Electron emission from low-energy Xe^+ ions interacting with a MgO thin film deposited on a Mo substrate

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Experimental electron spectra arising from low-energy Xe^+ ions scattering off a MgO(100) thin film on a Mo(100) substrate are reported. The ionization energy of Xe is so low that Auger neutralization of Xe^+ at the insulating film is virtually impossible. The ions are therefore predominantly neutralized by resonant processes leaving behind holes in the valence band of MgO. Recently we have proposed that holes created in a thin insulating film are transported to the substrate where they are neutralized. We have performed computer simulations of the electron emission arising in the Auger neutralization of the holes at the Mo substrate and found good agreement with the experimental spectra. The present results support our previously proposed model.

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I. INTRODUCTION

Since the 1950's research efforts have been devoted to the study of the emission of electrons arising in the scattering of low-energy ions from solid surfaces. Most of the experiments have been performed on metal surfaces.[1–10] For ions with energies in the range of a few eV up to a few hundred eV, the detailed mechanisms leading to electron emission are now rather well understood. For insulator surfaces, on the other hand, the experiments are more complicated: the target is a bad electric conductor and may charge up during the experiments. Yet, it is precisely the interaction of ions, as important constituents of plasmas, with insulators that has recently become important in a number of industrial applications. For example, insulators are used as protective layers in plasma display panels (PDP's), which are of crucial importance to achieve large, flat, and light-weight displays.[11] In the last fifteen years a number of experiments with atomic beams on insulating surfaces has been reported. To prevent charging either very thin films of insulating material deposited on well conducting substrates were used or the samples were heated (making use of ionic conductivity). Most of these studies have focused on scattered particles and on electron emission induced by fast ions, fewer studies on electron emission induced by low-energy ions.[12–25] Only recently ion-induced electron studies have started that may be of direct interest for PDP related research.[26–32]

We have recently published electron spectra obtained by the scattering of low-energy noble-gas ions from bulk MgO(110) (Ref. 31) and from a thin film of MgO(100) deposited on a Mo(100) substrate.[32] For these two systems, the results were found to be quite different: for bulk MgO the electron spectra seemed to be independent of which noble-gas ion was used (He^+ or Ne^+), for a MgO thin film the spectra definitely did depend on noble-gas ion (He^+, Ne^+, or Ar^+). The present paper involves the interaction of noble-gas ions with a MgO thin film and therefore only the latter results will be briefly discussed. A one-electron energy diagram, showing the ionization energies of noble-gas atoms, the valence band of the MgO thin film, and the conduction band of the Mo substrate are shown in Fig. 1. The mutual positioning of the valence band of MgO and the conduction band of Mo will be discussed later. Whereas for metal surfaces it is generally accepted that electron emission is dominated by Auger neutralization of the incoming ions, for an insulating, thin film, comparison of experiments with model simulations clearly showed that neither the high electron emission coefficients nor the electron spectra could be interpreted in terms of Auger neutralization of the incoming (He^+, Ne^+, Ar^+) ions at the thin film alone.[32] To explain the discrepancies, we proposed an additional mechanism for elec-

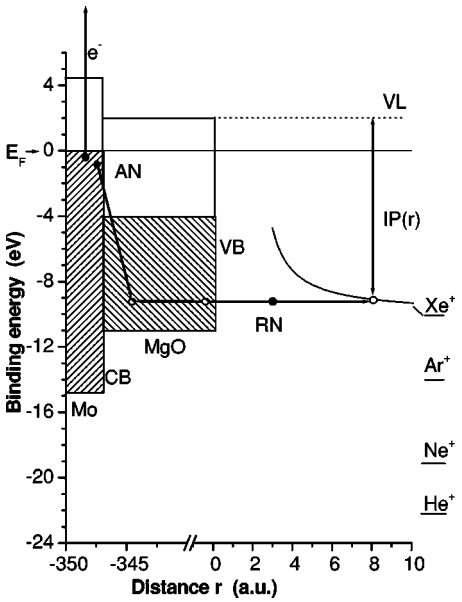

FIG. 1. Schematic energy-level diagram for resonant neutralization (RN) of Xe^+ in front of a MgO film on a Mo substrate. The hole created in the valence band (VB) of MgO is transported to the Mo substrate, where it is removed by either a resonant (not indicated) or an Auger process (AN). The latter process, involving electrons from the conduction band (CB) of Mo, leads to the observed electron emission. VL denotes the vacuum level of MgO.

tron emission: the holes, created in the insulating film by neutralization of the incoming ions, are transported to the film-substrate interface. At the interface they are neutralized either via resonant or via Auger processes, the latter giving rise to additional electron emission. The measured electron spectra, therefore, originate in two distinct processes, Auger neutralization of the primary noble-gas ions at the MgO film and Auger neutralization of the transported holes at the conducting substrate.

In the present paper, electron spectra obtained by the scattering of low-energy (47 eV) Xe^+ ions from a thin film of MgO(100) deposited on a Mo(100) substrate will be presented. Because of the very low kinetic energy of the incoming ions, kinetic effects are expected to be small. For example, in the mechanism proposed by Vogan *et al.*,[30] for ions with kinetic energies of a few hundred eV incident on oxidized Mg, an MgO^- molecule is excited, a process for which more than 10 eV is needed. For our experimental situation, the energy available in the center-of-mass system is so low that this process is not very likely (for a binary collision between a Xe^+ ion and an O atom this energy amounts to about 5 eV, between a Xe^+ ion and a MgO^- molecule as a whole to about 11 eV). Electron emission, therefore, is expected to originate predominantly in the potential energy of the incoming ions: an incoming Xe^+ ion is most likely neutralized by a resonant process, whereby an electron from the valence band of MgO is captured. Auger neutralization at the MgO film, on the other hand, is virtually impossible because of the large band gap of MgO compared to the potential energy of Xe^+ (see Fig. 1). According to our model, a hole left behind in the MgO thin film is transported to the Mo substrate, where its neutralization via an Auger process leads to electron emission. Measured electron energy distributions therefore present a clear test for the proposed model, since they only arise from neutralization of holes at the substrate. We have made simulations of electron spectra and in the following it will be shown that these simulations agree quite well with the measured spectra.

II. EXPERIMENT AND EXPERIMENTAL RESULTS

The experiments were performed in a UHV chamber at a base pressure of 5×10^{-10} mbar. The MgO thin film was prepared by evaporation of Mg in an O_2 atmosphere of 5×10^{-7} mbar.[33] During the evaporation process the substrate was kept at 250 °C. Prior to depositing the MgO film the Mo(100) substrate was prepared by cycles of sputter cleaning and annealing. The quality of the MgO thin film was monitored by low-energy ion scattering (LEIS) and by ultraviolet photoelectron spectroscopy (UPS). The thickness of the film was slightly more than the one used in our previous measurements (1–5 nm).[32] The latter was estimated by LEIS and by UPS, i.e., MgO was deposited until no signal of the Mo substrate was visible any more. For the present MgO film, we used an evaporation time which was about a factor of 4 larger and we therefore estimate the film thickness to be 5–20 nm. All spectra that will be shown were taken with an electrostatic double-parallel-plate analyzer that is located

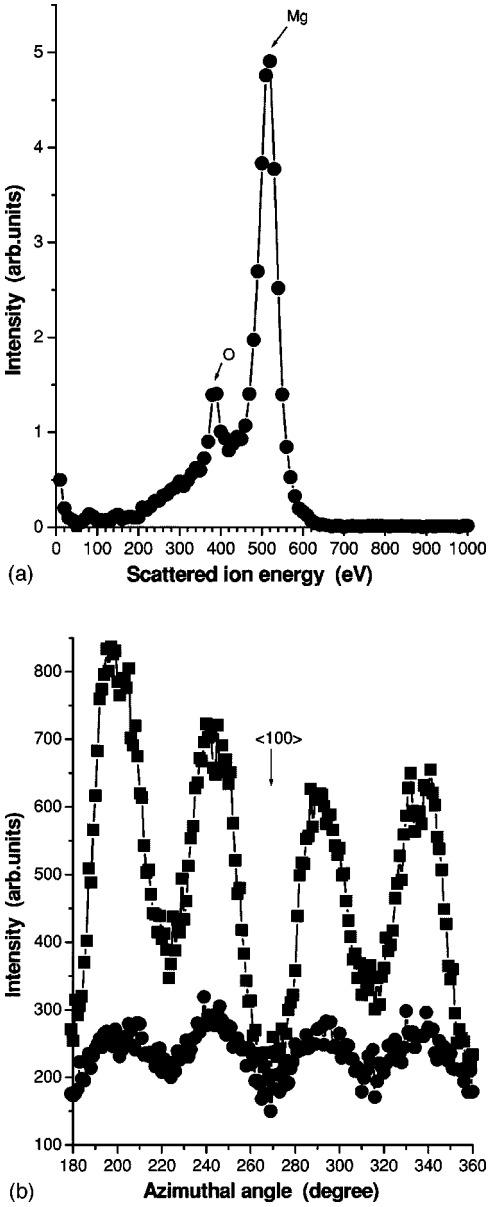

FIG. 2. Low-energy-ion-scattering spectra obtained with 1 keV He^+ ions incident on the MgO(100) thin film. (a) Energy distribution of scattered ions with the beam incident in the ⟨100⟩ direction at an angle of 45° with the surface, and a scattering angle of 135°. Scattering from Mg and O ions is indicated in the figure. Note that scattering from Mo is negligible (at energies around 750 eV). (b) Intensity of scattered ions as a function of the azimuthal angle of incidence with the ion beam incident at 5° with the surface (scattering angle 95°). (■) He^+ ions scattered from Mg ions, (●) He^+ ions scattered from O ions.

normal to the sample. Typical LEIS spectra are shown in Figs. 2(a) and 2(b). The spectra were obtained with 1 keV He^+ ions incident on the surface at an angle of 45° [Fig. 2(a)] and at an angle of 5° with the surface [Fig. 2(b)]. The energy scan [Fig. 2(a)] shows that the surface predominantly consists of Mg and O. The azimuthal scans [Fig. 2(b)], performed with the energy set to the Mg and O peaks, clearly

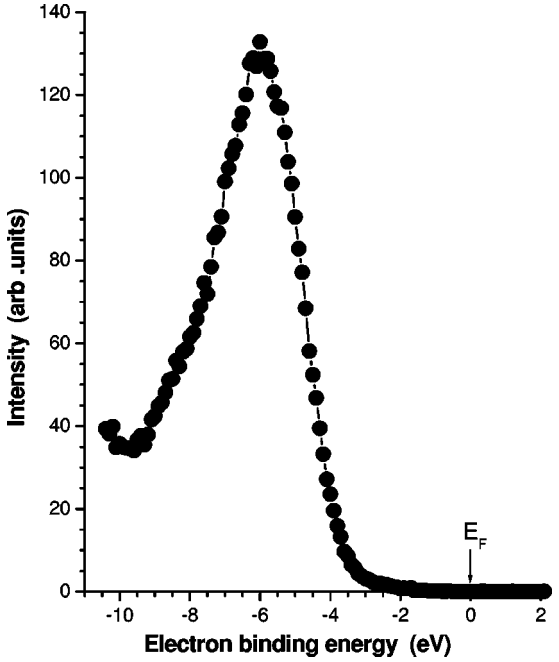

FIG. 3. UPS spectrum obtained with HeI photons (21.22 eV) incident on the MgO thin film in the ⟨100⟩ direction and at 45° with respect to the surface (observation angle normal to the surface).

show that the MgO thin film has a (100) crystalline structure. A typical UPS spectrum is shown in Fig. 3. The intensity in the energy range of 4 to 10 eV below the Fermi energy is ascribed to the $2p$ electrons of O in the valence band of MgO.[34–37] The minor intensity closer to the Fermi energy can be ascribed to electron emission from defect states.

The Xe^+ ions, with a kinetic energy of 40 eV with respect to ground potential, were directed on the thin film of MgO in the ⟨100⟩ direction at an angle of incidence of 40° with the surface. Before the measurements started, the sample was annealed for 20 min at 400 °C to desorb water and hydroxyls from the surface.[33] The experiments were carried out with the surface at an elevated temperature of 300 °C. To minimize the influence of the earth magnetic field on the low-energy part of the electron spectrum, the sample was biased at −7 V. The acceleration of the ions by this potential was not taken into account in the numbers given above. A typical measured electron spectrum is shown in Fig. 4(a). The peak at electron energy of about 6 eV corresponds to 0-eV electrons at the MgO surface. For the clean Mo surface, we observed this peak at about 8 eV, implying that the vacuum level of Mo is about 2 eV higher than the one from the MgO thin film. This is the reason that in Fig. 1 the vacuum level of Mo has been shifted by about 2 eV with respect to the one of MgO. The experiments have been performed at an elevated temperature, since we found that at room temperature the shift of the 0-eV peak was slightly more than 2 eV. The corrected spectrum, i.e., the spectrum corrected for the transmission function of the analyzer and for the acceleration of the electrons from sample to analyzer, is shown in Fig. 4(b). The spectrum has been normalized to the measured value of the total electron emission coefficient γ of 0.03 ± 0.02 (electrons per incoming ion). The latter value has been determined from the sample current and from the current of primary ions as measured in a Faraday cup. The normalized figure clearly shows that, although Auger neutralization at the MgO film is virtually impossible, Xe^+ incident on a thin

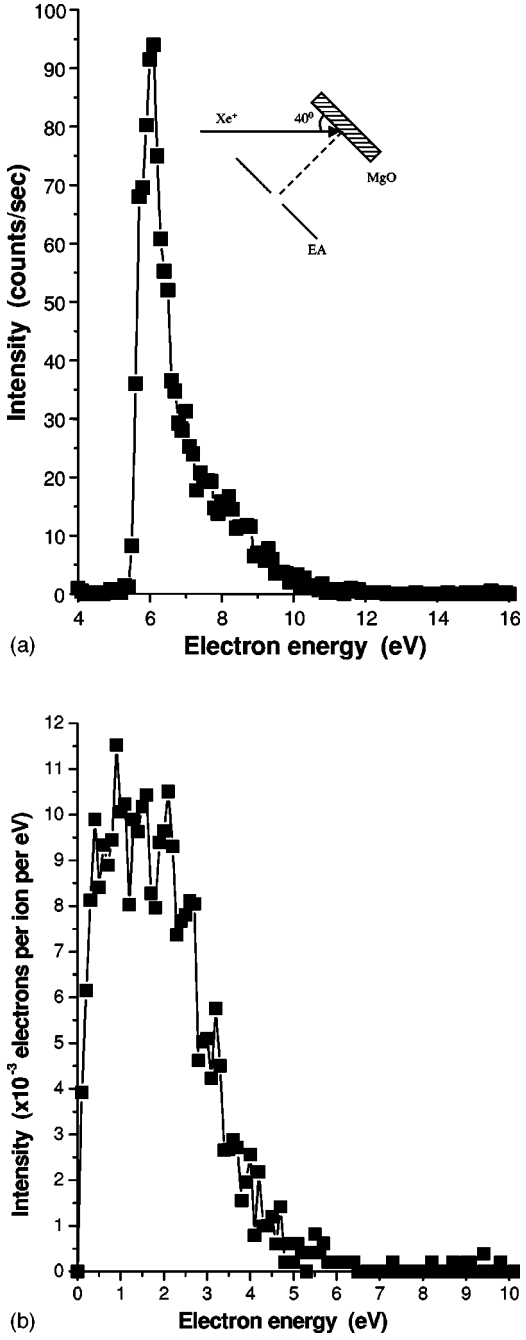

FIG. 4. (a) Electron spectrum (as measured) obtained with a 1.1 nA beam of 40 eV Xe^+ ions incident on the MgO(100) thin film in the ⟨100⟩ direction and at 40° with the surface. The energy is given with respect to the vacuum level of the analyzer. Electrons were detected normal to the surface. The crystal was held at 300 °C. A potential difference of 7 V was applied between analyzer and sample. (b) Same as (a), but after correction for the transmission function of the analyzer and for the 7 V acceleration. The energy is given with respect to the vacuum level of the MgO film. The area under the curve has been taken equal to the measured value for γ.

film of MgO does give rise to significant emission of electrons with energies up to 4–5 eV.

III. MODEL SIMULATIONS

We have performed computer simulations of the energy distribution of electrons arising in the neutralization of Xe^+ at a thin film of MgO on a Mo substrate. We assumed that each Xe^+ ion, impacting on the surface, is neutralized by resonance neutralization leaving behind a hole in the valence band of MgO (see Fig. 1). The binding energy of the hole is determined by the ionization energy of Xe of 12.1 eV (Ref. 38) and a shift due to the interaction of the ion with the MgO film. This interaction is not simply given by the well-known (upward) classical image potential shift as for metal surfaces,[39] since the dynamic dielectric function has to be taken into account. Recently it has been shown that for LiF this may lead to a downward shift.[40,41] Since for the present system no such calculations are available, we decided to use three different values for the hole binding energy: one equal to the ionization energy of Xe, one shifted upwards by 1 eV and one downwards by 1 eV.

The hole is subsequently transported to the Mo substrate where it is neutralized. During transportation through the MgO thin film, the hole may thermalize via exchange of energy with the environment. To which extent thermalization takes place depends on the film thickness and on the details of the transport mechanisms involved. For the time being we assume that the film is thin enough so that thermalization is negligible. Upon arrival at the substrate, the hole is neutralized either via Auger neutralization or via resonance neutralization. The latter process does not lead to electron emission and only affects the total electron emission yield via competition with Auger neutralization.

The next step is to calculate the electron emission arising when a hole with a specific binding energy is neutralized at the Mo substrate by an Auger process. The situation is quite similar to when a noble-gas ion is directly incident on a Mo surface. We have first simulated the latter process, the advantage being that neutralization of noble-gas ions at metal surfaces is rather well established and that experimental spectra for Mo(100) are available.[42] When successful in performing these simulations sufficiently accurate, they can easily be extended to the neutralization of holes at the Mo substrate. Only a brief discussion of the simulations will be given here, the details for other metal surfaces have been discussed elsewhere (see, e.g., Ref. 43). 40 eV He^+, Ne^+, Ar^+, and Xe^+ ions are directed on the Mo(100) surface at 40° in the ⟨100⟩ direction. The trajectories close to the surface are determined by the long-range image-charge attraction and by the short-range (binary) Molière potential (taking into account 1000 Mo atoms). After calculating the trajectories of the ions, the (distance-dependent) rate equations for Auger neutralization can be solved numerically. The transition rate for Auger neutralization was approximated by an exponential function

$$G = G_0 \exp(-az), \quad z \geq 0,$$
$$G = G_0, \quad z < 0$$

with z the distance between the ion and the image plane of the surface and G_0 and a constants that were chosen to be 0.02 and 1.84, respectively (both in atomic units). The value for G_0 is very close to recently established rates for Auger neutralization of He^+ close to metal surfaces.[9,39,43–45] For a, on the other hand, the latter publications give a range of possible values and we chose a value close to the average. It should be noted that some of the aforementioned rates were obtained for Al (Refs. 9, 43, and 44) (jellium like metal) and some for Ag (Refs. 39 and 45) (transition metal). Based on the agreement between these two metals, we decided to use the same rates for Mo. Furthermore, since, to our knowledge, there are no recent systematic and reliable studies available concerning the rates for the other noble-gas ions used in our studies, we have used the same rates for all four incident ions. We are confident that for the present purpose of our simulations these rates are sufficiently accurate. The solutions of the rate equations directly yield the probabilities for Auger neutralization as a function of distance z. The electron spectra can then be evaluated as follows. For neutralization at a specific distance z, to first order, the energy distribution equals the self-convolution of the surface density of states (SDOS) of Mo(100).[46] It is shifted with respect to the vacuum level according to the local ionization potential of the ion, which is distance dependent because of the interaction of the ion with the surface. An overall electron spectrum is obtained by integrating the distance-dependent spectra over the distance z, with the neutralization probability as weighting factor. We found that Auger neutralization predominantly takes place very close to the surface (see also Refs. 39 and 43–45). The electrons, therefore, have to escape from a surface barrier. We calculated the escape probability by assuming a cosine angular distribution for the emitted electrons and a steplike potential barrier. The height of the step we took as a free parameter in the calculations.

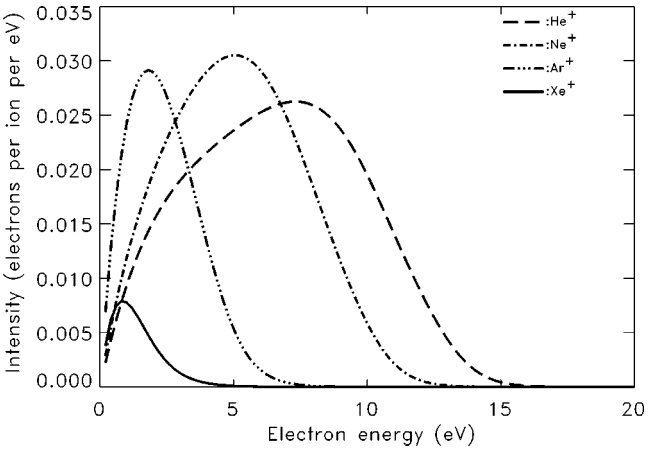

FIG. 5. Simulated electron energy distributions obtained for 40 eV noble-gas ions incident on a Mo(100) single crystal surface at 40° in the ⟨100⟩ direction.

The results of the simulations are shown in Fig. 5. We found the potential barrier to be a critical parameter, the results shown were obtained for a value of 4.5 eV. The simulated spectra resemble the measurements performed by Hagstrum [42] quite well: in width, shape, and absolute intensity. For the present purpose of the simulations these results are sufficiently accurate.

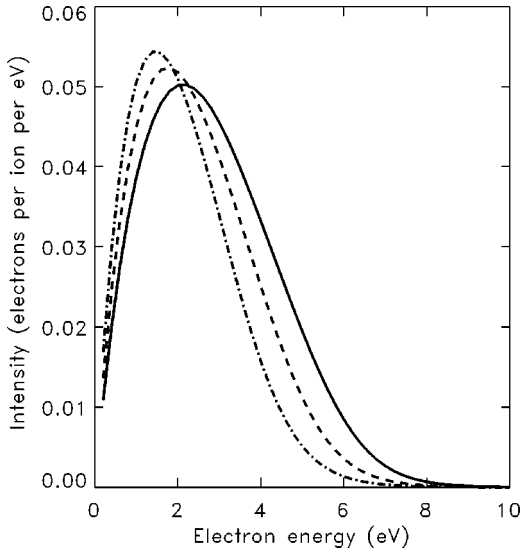

FIG. 6. Simulated electron energy distributions obtained with 40 eV Xe^+ ions incident on the MgO(100) thin film deposited on the Mo(100) substrate (same conditions as used in the experiments shown in Fig. 4. Upon neutralization, the holes have binding energies of 11.8 (solid curve), 10.8 (dashed curve), and 9.8 eV (dash-dotted curve) with respect to the vacuum level of MgO.

The next step in the simulations is to replace the noble-gas ions by the holes. As discussed before, a hole created in the MgO thin film is transported to the Mo substrate. Since we do not know the exact mechanism for hole transportation, it does not make sense to calculate the probability for neutralization along a "trajectory," as we did for noble-gas ions. We therefore assumed that neutralization of the holes takes place at a fixed distance above the Mo substrate, i.e., at a distance that corresponds to the average distance of neutralization for incident noble-gas ions and with a similar shift in binding energy due to image-charge interaction [1.3 eV (Ref. 39)]. Therefore, upon neutralization, the holes have binding energies of 9.8, 10.8, and 11.8 eV with respect to the vacuum level of MgO (binding energies of the holes upon creation, for which we used three values, minus the image-charge shift at the Mo substrate). The electron spectra, resulting from Auger neutralization of the holes at the substrate, can now be evluated as self-convolutions of the SDOS of Mo. It should be noted that the shift of the SDOS of Mo of about 2 eV with respect to the SDOS of MgO has been taken into account (see Fig. 1). This shift also affects the surface barrier, for which we used a value of 2.5 eV. Since the mean free path of low-energy electrons in MgO is large, we have furthermore assumed that the MgO thin film is fully transparent for electrons emitted from the Mo substrate. The results of the simulations are shown in Fig. 6. The energy range of emitted electrons and the shape of the simulated spectra agree quite well with the experimental results [Fig. 4(b)]. We take this as support for our model that holes are transported through an insulating film to the substrate where they give rise to electron emission. The absolute intensity of the simulated spectra is about a factor of 5 larger than the experimental one, which may largely be due to competition of Auger neutralization with resonant neutralization (of the holes at the substrate), not taken into account in the simulations. It seems that the simulation with the hole with the lowest binding energy agrees best with the experimental energy distribution.

IV. DISCUSSION

From our measurements we concluded that there is a potential difference of approximately 2 V between Mo substrate and MgO thin film. This conclusion was reached by comparison of the positions of the 0-eV electron peaks in the accelerated spectra for two situations, bombardment of a clean Mo surface and a Mo surface covered with a MgO thin film [see Fig. 4(a)]. In Fig. 1 we drew the vacuum level of MgO as a horizontal line, as if charges are only present at the interface. Of course, it may also be that charges are present throughout the MgO film, leading to potential gradients, and therefore to electric fields within the film. Since positive charges in the MgO film are compensated for by negative charges at the Mo surface (image charges), the direction of the net electric field would be towards the Mo substrate.

The exact origin of this small charging effect is not of importance for the present publication. Since we did not observe any shift of the 0-eV peak during the measurements, the holes created in the MgO film by resonant neutralization of Xe^+ are continuously being removed. In our model we have assumed that the holes are transported to the substrate, where they are neutralized. The holes are "hot" since they are localized deep inside the valence band of MgO. Since the SDOS in this energy regime mainly arises from the $2p$ electrons of O, the holes are localized on O sites and are therefore equivalent to O^- ions in the O^{2-} sublattice. Transportation of holes is likely to proceed via hopping of electrons in the reverse direction. Many hops will eventually lead to thermalization of the holes and delocalize them over the valence band.

The number of hops needed to transport holes through the film to the substrate is determined by the film thickness and by the detailed hopping mechanism. The thin film used in the present measurements contains tens of monolayers. Since an electric field in the direction of the substrate may be present, the holes could "drift" towards the substrate. Assuming that hopping only takes place between adjacent monolayers, this would imply that the holes reach the substrate after—as a minimum—tens of hops. If hole transportation is not dominated by drift but by a random-walk-type process, the average number of hops would be much larger, i.e., of the order of a few hundred to a few thousand (proportional to the square of the number of monolayers). Since thermalization of the holes is strongly related to the number of hops, experimental information on the degree of thermalization may reveal details of the transport mechanism. For the present results, however, this is not possible. Although we found best agreement with experiment for the simulation with the hole with the lowest binding energy, we cannot determine the degree of thermalization: a hole with this binding energy may be directly created in the neutralization process or via a hole with initially a larger binding energy and subsequent thermalization. Further systematic experiments, e.g. as a function of film thickness, are needed as well as theoretical studies.

Finally, electron-emission studies have recently been published for 10–100 keV protons impacting on insulating rare-gas solids on a Au substrate.[47] Assuming isotropic excitation of electrons in the insulating film, one would expect that 50% of them would be directed towards the vacuum side. However, from the analysis of their spectra, the authors found significantly larger fractions. They ascribe these large fractions to electric fields present in the insulating films that direct the electrons away from the substrate. We propose that transportation of holes to the Au substrate, where they are neutralized by Auger processes giving rise to additional electron emission, also contributes to these large fractions.

V. CONCLUSIONS

We have presented electron spectra arising from low-energy Xe^+ ions scattering off a thin film of MgO on a Mo substrate. We have shown that our simulated electron spectra, arising from the neutralization of holes at the Mo substrate, agree quite well with the experimental spectra. The results support our previously proposed model that holes created in the MgO film are transported to the Mo substrate, where they are neutralized by Auger processes. For the thin film used in the experiments, we are presently not able to determine whether or not the holes thermalize during the transportation process. Further research is needed to get this more detailed information.

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