Scattering and recoiling mapping of the Kr-Pt(111) and Ne-Ni(111) systems by SARIS*

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The technique of angle resolved mapping of scattering and recoiling imaging spectra (SARIS) combined with computer simulations is demonstrated to be a valuable tool for characterization of atomic collision events on surfaces. The energy distributions of scattered Kr and Ne and fast recoiled Pt and Ni atoms from Pt(111) and Ni(111) surfaces were measured as a function of exit angle. The use of a large area microchannel plate (MCP) detector and time-of-flight (TOF) techniques decreases the collection time and increases the number of detected trajectories above that of other designs. Classical ion trajectory simulations using the three-dimensional scattering and recoiling imaging code (SARIC) are used to simulate the kinematics of the scattering and recoiling particles. It is shown that SARIS mapping allows one to probe the kinematics of both scattered and recoiled particles, the probability for their occurrence in specific trajectories, and the atomic layers from which the particles originate. [DOI: 10.1380/ejsnt.2004.93]

Keywords: Low energy ion scattering spectrometry; Scattering and recoiling imaging spectrum (SARIS); Time-of-flight (TOF) technique; Ion trajectory simulation; Pt; Ni

I. INTRODUCTION

Ion beams impinging on solid surfaces have been extensively investigated for applications to materials processing, fabrication techniques, and analysis of solid structures. Low energy ion scattering spectrometry with time-of-flight (TOF) detection has been used extensively to study the composition and structure of surfaces. Recently developed large solid angle detection instruments for scattering and recoiling imaging spectrometry (SARIS) [1, 2] provide spatial- and time-resolved, element-specific images from surfaces that directly expose the three-dimensional anisotropy of keV scattered and recoiled atoms. The technique has been used for structural information, compositional analysis of surfaces, and ion fraction mapping [3–6].

It is known that the ordered arrangement of atoms may strongly affect the energy and spatial distribution of recoils ejected from targets under ion bombardment. In keV ion bombardment the majority of the sputtered atoms have energies of only a few eV. These abundant low-energy atoms can arise from several atomic layers and can overshadow the features of high-energy recoiled particles from first few surface layers. Most angle-resolved secondary particle spectrometric studies have focused on the properties of particles sputtered from the surface with kinetic energies less than ~ 200 eV. To our knowledge, only a few angular resolved experimental studies have been performed on the ejection of high-energy particles [7–16]. Computer simulations of ion-surface collision processes have undergone extensive development in the past two decades. These simulations are a complementary source of information that provides valuable insight into the microscopic collision details. The recently developed scattering

and recoiling imaging code (SARIC) [17, 18] is a classical ion trajectory program that simulates two-dimensional scattering and recoiling patterns and provides quantitative interpretations of ion scattering and recoiling images from SARIS.

The purpose of this paper is to introduce high-precision angle-resolved mapping of scattered and recoiled particles with a large area detector, combined with computer simulations, as a quantitative tool for characterization of scattering and recoiling events on surfaces. In contrast to analysis of scattering features, there have been very few studies [13, 14, 19–21] focused on the relationship between the kinetic energies of recoiled particles and the emission angles, which, in the azimuthal distribution of these particles, reflects the geometric structure of the surface. Herein we present experimental and simulated results of Kr⁺ incident on Pt(111) and Ne⁺ incident on Ni(111) surfaces for the angle-resolved mapping of recoiled particles with a large area detector, combined with computer simulations as a quantitative tool for characterization of scattering and recoiling events on surfaces. Most of the details of the experimental/simulation techniques have been published elsewhere [16].

II. METHODS

The experiments were performed in an ultra high vacuum chamber with a base pressure $\sim 5 \times 10^{-10}$ Torr. All measurements were made with the sample at room temperature in a SARIS spectrometer that has been described elsewhere [1–5, 16]. Briefly, a pulsed ion beam [22] scatters and recoils atoms from the surface. The velocities of the keV ejected atoms and ions are analyzed by measuring their flight times from the sample to a rectangular position sensitive MCP detector [23] with a sensitive area of 3.5×4.5 cm². The detector is gated so that it can be activated in windows of ~ 4 μ s duration that are appropriate for collection of specific scattered or recoiled atoms. The velocities (energies) of scattered and recoiled particles are analyzed by measuring their flight times from the sample to the MCP using a multiple-stop time-to-digital

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FIG. 1: Geometry of the SARIS experiment and SARIC calculation. α - incidence angle, ξ - angle between incident beam and plane of MCP, β - variable emission angle, $\theta_p = \alpha + \beta_p$ - scattering/recoiling angle varying between θ_{min} and θ_{max} and corresponding to pixel p on the MCP, and $h = 13$ cm - distance to the detector (at the position of the normal at θ_0) which is used for the SARIC calculation.

converter. The detection efficiencies of neutrals and ions is comparable in this energy range.

The Pt and Ni single crystals in the form of 1×9 mm disks were polished within 0.5° of the $[111]$ direction and cleaned by repeated cycles of 3 keV Ar^+ sputtering and annealing. The surfaces were considered clean and well ordered when no impurity features were observed in the SARIS images and the LEED images exhibited sharp (1×1) patterns. The pulsed, mass-selected ion beam has a duoplasmatron ion source [22] that produces beam spot sizes down to 1 mm^2 with energies variable over the range 3-25 keV and a final energy spread of < 50 eV. A two step pulsing system produces pulsed beam widths < 30 ns and an average pulsed beam current of 10-100 pA. The 64×64 pixel MCP is mounted on a triple-axis goniometer [24] so that it can be positioned at different angles relative to the sample surface. Details of the angular notations are shown in Fig. 1.

Ion trajectory simulations from the SARIC [17, 18] program were used to calculate the angle-resolved energy distributions of scattered atoms and recoils. It describes the interactions between atoms and follows the trajectories of all scattered and recoiled atoms in three-dimensions, thereby capturing both in- and out-of-plane single and multiple collision events. Surface Debye temperatures, as estimated by Jackson [25], were used to generate the three-dimensional thermal vibrations of atoms around their equilibrium positions as in our previous work [26].

III. RESULTS

A. Contour plots of angular distributions for $\text{Kr}^+ \rightarrow \text{Pt}(111)$

Experimental two-dimensional contour plots of the scattering and recoiling intensities as a function of the scattering and recoiling angles and flight times for 10

FIG. 2: Experimental SARIS (a, b) and simulated SARIC (c, d) two-dimensional contour plots of the scattering (a, c) and recoiling (b, d) intensities as a function of the scattering/recoiling angle and flight time for the Pt(111) surface. Beam: 10 keV Kr^+ ; Incidence angle: 27° . The number of detected trajectories increases from the white to the black color. The main features can be separated into scattering (s_i) and recoiling (r_i) traces. (e, f) Comparison of experimental results (open circles), SARIC calculations (solid circles), and various curves obtained using Eqs. (1) and (2). Seven observed collision sequences are shown schematically with explanations given in text.

keV Kr⁺ scattering from Pt(111) are shown in Fig. 2 as extracted from SARIS frame analysis. A horizontal cut through the figure gives an energy distribution at a fixed emission angle and a vertical cut gives an angular distribution at fixed energy (or fixed TOF). Figure 2(a) presents the experimental angular distribution of scattered Kr particles, while Fig. 2(b) consists of the distribution of recoiled Pt particles. Here we use the term ‘particles’ to represent scattered and recoiled atoms plus ions. The main features can be separated into scattering ($s_1 - s_4$) and recoiling ($r_1 - r_3$) traces. As will be shown later, s_1 and r_1 can be described as quasi-single scattering and recoiling collision events, while $s_2 - s_3$ and $r_2 - r_3$ include two or more large-angle collision events. s_4 is a small quasi-single scattering contribution from the ⁸³Kr isotope. Angle versus TOF scattering and recoiling

mapping distributions were also obtained from the simulations. The calculated contour plot distributions of the scattered and recoiled particles can also be separated into three scattering ($s_1 - s_3$) and four recoiling ($r_1 - r_4$) traces as shown in Figs. 2(c)(d).

B. Separation of collision sequences and fractional yields

Classical kinematical analysis is particularly useful in studying the details of the scattering and recoiling events since the observed particles leave the surface as a result of individual primary impacts, the associated cascades are not complex, and the ejected atoms are mainly from the first layer. The well known kinematical description of collisions [2, 27, 28] provides information about the final energies and scattering angles of interacting particles. The energies of scattered and recoiled atoms in an elastic collision can be determined from the conservation of energy and momentum as

$$E_S = E_0 \times \prod_i f_S(\theta_i), \quad (1)$$

and

$$E_R = E_0 \times \prod_{i,j} \{f_S(\theta_i) \times f_R(\theta_j)\}, \quad (2)$$

with

$$f_S(\theta_i) = \frac{\left(\cos \theta_i \pm \sqrt{(M_2/M_1)^2 - \sin^2 \theta_i}\right)^2}{(1 + M_2/M_1)^2}, \quad (3)$$

and

$$f_R(\theta_j) = \frac{4(M_2/M_1) \cos^2 \theta_j}{(1 + M_2/M_1)^2}, \quad (4)$$

where E_0 is the energy of the incident ion with mass M_1 , M_2 is the mass of a target atom which is initially at rest, $\theta_{i,j}$ are the partial scattering or recoiling angles, and $f_{S,R}$ is the fraction of energy transferred during the scattering or recoiling event. For in-plane geometry,

$$\sum_{i,j} \theta_{i,j} = \theta = \alpha + \beta, \quad (5)$$

where θ is the angle between the direction of the incident beam and the direction of the outgoing particle, α is the angle of incidence, and β is the emission angle. When the scattering/recoiling plane is not normal to the target surface, the partial angle is determined by

$$\cos \theta_i = \cos \alpha_i \cdot \cos \beta_i \cdot \cos \phi_i - \sin \alpha_i \cdot \sin \beta_i, \quad (6)$$

where α_i is the partial incident angle, β_i is the partial emission angle, and ϕ_i is the partial azimuthal angle. It is easy to see that for particles experiencing out-of-plane collisions, $\sum_{i,j} \theta_{i,j} > \theta$. When the energy and mass of the analyzed particles are known, the energy E of the particles is connected with the time-of-flight TOF_p corresponding

to pixel p on the MCP and the measured flight time (T_M) by the relation

$$T_M = TOF_p + T_0 + \Delta, \quad \text{with } TOF_p = l_p \sqrt{\frac{M}{2E}}, \quad (7)$$

where M is the particle mass, l_p is the flight length, *i.e.* the distance between the target and pixel p on detector (see Fig. 1), T_0 is the time it takes the particle to travel between the pulsing aperture and the sample, and Δ is the fixed electronics delay.

Figures 2(e)(f) compares TOF distributions predicted by SARIC simulations (solid circles) and measured by SARIS experiments (open circles) with various curves from Eqs. (1) and (2). The definitions of the experimental and SARIC traces ($r_1 - r_4$, $s_1 - s_3$) are the same as in Figs. 2(a-d). The experimental and calculated peak positions are very close to those of the theoretical binary collision curves that include a maximum of two collisions. The relevant processes are shown schematically in Fig. 2. Curves SS and DR correspond to processes s_1 and r_1 , respectively, defining positions for the energies of particles after a single collision. If several large impact parameter, or "Quasi-single" collisions, with angles $\sim 1^\circ - 2.5^\circ$ are included for incoming and outgoing particles, improved agreement between the SARIS/SARIC results can be obtained. The rest of the higher energy traces in Fig. 2 cannot result from a single binary collision event; at least two binary collisions are necessary to produce these traces. A more detailed understanding of such high energy events can be achieved if the actual trajectories of the scattered and recoiled particles are determined. Such trajectories have been extracted from the SARIC simulations. In-plane collisions can be defined as a double scattering process (DS) from atoms lying in a single row corresponding to trace s_3 . For recoil, a possible collision sequence is the following: a primary ion recoils a Pt atom which scatters off a second Pt atom in the same surface row (curve FR₂ or trace r_3). Curve FR₃ corresponds to a collision sequence in which Kr scatters parallel to the surface and then recoils a Pt atom. For out-of-plane collisions including atoms from two parallel rows, one can observe only fixed zig-zag collisional events. From comparison of SARIS and SARIC results with curves from Eqs. (1) and (2), we find that only two angles are possible in zig-zag collisions, *i.e.* $\sim 20^\circ$ (for ZS) and $\sim 22^\circ$ (for FR₁). These angles do not belong to any specific crystallographic directions and are most likely related to the nature of the screening function for a given collision pair.

C. Contour plots of angular distributions for $\text{Ne}^+ \rightarrow \text{Ni}(111)$

Figure 3 presents SARIS/SARIC results for the two-dimensional contour plots of the scattering and recoiling intensities as a function of the scattering/recoiling angle and flight time for 20 keV Ne^+ at 27° incidence angle and three different azimuths of the Ni(111) surface. The contour plots (a-c) are experimental SARIS results from the MCP-detector, while the contour plots at (d-f) are simulated SARIC spectra. The simulated plots are in good agreement with the experimental contours, *i.e.* the

FIG. 3: Experimental SARIS (a, b, c) and simulated SARIC (d, e, f) two-dimensional contour plots of the scattering and recoiling intensities as a function of the scattering/recoiling angle and flight time for the $[1\bar{1}2]$, $[0\bar{1}1]$, and $[1\bar{2}1]$ azimuths of a Ni(111) surface. Beam: 20 keV Ne^+ ; Incidence angle: 27° . The number of detected trajectories increases from the white to the black color. On top schematically is shown. The geometry of the experiment and positions of open directions or 'atomic lenses' are shown above the images.

SARIS experimental images are accurately reproduced by SARIC simulations after including correction factors such as detection efficiency and detector position [3, 16]. Features at $t < 0.5 \mu\text{sec}$ correspond to scattered Ne atoms while those at $t > 0.5 \mu\text{sec}$ correspond to recoiled Ni atoms. A typical quasi-single collision recoiling trace is observed for the $[1\bar{1}2]$ azimuth (Figs. 1(a)(d)). For the $[0\bar{1}1]$ (Figs. 1(b)(e)) and $[1\bar{2}1]$ (Figs. 1(c)(f)) azimuths the angular distributions of recoiling atoms are extremely anisotropic. A 'single-recoil collision' trace along with focused 'recoil spots' are observed. Preferential ejection of recoiled atoms is observed at exit angles $\beta = 40^\circ - 50^\circ$ for $[0\bar{1}1]$ and $\beta = 30^\circ - 35^\circ$ for $[1\bar{2}1]$. Analysis shows that the recoil spots are related to atoms recoiled from the second layer. They clearly do not coincide with any crystallographic direction, while the preferential ejections of low-energy sputtered atoms are usually observed along low-indexed lattice directions [29]. The observed positions of the recoil spots are close to the center of open directions ('atomic lens' [2] created by first-layer atoms) as shown at the top of Fig. 3. For the $[0\bar{1}1]$ azimuth, the projection of the open direction is localized between 28.7° and 58.5° (center $\sim 44^\circ$), while for $[1\bar{2}1]$ the open direction is localized between 19.5° and 54.7° (center $\sim 37^\circ$).

In order to obtain further information on recoil spot

formation, we have considered the depth from which Ni atoms are recoiled when 20 keV Ne atoms are incident on Ni(111) along the $[1\bar{2}1]$ azimuth. Additional simulations were performed in order to determine whether or not this preferential ejection direction depends on the subsurface layers. The contributions of the recoil yield from different layers were calculated from SARIC for the same exit angles and targets consisting of 1, 2, 3, and 4 atomic layers. Figure 4 shows the resulting angular-TOF distributions of the recoil fractions from the first (4a), second (4b), third (4c), and fourth (4d) atomic layers. Figure 5 shows the resulting angular yields obtained by integrating the contour plots at Fig. 4 for each atomic layer. The insert in Fig. 5 shows a bar graph of the total integrated yield from each atomic layer.

From Figs. 4 and 5, it is clear that the first three atomic layers contribute most of the recoiled atoms and that the contributions of each of these three layers are very different. The first atomic layer (Fig. 4(a)) yields $\sim 22\%$ of the recoils and exhibits a 'typical' kinematical trace of recoiled atoms (similar to that observed for Kr-Pt(111) [16]) with traces of quasi-direct recoil and fast-recoils. As distinct from the Kr-Pt(111) system (Fig. 2), here the fast recoil traces represent a very small fraction of the scattered atoms. They can be observed on the left side

FIG. 4: Simulated SARIC angular-TOF distributions of the recoiled Ni atom fractions from the first (a), second (b), third (c), and fourth (d) atomic layers. The fraction of detected trajectories increases from the white to black color in a logarithmic scale.

FIG. 5: Angular yield obtained by integrating intensities from the contour plots of Fig. 4 and normalized to total yield. Insert - bar graph of total integrated yield from each atomic layer.

of Fig. 4(a) by using a logarithmic scale. The second atomic layer (Fig. 4(b)) yields $\sim 40\%$ of the recoils in a highly focused recoil spot. The direction of the maximum near 32° (Fig. 5) cannot be related to any low-index crys-

tallographic vectors between the 2nd and 1st layers. This observation again confirms that the position of the 'recoil spot' is only related to the 'atomic lens' formed by atoms of the first atomic layer. The third atomic layer (Fig. 4(c)) yields $\sim 33\%$ of the recoils, although the recoil distribution is diffuse and exhibits no focused recoil spots. This indicates that atoms recoiled from the third atomic layer are scattered by first and second layer atoms, thereby obliterating any focused recoiled patterns.

IV. DISCUSSION

Our results show that angular distributions of scattering and recoiling particles can be simplified by using a kinematical description obtained from TOF versus angular traces. A combination of SARIS experiments and SARIC simulations provides a sensitive probe, which can yield, within experimental error, a conclusive description of the three-dimensional collision behavior of energetic atoms scattered from the outermost atomic layers of a surface. SARIS and SARIC provide a quantitative separation of the observed multippeak features in the scattering and recoiling spectra and accurate analysis of the collision sequences. An important result of this work is that the most intense recoiling features are due to atoms recoiled from the first two to three atomic layers. The 'recoil

spots' are the results of preferential ejection of second-layer atoms along the open directions, or 'atomic lens', where atoms can either recoil directly into the atomic lens or it can scatter from a neighboring and aligned into the atomic lens.

Much research has focused on studying the scattering features in experimental spectra. For example, experimental energy spectra have been analyzed in terms of "quasi-single" peaks and "quasi-double" shoulders [27]. Generally, better agreement between experiments and simulations can be achieved if the full three-dimensional nature of the collision is recognized. For example, computer simulations have been used to identify peaks due to "planar" and "zig-zag" collision sequences [26, 30–32]. These results support our conclusion about the kinematic nature of separation and description of the observed peaks and traces in Figs. 2 and 3.

V. CONCLUSIONS

This study demonstrates that angle-resolved SARIS mapping combined with computer simulations is a valu-

able tool for characterization of scattering and recoiling events on a surface. The measurements allow identification of direct and indirect, *i.e.* multiple collision, scattering and recoiling particles in the energy distributions. Use of a large area MCP detector and TOF techniques decreases the collection time and increases the number of detected recoils above that of other designs. The scattering and recoiling contour map dependencies provide the kinematics of scattering and recoiling particles, their probability of being detected, and the probability for their occurrence in specific trajectories.

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