Scattering of Low-Energy Ions from Clean Surfaces: Comparison of Alkali- and Rare-Gas-Ion Scattering

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(Received 3 April 1980)

The first experimental comparison of Li^+ and He^+ scattering (primary energies between 100 and 1200 eV) from a clean Ni(110) surface shows strong variations of the Li^+ intensity with crystal orientation, an effect which we attribute to multiple scattering. In the He^+ case, only those He^+ which scattered from surface atoms in single binary collisions survived as ions. The energy dependence of differential scattering cross sections is obtained from the experiments as well as the ratio of the neutralization probabilities of Li^+ and He^+ in the single-scattering events.

PACS numbers: 79.20.Nk

We report the first results from experiments and numerical calculations comparing low-energy ion scattering of Li^+ and He^+ from a clean Ni(110) surface. Large differences in absolute yields are observed between He^+ and Li^+ which are quantitatively explained by differences in the neutralization probabilities. The Li^+ yield exhibits strong crystallographic effects, i.e., in the direction of the (110) surface half channels the backscattered intensity is enhanced by a factor of 30 under certain experimental conditions. Calculations show that this enhancement is caused by multiple-scattering events. For He^+, the comparison of the calculations with the experiment gives strong evidence for trajectory-dependent neutralization effects.

The scattering of Li^+ at energies below[1] 20 eV and the He^+ scattering in the energy range from[2] 100 eV to 2 keV have been described by the binary-collision model. However, the He^+ yield is to a large extent dominated by neutralization which complicates the analysis of the experiments, whereas for alkali ions we expected ion yields close to those of Ref. 1 because of their low ionization potentials in comparison to the work function of solids.[3] Since the elastic part of the ion-surface interaction can be calculated within the binary-collision model, Li^+ can be used as a probe for the elastic interaction, thus allowing more detailed conclusions about the neutralization behavior of He^+. In our case the Li^+ scattering in the neighborhood of the (100) and (110) surface half channels is heavily influenced by trajectories which include zigzag-type motions. The intensity enhancement caused by these trajectories is not obtained for He^+, indicating different neutralization for different trajectories.

The experiments are performed in an UHV system[4] which allows doubly differentiated analysis of ion scattering (energy and scattering angle) for primary energies from 100 to 2000 eV. A commercial Li^+ source (Spectra-Mat, Inc.) has been adapted[5] to fit into our rare-gas electron-impact source, such that rare-gas-ion and Li^+ scattering experiments can be done under identical target and scattering conditions by selecting the beams with the sector field magnet. Li^+ currents in the picoampere region are sufficient to obtain spectra, and are generally a factor of 10 to 100 lower than the He^+ currents. This reflects grossly the difference in neutralization probabilities. These low currents and current densities (beam size 2 mm diam) allow sufficient time to complete the experiment without detectable damage or contamination of the target. The Ni(110) was mechanically and electrolytically polished, oriented by x-ray diffraction, and cleaned and annealed *in situ*. Target preparation and cleanliness were checked by low-energy electron diffraction, Auger-electron spectroscopy, and ion scattering.

Figure 1 shows Li^+ and He^+ spectra for an orientation of the plane of scattering 3 deg off the [110] direction. The positions of the main peaks coincide with the energy given by the binary scattering of two mass points. This was previously observed for He^+ and also for Li^+ at lower energies (20 eV and below).[1,2] For certain azimuthal regions, i.e., around the (110) and (100) surface half channels, the Li^+ spectra show high-

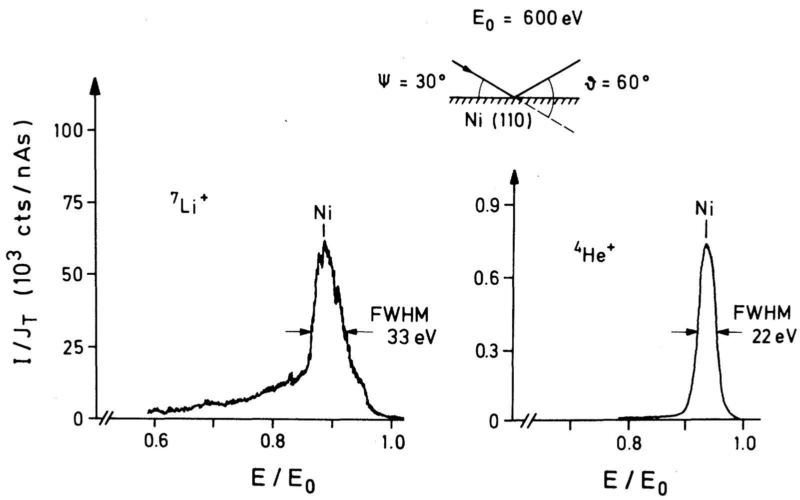

FIG. 1. Ion backscattering of Li^+ (left) and He^+ (right) from clean Ni(110). The plane of scattering is perpendicular to the surface and 3° off the [110] surface direction ($\varphi = 3°$; see Fig. 2). Note the differences in the ordinates and in full width at half maximum.

energy shoulders typical of multiple-scattering events. The low-energy tail observed for Li^+ is similar to H^+ backscattering[6] and higher-energy rare-gas–ion scattering.[7] It is ascribed to particles which are backscattered after penetrating at least beyond the top atomic layer of the solid, i.e., a distinction is made between the "surface peak" and "scattering from the bulk." Figure 2 shows the azimuthal dependence of the Li^+ and He^+ surface peak intensities at 600 eV, an impact angle of $\psi = 30°$, and a laboratory scattering angle of $\theta = 60°$. The He^+ intensity is virtually independent of the crystal orientation (as are the energy and width of the surface peak), whereas the Li^+ intensity depends strongly on the crystal orientation (the peak form also changes). Included in Fig. 2 are the results of numerical calculations based on the binary-collision model. The program[8] simulates the experiment with respect to beam and analyzer properties. The target is a three-dimensional Ni(110) crystal with a thickness of two layers, to minimize computing time. Thermal vibrations are included. The interaction potential used is a Thomas-Fermi-Molière potential. Neutralization is not included. For both He and Li, the calculations predict a strong azimuthal dependence which is experimentally found for Li^+ only.

The program allows an analysis of the scattering process with respect to different types of trajectories. In the region of the intensity minimum (around $\varphi = 50°$ in Fig. 2) the peaks of the spectra are built up by single–binary-scattering events, whereas in the region of the surface half channels multiple-scattering trajectories involving the first and second layer give the main contribution to the intensity in the peaks. (Details of these results will be published elsewhere.[8]) Experimental evidence for the calculated results is given by the energy spectra (Fig. 1) and the azimuthal dependence of the backscattered Li^+-ion intensity (Fig. 2). Further evidence is obtained from the energy dependence of the intensity as shown in Fig. 3. If the scattering in the $\varphi = 50°$ region is mainly due to single binary collisions, then the measured intensity should follow the energy dependence of the binary-collision cross section. It is indeed possible to fit the He^+ scattering intensity $I \propto (d\sigma/d\Omega)P$ to a calculated differential scattering cross section $d\sigma/d\Omega$ by dividing the measured intensities by an ion survival probability[9] $P = \exp(-A/av_\perp)$ as shown in Fig. 3. Here $v_\perp$ is the ion velocity perpendicular to the surface and the "survival parameter" A/a is found to be 1.78×10^7 cm/s. This value is comparable to previous results for different scattering angles [2.88×10^7 cm/s for $\psi = 45°$, $\theta = 90°$ (Ref. 10) and 3.78×10^7 cm/s for $\psi = 90°$, $\theta = 132°$ (Ref. 11)]. For the calculation of the scattering cross section a Thomas-Fermi-Molière potential with a Firsov screening parameter was used. This is apparently appropriate to describe the scattering, at least in our parameter range. A consistent result without further fit is obtained if we calculate the

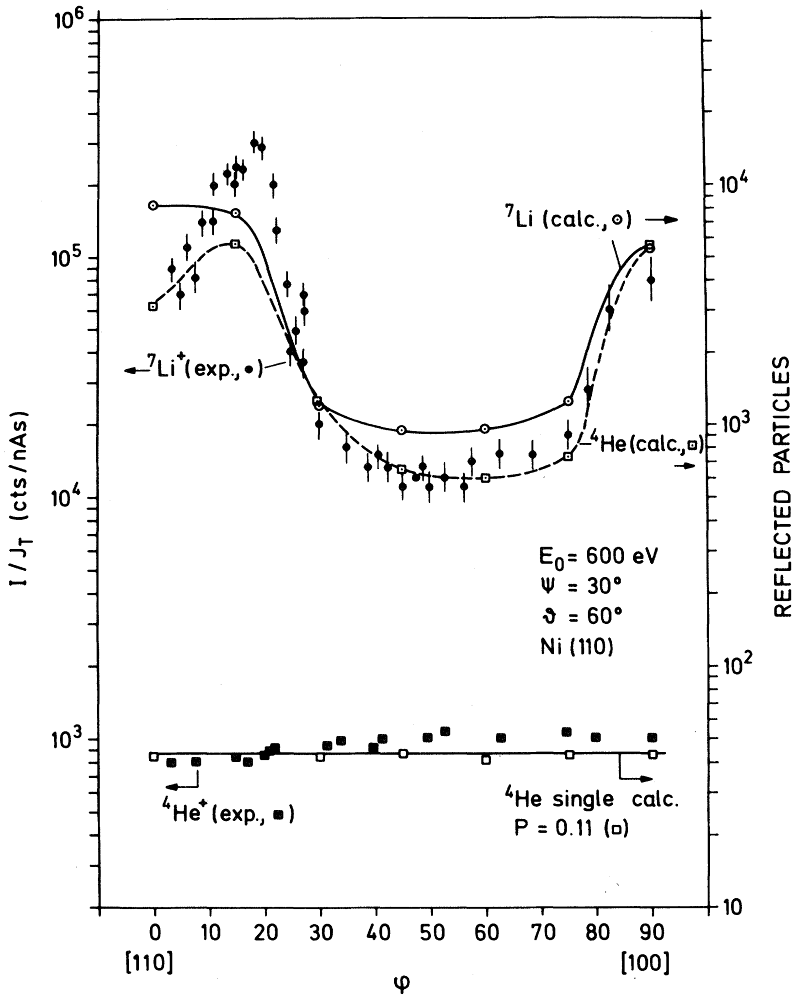

FIG. 2. Azimuthal dependence of the experimental Li^+ (solid circles) and He^+ (open squares) intensities (left ordinate), and comparison with numerically calculated results (lines) (right ordinate). Experiment and calculation are matched for the He^+ scattering with use of $P = 0.11$ (resulting from Fig. 3) to reduce the calculated single-scattering component (lower curve) contained in the total scattering (upper curve).

cross section for Li^+-Ni scattering and compare it with the experimental intensities in the "single-scattering regime," i.e., for an azimuthal angle of $\varphi = 53°$. Without invoking any neutralization (i.e., $P = 1$) and with use of the same factor as in the He^+ case to compare cross sections (Å^2/sr) with intensities (counts/nA·s), we get an exact agreement of the measured and calculated values, as illustrated in Fig. 3.[12] This result strongly supports the idea that the Li^+ scattering peak intensity around $\varphi = 50°$ mainly arises from single-scattering events without neutralization. For the single scattering of He^+ the ion survival probability is 0.11 with $A/a = 1.78\times10^7$ cm/s, whereas all other trajectories are subject to neutralization by factors of 10^{-3} to 10^{-4} (Fig. 2), comparable to the charge-state fraction observed for "scattering from the bulk."[6]

There is an interesting analogy between our results and those reported recently for 2.4- and 5-keV neon ions and neutrals backscattered from Ni(001),[13] in which neutralized neon shows a strong dependence on crystal orientation in contrast to the ions.

In summary, our results demonstrate strong differences between Li^+ and He^+ scattering from a Ni(110) surface. They can be explained by considering the single- and multiple-scattering contributions. For Li^+ both contributions exhibit an equally low neutralization probability. Multiply scattered He^+ ions, however, have an extremely low probability to escape from the surface as

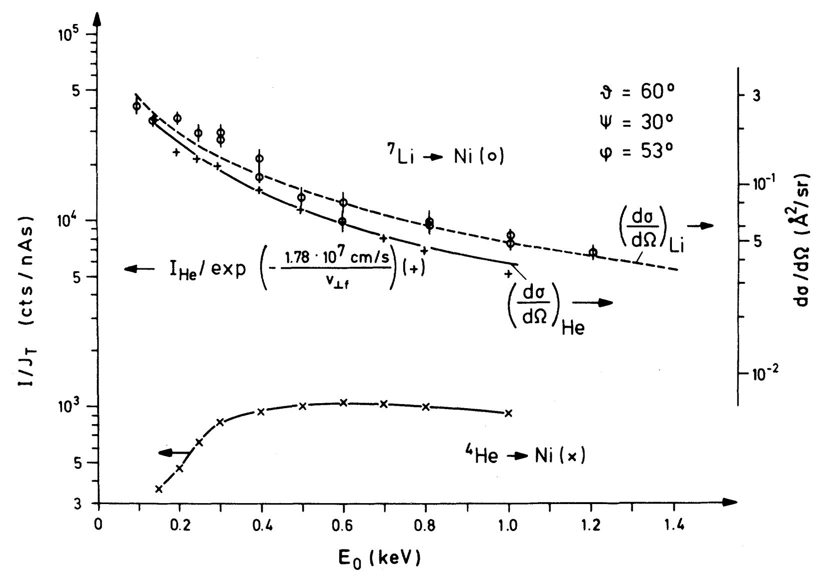

FIG. 3. Energy dependence of the He^+ and Li^+ intensities (left ordinate) compared with the calculated differential scattering cross sections for single scattering (right ordinate). The exponential yields $P = 0.11$ for He^+ at 600 eV independent of the azimuthal angle. $v_{\perp f}$ is the normal velocity component of the scattered He^+ ions.

ions, such that virtually all backscattered ions arise from single-scattering events from the top atomic layer. Our results also yield absolute numbers for the survival parameter and the scattering cross sections.

Part of this work was performed within the Sonderforschungsbereich 128 of the Deutsche Forschungsgemeinschaft. We thank E. Hulpke for information about the Li source and K. Snowdon for helpful discussions.

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