surface trench. In total 24% of all ions hitting the flat
terrace at an angle of 78.5° penetrate the crystal surface and create a channel during subsequent subsurface channeling. For \( \vartheta = 80^\circ \) within the limited statistics of our MD simulations we do not find trench formation by terrace impacts.

The slightly smaller \( \vartheta \) for trench formation by terrace impacts found in the MD simulations compared to experiment may be rationalized by (i) the absence of vibrations in the MD simulation that ease ion penetration and (ii) the experimental uncertainty in polar angle of about one degree. A slight deviation from the precise [110] direction may also ease ion penetration.

8. Influence of temperature on subsurface channeling

Finally, we discuss briefly the temperature dependence of subsurface channeling for the case of 5 keV Xe\(^+\) for \( \vartheta = 86^\circ \). Figure 18 shows two experiments performed at (a) 115 K and (b) 323 K. In both cases damage patterns of long channeling events are visible. However, the number of adatom clusters visible is drastically decreased in case (b). While the surface trench formed at low temperatures appears to be continuous and is decorated by adatoms, near room temperature disconnected vacancy islands extending along a straight line are visible. Apparently subsurface channeling still takes place at 323 K, but adatom and adatom clusters diffuse and anneal efficiently with surface vacancies. Moreover, vacancy grooves reshape by thermally activated processes and break up into compact surface vacancy clusters. Due to the relevance of thermally activated processes for the appearance of the damage patterns, comparison to MD simulations is no longer meaningful as the time scale of thermal diffusion processes (seconds) is out of range for MD simulations. Ion exposure of Pt(111) at 450 K no longer shows features that can be unambiguously attributed to subsurface channeling. For such temperatures subsurface channeling mirrors itself only indirectly in the evolution of surface morphology after larger ion fluences [18, 24, 42].

9. Conclusion

Using the grazing incidence geometry, we systematically analyzed individual trails of keV ions by STM after low-temperature and low-fluence ion bombardment. A one-to-one comparison of
these frozen damage patterns to MD simulations is made. Under grazing incidence ions enter the crystal at ascending step edges and perform channeling in axial channels parallel to the surface plane. This subsurface channeling may be understood along the same lines as bulk channeling, in view of energy and ion species dependence as well as with respect to hyperchanneling and channel switching. This leads to a unique opportunity to study hyperchanneling versus unstable channeling, as well as energy, angular and temperature dependence of channeling by analyzing the surface damage. Subsurface channeling is distinct from bulk channeling by the ease of damage production at the surface, which creates the ion trail, i.e. the surface image of the ion trajectory. For \( \text{Ar}^+ \) and \( \text{Xe}^+ \) ions we identify trails with lengths of more than 1000 Å.

Most striking, for 5 keV \( \text{Xe}^+ \) we observe continuous vacancy trenches along the ion trajectory. For decreasing angle of incidence we observe the breakdown of surface channeling and ion penetration on the flat terrace followed by subsequent subsurface channeling. We believe that our investigations open up a new window for the investigation of the ion–solid and ion–surface interaction.

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Appendix. Calculation of the channeling fraction \( \eta \)

The channeling fraction can be estimated by following Onderdelinden’s analysis \([40]\), which is based on the channeling theory of Lindhard \([36]\). The description relies on the continuum approximation, which assumes that an ion hitting a string or a plane of atoms does not scatter at individual atoms but at many atoms simultaneously. If an ion hits a string of atoms under very grazing incidence conditions, this assumption is certainly valid in channeling. An increase in the angle of incidence \( \alpha \) with respect to the strings of atoms leads to an increase in the transverse energy. It is clear that at some point the continuum approximation breaks down and the ion scatters at individual atoms. The maximum transverse energy determines the maximum angle \( \alpha_{\text{crit}} \), which is identical to the well-known critical angle for channeling,

\[
\alpha_{\text{crit}} = \left( \frac{3e^2a^2Z_1Z_2}{4\pi \varepsilon_0 E_i^3t_{uvw}^3} \right)^{1/4}.
\]  

(A.1)

Here, the distance between two atoms in the string is denoted by \( t_{uvw} \), and the Thomas–Fermi screening length is given by

\[
a = \left( \frac{9\pi^2}{128} \right)^{1/3} \frac{a_0}{\left( Z_1^{2/3} + Z_2^{2/3} \right)^{1/2}},
\]

(A.2)

where \( a_0 \) is the Bohr radius and \( Z_1 \) and \( Z_2 \) are the atomic numbers of the target and the ion. In our case \( \alpha_{\text{crit}} \) is 18.7° for 5 keV \( \text{Xe}^+ \) and 14.9° for 5 keV \( \text{Ar}^+ \).

The ion beam is divided into two components, namely the channeling fraction \( \eta \) and the non-channeling fraction \( \chi = 1 - \eta \). The non-channeling fraction \( \chi_{uvw}^0 \) for a perfectly aligned beam along the crystallographic direction \([uvw]\) equals

\[
\chi_{uvw}^0 = \pi N t_{uvw}^{3/2} \left( \frac{3e^2a^2Z_1Z_2}{4\pi \varepsilon_0 E_i} \right)^{1/2},
\]

(A.3)
where $N$ is the atomic density. The non-channeling fraction $\chi_{uw}$ for an ion beam that hits the atomic string under a small angle $\alpha$ is

$$\chi_{uw} = \frac{\chi_{uw}^0}{1 - (1 - \chi_{uw}^0) \cdot \left(\frac{\alpha}{\alpha_{crit}}\right)^2},$$  \hspace{1cm} (A.4)

where $f$ is a fitting parameter. In this case it is set to unity. This results in the channeling fraction $\eta$ along a certain crystallographic orientation of the crystal

$$\eta = 1 - \frac{\chi_{uw}^0}{1 - (1 - \chi_{uw}^0) \cdot \left(\frac{\alpha}{\alpha_{crit}}\right)^2}.$$  \hspace{1cm} (A.5)

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