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INNER-SHELL PROCESSES AS PROBES OF MULTICHARGED ION NEUTRALIZATION AT SURFACES

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Abstract - We have measured energy distributions for electrons emitted during grazing collisions of multicharged ions with Au and Cu single crystals in the projectile energy range 20-90 keV. The measured electron spectra are characterized by discrete peaks resulting from Auger transitions, superimposed on a broad continuum electron distribution. Auger electron emission from both projectile and target atoms has been observed. The projectile Auger electrons result from the decay of inner-shell vacancies either carried into the collision or produced by vacancy transfer from empty outer projectile levels via pseudocrossings or rotational coupling of molecular orbitals. The latter mechanism may also lead to the creation of target inner-shell vacancies which give rise to Auger electron emission characteristic of the target. An analysis of these Auger electron features is presented which is aimed, on the one hand, at elucidating detailed production mechanisms, and, on the other, at obtaining information on the time scales describing the neutralization of multicharged ions during their interaction with metal surfaces.

1 - INTRODUCTION

The study of multicharged ion-surface interactions has received significant attention in recent years. One reason for the increased interest is the large neutralization potential energy that the multicharged projectiles carry into the collision. The detailed mechanisms by which the dissipation of this potential energy affects ion neutralization, sputtering, or particle reflection are still incompletely understood, making this a fertile area of experimental as well as theoretical investigation.

One way of investigating the neutralization of multicharged ions during interactions with surfaces is through the measurement of electrons emitted during the interaction. Multicharged ion neutralization and electron emission are in fact closely related, as evidenced by the large fraction of the possible neutralization processes (see Refs. 1 and 2 for reviews) that also result in electron emission. In order for complete neutralization (i.e., complete dissipation of the multicharged ion's initial potential energy) to occur, long interaction times with the surface are required, which can be attained by the use of very low projectile kinetic energies. This approach has been used by de Zwart /3/, Varga et al. /4,5/, and by Delaunay et al. /6-9/, who have investigated "potential" electron emission for ions incident on metal surfaces at normal or close to normal angles with energies as low as 6 eV. At ORNL, measurements /10-13/ of electron emission have been performed for higher-energy multicharged ions (typically 10xq keV) incident on metal surfaces at grazing angles (typically 5°). By

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the use of such small angles of incidence, similar long interaction times with the surface can be attained. By varying the angle of incidence, and thereby the perpendicular component of projectile velocity, the interaction times can be varied over a large range. Furthermore, by varying both the projectile energy and angle of incidence, the penetration depth of the ions can be varied; specifically, the regime of specular reflection can be approached, in which essentially no penetration of the surface occurs. In this regime, electron emission above the surface can be studied in isolation, i.e., without the complications arising from electron emission below the target surface. At the higher projectile energies used in the grazing incidence measurements, inner-shell binary-collision processes become possible during the ion-surface interaction, which can be used as probes of the neutralization process. At the same time, however, interpretation of the measured electron energy distributions becomes more difficult, since at these energies "kinetic" electron emission processes /14/ may make significant contributions to the total electron yield. The contribution of "kinetic" emission is confined to the production of low energy continuum electrons (energies <50 eV). Consequently, the discussion below will be restricted to the discrete features in the measured electron energy distributions observed at higher electron energies, where "kinetic" emission effects are expected to be negligible. Specifically, a qualitative discussion of the observed target and projectile Auger features will be presented, based on molecular orbital (MO) energy level calculations. In addition, a comparative analysis of projectile K-Auger features will be presented to illustrate, again in a qualitative way, the use of inner-shell processes as probes of the time scales over which neutralization of multicharged ions near surfaces occurs. The discussion will in part be based on electron energy distribution measurements obtained using an improved experimental apparatus, a brief description of which is also provided below.

2 - TARGET AND PROJECTILE INNER-SHELL EXCITATION

Figure 1 shows electron energy distributions measured for 60 keV N + ions incident on Au and Cu single crystals at 5° using a large acceptance-angle cylindrical mirror analyzer (CMA). Details of the experimental apparatus have been previously described /11,13/. The Au target electron spectra for H-like and He-like incident ions are characterized by a broad feature around 350 eV. As has been previously discussed /11-13/, this feature is due to projectile KLL transitions which fill the K-shell vacancies carried into the collision by each incident ion (in the case of the H-like ions), or by those ions in the metastable 2s2 3S state (in the case of the He-like ions). Note the absence of this KLL feature for the Li-like incident projectiles. Turning now to the Cu target electron energy spectra, it is seen that even for the Li-like incident projectiles, which have filled K-shells, the projectile KLL feature is present. This observation is interpreted as evidence for projectile K-shell excitation in this collision system. Projectile K-shell excitation is also observed for F + ions incident on Cu /15/, as can be seen from the electron energy spectra shown in Fig. 2. The latter spectra were also obtained using a CMA electron spectrometer.

In order to obtain insight into the reasons underlying this interesting difference observed for Au and Cu targets, adiabatic MO energy level calculations were carried out on the N + Au and N + Cu collision systems using the variable screening model developed by Eichler and Wille /16/. Representative results of the calculations for N + ions are shown in Fig. 3. The relevant curves, which represent the purely electronic eigenenergies of the N + Au and N + Cu quasimolecules, respectively, as a function of internuclear separation, are labelled by the atomic levels that they correlate to in the separated atom limit. In the figure, a significant difference between the sequence of energy levels for Au and Cu targets is immediately apparent. For the N + Au system, the potential curve correlated to the ls level of the projectile is separated from those correlating with the 2s and 2p projectile levels by the filled 4s, 4p, and 4d Au target levels. Transfer of an electron out of the projectile K-shell (i.e., projectile K-shell excitation), which proceeds via pseudocrossings or rotational couplings of the initial state and adjacent MO's is therefore inhibited, since all the neighboring orbitals correlate to target levels which are already filled. On the other hand, transfer of an initial K-shell vacancy to neighboring n=4 target levels is facilitated. As has been discussed previously /11-13/, such projectile-to-target vacancy transfer reactions may give rise to the NNV and NVV target Auger transitions at 220 and 70 eV, respectively, evident in the N + Au electron energy spectrum shown in Fig. 1.

In contrast to this situation, it is seen that for the N + Cu system, there is no similar interposition of orbitals correlated to filled target levels between the MO's correlated to the projectile ls, 2s, and 2p levels. There is thus a more direct pathway along which a projectile K-shell electron might be transferred to the only partially filled L-shell, consistent with the experimental evidence of K-shell excitation noted earlier for this collision system. MO calculations of the F + + Cu systems show a similar sequence of
projectile-correlated orbitals, and thus indicate a similar mechanism for projectile K-shell excitation for those collision systems.

Due to the large Doppler broadening (typically about 90 eV for the above projectile N KLL features) resulting from the 90° orientation of the CMA spectrometer axis with respect to the projectile beam direction, the resolution of the projectile KLL features in the above spectra is significantly degraded, making interpretation difficult. Despite the limited resolution, however, a systematic difference in peak positions is observed between the KLL features observed for H-like incident ions, which carry an initial K-vacancy, and those observed as a result of K-shell excitation during the interaction with the surface. In comparing the spectra for F8+ and F6+ incident on Cu in the bottom of Fig. 2, it is seen that the KLL feature resulting from K-shell excitation (i.e., for incident F8+), while characterized by a similar fall-off toward higher energies, does not extend as low in electron energy as that observed for incident F6+. As a result, the KLL "peak" arising due to K-shell excitation appears to lie about 25 eV higher in energy than that observed for H-like incident ions. A similar difference in KLL "peak" positions is observed in the case of N6+ and N4+ ions incident on Cu (see Fig. 1). It is noted, on the other hand, that the KLL "peak" for N5+ ions incident on Au, also shown in Fig. 1, is not shifted relative to that observed for incident N6+ ions. It is recalled that for the N5+ incident ions, the KLL "peak" arises from the small fraction of 1s2s3S metastable ions in the incident beam. Thus for both of the latter ions, the KLL "peaks" are the result of the filling of an initial K-shell vacancy present in the incident beam. It is thus seen that by using as a reference the projectile Auger "peak"
Fig. 2 - Electron energy distributions for F ions incident on Cu; $F^{8+}$ and $F^{6+}$ projectile energies are 80 keV; energies of $F^{4+}$ and $F^{2+}$ ions are 52 and 26 keV, respectively.

measured for an incident charge state beam known to carry the appropriate initial inner-shell vacancy, it can be inferred whether similar "peaks" observed for lower charge state ions (in whose ground states the inner shell of interest is filled) are the result of metastables present in the incident beam or projectile inner-shell excitation during the interaction with the surface.

Returning to the earlier discussion of target inner-shell excitation, it is noted that de Zwart has also observed target Auger transitions in 20 keV $Ar^{9+} + W$ collisions, as discussed in his Ph.D. thesis. He suggests that inner-shell vacancy transfer via MO pseudo-crossings may be the underlying excitation mechanism for this collision system also. It remains to discuss briefly the additional Auger features at about 270 and 500 eV evident in the Cu target spectra of Figs. 1 and 2, respectively. These features are identified as KV transitions of carbon and oxygen impurities, respectively, present on the Cu surface in minute quantities. The excitation mechanism in this case is 2pm-2pa rotational coupling, well known and studied in ion-atom collisions involving second row elements, in which a 2p vacancy is transferred from the heavier collision partner to the 1s shell of the lighter partner. This mechanism is illustrated in Fig. 4 for the N + C collision system. The vacancy transfer cross section increases steeply with decreasing $\Delta Z$, i.e., difference of
atomic numbers of the collision partners. This makes N an ideal probe of C surface contamination, while F ions are a sensitive probe for surface contamination by O. The sensitivity of a N beam probe to the presence of C on a Au surface is illustrated in Fig. 5, where an electron energy spectrum is shown for N\textsuperscript{6+} ions incident on a Au surface having a ~20\% monolayer coverage of carbon. The spectrum was obtained using a LEED system in a manner previously described /10/. The area of the C KVV feature is about 30\% of that of the N KLL feature. Since the total yield of N KLL electrons has previously been determined /11/ to be on the order of unity, the absolute yield of C KVV electrons is seen to be quite high (~30\%). For comparison, Fig. 5 also shows a 500 eV electron induced energy spectrum acquired for the same surface conditions. As can be seen, on the scale of the elastic scattering peak, the C KVV peak is not discernible. The production of "target" Auger electron emission by inner-shell vacancy transfer is thus in this case considerably more efficient than that produced by electron-impact ionization.

3 - APPARATUS IMPROVEMENTS

As has already been pointed out above, the energy spectra acquired using the fixed-position CMA (as well as the LEED system) electron spectrometers were of limited resolution due to Doppler broadening and extended-source effects. To remove this limitation, a compact, small-acceptance-angle, high-resolution hemispherical sector analyzer (1.82 cm radius of curvature) was recently installed in the UHV experimental chamber. The analyzer is mounted on a rotatable shaft to permit measurement of ejected-electron angular distributions, and is provided with a "zoom" lens to permit deceleration of the electrons prior to analysis. In addition to the new electron spectrometer, the present apparatus features a beam collimation/monitoring
section, which provides for independent, real-time monitoring of incident ion beam current, and thus permits more convenient normalization of the measured electron energy distributions to the incident ion flux. The beam collimator/monitor consists of a series of apertures which are used to limit the divergence of the beam incident on the final collimation aperture, where a small fraction of the incident ion beam is intercepted. Due to the upstream collimation, the fraction of intercepted to transmitted beam current (which is equal to the current incident on the target crystal) is almost independent of upstream beam tuning, i.e., is solely determined by the collimator geometry. In previous versions of the apparatus, the electron spectra were normalized to the unbiased target current, which, due to the large total electron yields, represented mainly the ejected electron flux and not incident ion flux.

The geometry of the present setup is schematically indicated in Fig. 6. Note that angle of incidence as well as electron ejection angle can now be independently varied, providing greatly increased experimental flexibility. With the exception of these two improvements, the apparatus is identical to that previously described /13/. To illustrate the resolution attainable with the new spectrometer, Fig. 6 also shows a scattered electron energy spectrum for ~500 eV electrons incident on Au at 45°.

4 - PROJECTILE KLL DECAY MEASUREMENTS

Using this new setup, energy spectra have been measured for 70 keV O\(^{7+}\) ions incident on a gold single crystal. Figure 7 shows a family of such energy spectra, for different angles of incidence in the range 10° to 80°. The detection angle remains fixed at 90° relative to
Fig. 5 - Top - electron energy distribution for $N^{6+}$ ions incident at $5^\circ$ on Au having a 20% monolayer coverage of carbon. The peaks around 250 eV and 350 eV are identified as C KVV, and N KLL peaks, respectively. The horizontal bar indicates the broadening introduced by the numerical differentiation of the LEED transmission current. Bottom - electron energy spectrum for 500 eV $e^-$'s incident normally on Au also with 20% monolayer C coverage. The spectra shown all have the same normalization, and were acquired with a selected spectrometer-pass-energy of 100 eV, resulting in an electron energy-independent instrumental resolution of about 5 eV. Doppler broadening in the vicinity of the projectile KLL peaks located at ~500 eV is about 10 eV. The total instrumental width due to these two effects combined is thus small compared to the observed width of the projectile KLL peaks (~100 eV). By varying the angle of incidence, the time interval between the start of projectile neutralization and penetration of the surface can be varied. Assuming that neutralization commences at the critical distance $l_{1/8}$ above the surface at which the Coulomb barrier between projectile and metal falls below the Fermi level, equal to about 21 a.u. for $O^{7+}$ ions, the above-surface interaction times cover the range 1 to $7 \times 10^{-15}$ s, the shortest time corresponding to the largest angle of incidence ($80^\circ$). The following trends are noted in the dependence of the projectile KLL peak on time spent above the surface. The size of the KLL peak decreases monotonically with decreasing interaction time, and becomes barely discernible above the continuum background in the spectrum for the $80^\circ$ angle of incidence. The position
of the KLL peak, however, does not appear to change as a function of the above-surface interaction time. These trends are consistent with the following picture. At the already defined critical distance from the surface, multiple resonant neutralization from the valence band of the metal occurs (on a time scale of the order $5 \times 10^{-16}$ s /19/), which populates highly excited Rydberg levels of the incident ion (e.g., $n=9$ for incident $O^{7+}$). A cascade of electrons to lower $n$ levels occurs as the multiply excited ion autoionizes, in parallel, of course, with further resonant neutralization processes to progressively lower $n$ as the ion continues to approach the surface. As soon as at least two electrons have reached the L-shell, KLL transitions will occur. If the rate of filling the L-shell is much less than the KLL rate for the Li-like ion, no further filling of the L-shell is possible, and the observed KLL peak should be that for $O^{5+}$. If, on the other hand, the L-shell filling rate exceeds that of KLL decay, then the observed KLL peak should be a composite structure, consisting of KLL contributions from all charge states $s$. In this picture the KLL peak position is thus argued to depend only on the relative magnitudes of two intrinsic time scales characterizing the neutralization process, and not to have a dependence on the extrinsic interaction time scale selected by a particular angle of incidence, in accord with observation.

To permit a more quantitative discussion, atomic structure calculations were performed, using the codes of Cowan /20/, to determine the dependence of KLL Auger energies and transition rates on the number of electrons present in the L-shell of the O projectile. The results of the calculations are summarized in Table I. The range of calculated configuration-average KLL transition energies for each possible projectile charge state has also been indicated under the KLL peaks in Fig. 7. As can be seen, the observed KLL structure encompasses KLL transitions from all possible projectile charge states, including the neutral, which features
Fig. 7 - Electron energy distributions for 70 keV $O^{7+}$ ions incident on Au, for six different angles of incidence. Horizontal lines under the KLL peaks give calculated ranges of KLL transition energies for all charge states $\leq 5^+$. 

<table>
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<th>Initial Charge State</th>
<th>Initial Configuration</th>
<th>Final Configuration</th>
<th>Configuration Average Auger Electron Energy (eV)</th>
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a "super-filled" L-shell, since it can bind an extra electron due to the K-shell vacancy. The possibility of K-Auger transitions from a "super-filled" L-shell is one mechanism that may explain the extent of the observed KLL feature to energies above the KLL peak at about 495 eV observed subsequent to K-shell photoionization of neutral O. An additional mechanism for yielding higher than "normal" Auger transition energies, based on interaction of the Auger electron with the image charge of the (incompletely screened) emitter has been discussed by Folberts and Morgenstern /21/.

A consequence of this interpretation of the width of the observed KLL structure is that the filling rate of the L-shell significantly exceeds the rate of the fastest KLL transitions, as discussed earlier. Referring to Table I, the fastest KLL decay rate is calculated for neutral O (with the "super-filled" L-shell) where it is larger than $2 \times 10^{14}$ s$^{-1}$. The limiting rate being that of the KLL transition, it is the time scale defined by this rate that must be compared to the neutralization time available above the surface. It is seen that at 10° angle of incidence, the interaction time corresponds to about 1.2 KLL decay lifetimes, while at 80°, the available time corresponds to only about 0.2 KLL decay lifetimes. This explains the gradual disappearance of the observed KLL peaks with increasing angle of incidence. To verify that the observed KLL transitions indeed occur on the incident ion trajectory, and not late in the interaction subsequent to the reemergence of (some of) the ions from the surface along some different direction, the Doppler shift of the KLL peak was investigated as a function of viewing angle. Figure 8 shows the KLL peak for O$^{7+}$ incident on Au at 10° as observed at three different observation angles. The well-defined Doppler shift of the observed KLL peaks shows clearly that the Auger electron emission occurs while the projectile is still traveling along the incident beam direction, i.e., prior to any deflection of the projectile by close encounters with target atoms. A similar conclusion was reached by de Zwart /3/ in analyzing Ar LMM transitions during 500 eV Ar$^{9+}$ collisions with a W surface.

In the light of the above interpretation of the observed KLL widths, a reason for the difference, noted in the previous section, between the KLL peak positions observed subsequent to K-shell excitation and those observed for H-like incident projectiles can now be suggested. Since the excitation process requires a small impact parameter binary collision with a target atom, and thus occurs late in the multicharged ion-surface interaction, the ion will be

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**Fig. 8** - Electron energy distributions for 70 keV O$^{7+}$ ions incident on Au, for three different observation angles.
almost completely neutralized at the instant of inner-shell excitation. The subsequent KLL transitions will thus occur in a narrower electron energy range, characteristic of, say, neutral or singly charged \(0^+\), than that observed for H-like incident ions, where KLL transitions from all possible charge states occur. The high energy sides of the KLL peaks for the two cases, which correspond to KLL transitions from "super-filled" L-shells, thus coincide, as can be seen from the comparison in Fig. 2 between \(F^{5+}\) and \(F^{8+}\). The mechanism for obtaining a "super-filled" L-shell in the case of K-shell excitation is the excitation itself, in that the nearest (and most likely) unfilled orbital to which a projectile K-shell electron can be promoted is the orbital correlating to the projectile 2p level (see Fig. 3).

To determine the extent to which the shape of the KLL peaks is perturbed by electron emission of the projectile after penetration of the surface, the measurements of Fig. 7 were extended to lower angles of incidence. Results for \(N^{6+}\) ions incident on Au at \(10^\circ\), \(3^\circ\), and \(1^\circ\) are shown in Fig. 9. The electron energy spectra shown cover electron energies in the vicinity of the N KLL peak; the spectra were scaled to have the same KLL peak height, in order to illustrate the relative contribution of the broad feature below the projectile KLL peak as a function of angle of incidence. Clearly, the relative importance of this feature decreases with decreasing angle of incidence, indicating that it is not related to projectile KLL emission occurring prior to penetration of the surface. The trend shown in these measurements can be due to either the increased interaction time above the surface obtained with the smaller grazing angles (resulting in a larger KLL peak), or the decreased penetration of the projectiles, or both. The latter possibility is illustrated in Fig. 10, where classical trajectory Monte Carlo calculations using the MARLOWE code /22/ are shown for 60 keV \(N^{6+}\) ions incident on Au for two different angles of incidence. The simulation was carried out using the ZBL screened-Coulomb interatomic scattering potential /23/, and assuming an unreconstructed metal surface. The calculations show that at the present energies, the condition of specular reflection is approached for \(-1^\circ\) grazing angles of incidence. A similar conclusion can also be reached by calculating the "half-dip" angle for planar channeling (of which specular reflection is the surface analog) using the formalism presented in the review by Gemmel /24/. For 60 keV N ions incident on Au, this angle is calculated to be \(2.6^\circ\), which is in good agreement with the result obtained using the Monte Carlo simulation. Further measurements are planned to investigate this interesting scattering regime, in which the multicharged ion-surface interaction can be studied in isolation without having to consider the complications arising from surface penetration effects.

![Fig. 9](image-url)
Fig. 10 - MARLOWE calculation of mean penetration depth for 70 keV O projectiles incident on Au at 5° and 2°. Vertical arrows along abscissa correspond to crystal lattice planes in the (110) orientation; $R_N$ in the figure refers to particle reflection coefficient.

5 - SUMMARY

A qualitative discussion has been presented of inner-shell vacancy production mechanisms relevant to collisions of multicharged N, O, and F ions incident on clean Au and Cu surfaces as well as those having fractional-monolayer coverages of C and/or O. The discussion was based on calculated adiabatic MO energy levels, which give an insight into the possible pathways along which inner-shell excitation may occur, and into the sensitivity of these pathways to the collision partners making up the quasimolecule. A comparison was made of projectile KLL peaks resulting from the filling of K-shell vacancies carried into the collision, and those observed subsequent to projectile excitation. Analysis of the former provides information about the rate of filling of the L-shell during the neutralization process, while analysis of the latter gives information on the degree of filling of the L-shell at the conclusion of the neutralization occurring above the surface. A characteristic signature of K-shell excitation apparent in the measured electron energy spectra was discussed. This characteristic can be used to distinguish inner-shell transitions occurring in metastable ions from those occurring subsequent to inner-shell excitation occurring during the collision.

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