

Calculation of Secondary Electron Emission Yield γ From MgO Surface

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Abstract—Secondary electron emission yield γ values for rare-gas particles (He, Ne, Ar, Kr, and Xe ions of atoms and molecules, metastable atoms, and excimers) of MgO deposited under optimum conditions for the highest γ values were calculated assuming the Auger transitions between the valence band, and the F (oxygen ion vacancy + two electrons) and F^+ (oxygen ion vacancy + one electron) centers in the MgO surface. These calculated γ values are probably the same as γ values for MgO used in practice. As for combination of the MgO with these rare-gas particles, all the calculated γ values fall to nonzero; resonance neutralization cannot occur for the rare-gas particles except Ne and Xe₂ ions. Therefore, γ values of the MgO for these rare-gas particles, other than Ne and Xe₂ ions, are determined only by Auger neutralization. For Ne and Xe₂ ions, the influence of resonance neutralization effect on calculated γ values of ions is small. Therefore, γ values of the MgO for Ne and Xe₂ ions are also almost determined only by Auger neutralization. The γ values for the ions of atoms are a little larger than those for the ions of molecules. The γ values of the metastable atoms are also a little larger than those of the excimers. As for MgO without defect states, calculated γ values of Ar, Kr, and Xe ions of atoms and molecules fall to zero; calculated γ value of Xe₂ excimer at the lowest continuous spectrum also falls to zero; these calculated γ values for MgO without defect states are probably the lowest values theoretically. As for rare-gas ions of atoms, the calculated γ values have been compared with experimental results reported previously. These results will be useful in detailed investigations into the mechanism of discharge of plasma display panels (PDPs).

Index Terms—Plasma display panels (PDPs), protective layer, MgO, secondary electron emission yield γ , F center.

I. INTRODUCTION

THE secondary electron emission yield γ of the cathode is an important factor for improving the discharge characteristics of plasma display panels (PDPs) because of its close relationship with the discharge voltage. In PDPs, the electrodes are covered with glass, which is usually coated with an MgO film because of its low breakdown voltage and good durability [1].

The theoretical γ values of MgO without energy bands in the bandgap for Ne and Ar ions were calculated [2] from Hagstrum's theory [3], [4]. For an insulator without energy bands in the band gap, we have calculated the generalized relations between the γ values and physical parameters from Hagstrum's theory [2]–[4] and showed that the γ values of MgO without energy bands in the bandgap for Kr and Xe ions fall to zero [5], [6]. Additionally, the γ values of MgO with one defect state in the bandgap were calculated theoretically

[7], although the energy level of the defect state used in this calculation was determined arbitrarily. In order to investigate the energy bands in the band gap, the cathodoluminescence (CL) spectra of MgO were measured. The CL spectra from these energy bands depended on the substrate temperature during MgO film deposition [8]. Moreover, the influence of the oxygen feed during MgO film deposition on the CL spectra has been reported [9]. We also measured CL spectra of MgO films, deposited at several oxygen partial pressures and observed CL peaks at around 520 and 370 nm [10]. It has been suggested that the 525- and 375-nm bands are probably due to the F and F^+ centers, respectively, in the MgO surface [11], [12]. The breakdown voltages decreased with increasing CL intensities from the F and F^+ centers, especially from the F^+ centers. These result suggested that the γ values also increase with increasing numerical densities of the F and F^+ centers, especially for F^+ centers [10]. The γ values of MgO for Ne and Xe ions, which include the F and F^+ bands, were calculated assuming that the probabilities of transitions are proportional to the measured CL intensities from the F and F^+ bands in the MgO. Here, the γ values of the MgO film deposited at the oxygen partial pressure (1.2×10^{-4} torr) and substrate temperature (300 °C) reach the highest [10]. Throughout this paper, we call these deposition conditions the optimum conditions.

In this paper, for rare-gas ions and metastable atoms, the γ values of MgO deposited under the optimum conditions were calculated. Moreover, for ionized and metastable rare-gas molecules, the γ values of MgO deposited under the optimum conditions were also calculated. These calculated γ values, except γ values of Ne and Xe ions, have not been reported. These calculated γ values of MgO deposited under the optimum conditions were compared with those of MgO without energy bands in the band gap. Regarding rare-gas ions, experimental γ values were previously reported. Therefore, the calculated γ values of MgO were compared with these experimental results.

II. DERIVATION OF SECONDARY ELECTRON EMISSION YIELD γ

A. Conditions for Secondary Electron Emission

According to the research by Hagstrum [3], [4], it is known that secondary electron emission by low-velocity ions, as in conventional gas-discharge phenomena [13], does not depend on kinetic energy but mostly on the potential (internal) energy of the ion. In this case, the mechanism of electron emission consists of the following two processes:

- 1) Auger neutralization (one step);
- 2) resonance neutralization + Auger deexcitation (two steps).

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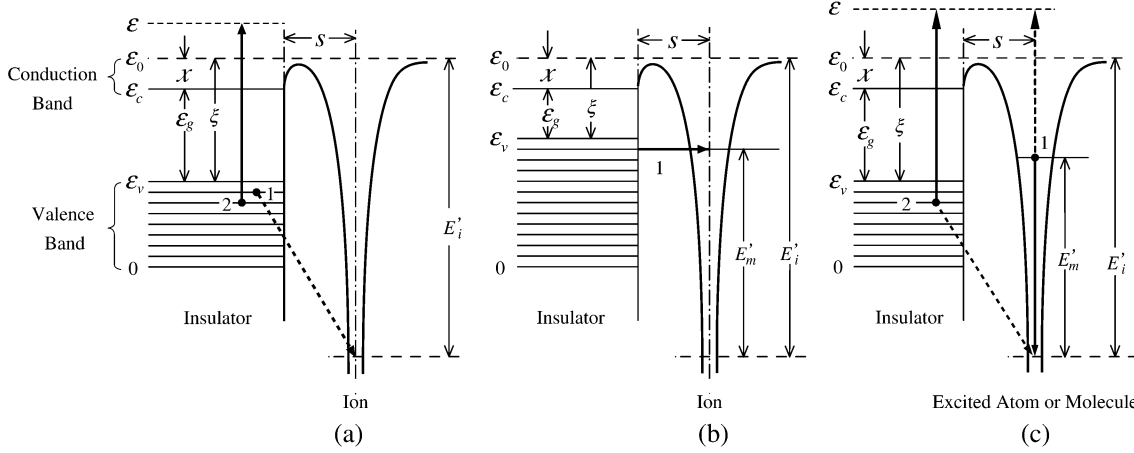


Fig. 1. Schematic diagram illustrating electronic transitions at an insulator surface. (a) Auger neutralization of an ion. (b) Resonance neutralization of an ion. (c) Auger deexcitation of an excited atom or molecule.

Here, Auger neutralization, resonance neutralization (the inverse of resonance ionization), and Auger deexcitation are tunnel effects, as shown in Fig. 1(a)–(c), where the latter two are concerned with the excited state of the atom, especially the metastable states. The notions of physical parameters used in Fig. 1, as defined in Table I, are also used throughout the paper. When defect states do not exist in the band gap of an insulator, the necessary condition that 1) and 2) occur is given by $E'_i \geq \xi + \varepsilon_g$ and $\varepsilon_0 \geq E'_i - E'_m \geq \xi$. Therefore, depending on the combination of an insulator and a gas, the following cases exist: only 1) or 2) occurs; both 1) and 2) occur; or neither 1) nor 2) occur. Moreover, the necessary conditions that the electron can be ejected by the above mechanisms are (i) $E'_i \geq 2\xi$ and (ii) $E'_m \geq \xi$.

B. Secondary Electron Emission Yield γ^N Based on Auger Neutralization

The electron energy distribution function $n(\varepsilon)$ in the valence band of the insulator is given by the product of the state density, $\rho(\varepsilon)$, and the Fermi–Dirac distribution function, $f(\varepsilon)$, where the latter can be regarded as a step function at room temperature, that is, $f(\varepsilon) = 1$ for $\varepsilon \leq \varepsilon_F$ and $f(\varepsilon) = 0$ for $\varepsilon \geq \varepsilon_F$. As in Fig. 1(a), when electron 1 moves to the ground state of an atom and electron 2 is excited at the same time, the energy distribution $E'_i(\varepsilon)$ of the excited electron is given by the following expression by using the Auger transform $T[\cdot]$ defined in it, with the assumption that the matrix element of this transition is independent of the energies of these electrons [4]

$$\begin{aligned} N'_i(\varepsilon) &\propto \rho_0(\varepsilon) \int_0^{\varepsilon_v} \int_0^{\varepsilon_v} n(\varepsilon_1)n(\varepsilon_2) \\ &\quad \times \delta(\varepsilon - \varepsilon_1 - \varepsilon_2 + \varepsilon_0 - E'_i)d\varepsilon_1d\varepsilon_2 \\ &\equiv \rho_0(\varepsilon)T\left[\frac{\varepsilon + \varepsilon_0 - E'_i}{2}\right] \end{aligned} \quad (1)$$

where, $\delta(\cdot)$ is the Dirac delta function and indicates the conservation of energy, and $\rho_0(\varepsilon)$ is the state density for the excited electron and is considered to be proportional to $(\varepsilon - \varepsilon_c)^{1/2}$. Next, for an electron, thus excited, to escape from the solid, it is necessary that $\varepsilon > \varepsilon_0$. Assuming that this escape probability

TABLE I
DEFINITION OF PHYSICAL PARAMETERS

ε	: energy of an excited electron
ε_0	: energy of vacuum level
ε_c	: energy of bottom of conduction band
ε_v	: energy of top of valence band
ε_f	: energy of top of F band from the vacuum level
ε_{f^+}	: energy of top of F^+ band from the vacuum level
$\varepsilon_g \equiv \varepsilon_c - \varepsilon_v$: band gap
$\chi \equiv \varepsilon_0 - \varepsilon_c$: electron affinity
$\xi \equiv \chi + \varepsilon_g \equiv \varepsilon_0 - \varepsilon_v$	
E'_i	: ionization energy at a distance s from the solid surface
E'_m	: excitation energy at a distance s from the solid surface

is $P_e(\varepsilon)$, we obtain the following expression for the secondary electron emission yield, γ^N , at a distance s

$$\begin{aligned} \gamma^N &= \int_{\max\{E'_i - 2\xi + \varepsilon_0, \varepsilon_0\}}^{E'_i - 2\xi + \varepsilon_0} P_e(\varepsilon) \sqrt{\varepsilon - \varepsilon_c} T\left[\frac{\varepsilon + \varepsilon_0 - E'_i}{2}\right] d\varepsilon \\ &\quad \int_{\max\{E'_i - \varepsilon_0, \varepsilon_c\}}^{E'_i - 2\xi + \varepsilon_0} \sqrt{\varepsilon - \varepsilon_c} T\left[\frac{\varepsilon + \varepsilon_0 - E'_i}{2}\right] d\varepsilon \end{aligned} \quad (2)$$

where $P_e(\varepsilon)$ for the electron excited by Auger neutralization is not isotropic. By taking this into consideration, the following formula has been proposed, introducing parameters α and β [4]

$$P_e(\varepsilon) = \frac{1}{2} [1 - (\varepsilon_0/\varepsilon)^\beta]^\alpha, \quad \varepsilon > \varepsilon_0. \quad (3)$$

Hagstrum determined $\alpha = 0.248, \beta = 1.0$ by adjusting to correspond with the experimental results of He^+ for Ge. These values are also used in the present calculation. Since a transition occurs when an ion travels a long way to the solid surface, the desired γ^N must be an average of γ^N over s . In practice, however, it is known from experiments that transitions occur collectively at a certain distance $s = s_m$ [3], [4]. Therefore,

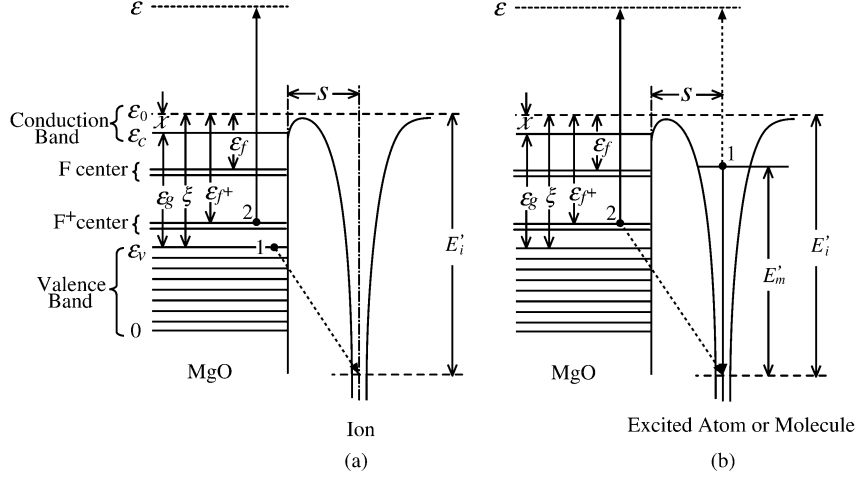


Fig. 2. Schematic diagram illustrating electronic transitions at an MgO surface that includes F and F^+ bands. (a) Auger neutralization of an ion. (b) Auger deexcitation of an excited atom or molecule.

substituting the ionization energy at $s = s_m$ for E_i' , we can obtain a good approximation of γ^N .

In practical calculations, the state density $\rho(\varepsilon)$ in $n(\varepsilon)$ must be given. But this varies, depending on the kind of insulator. This being the case, the calculations here are performed for two cases, a flatband and a parabolic band, to study the influence of the state-density profile on the γ value. Furthermore, by putting $x \equiv \varepsilon/\varepsilon_0$ and $\sigma \equiv \varepsilon_c/\varepsilon_0$ to normalize the variables, we obtain the following formula from (2)

$$\gamma'^N = \int_{\max\{\alpha_i, 1\}}^{\beta_i} P_e^*(x) \sqrt{x - \sigma} T^*(x) dx \quad \Bigg/ \quad \int_{\max\{\alpha_i, \sigma\}}^{\beta_i} \sqrt{x - \sigma} T^*(x) dx. \quad (4)$$

Where $\alpha_i \equiv E_i'/\varepsilon_0 - 1$, $\beta_i \equiv (E_i' - 2\xi)/\varepsilon_0 + 1$ and $P_e^*(\varepsilon) \equiv \frac{1}{2}(1 - x^{-\beta})^\alpha$. The function $T^*[x]$, which is finite only when $\alpha_i < x < \beta_i$, is given as follows, depending on the state density assumed for flatband

$$\begin{aligned} T^*[x] &= x - \alpha_i, & \alpha_i < x \leq (\alpha_i + \beta_i)/2 \\ T^*[x] &= \beta_i - x, & (\alpha_i + \beta_i)/2 < x < \beta_i. \end{aligned} \quad (5)$$

C. Secondary Electron Emission Yield γ^D Based on Auger Deexcitation

When an ion approaches a solid surface and resonance neutralization occurs, the ion becomes an excited atom. After this process, unless resonance ionization occurs with the condition $E_i' - E_m' < \chi$ for a smaller distance s , the excited atom is considered to return to the ground state by Auger deexcitation. Accordingly, as a component of the secondary electron emission yield, γ_i , by an ion, we have to consider γ^D as well as the above-mentioned γ^N . Specifically, when the transition ratio of Auger neutralization to resonance neutralization is g to $(1 - g)$, then γ_i is given by

$$\gamma_i = g\gamma^N + (1 - g)\gamma^D. \quad (6)$$

TABLE II
BAND PARAMETERS OF MgO USED IN THIS STUDY

Energy (eV)	ε_v	ε_g	χ	ε_0	ε_f	ε_{f+}
MgO	5.0	6.8	0.85	12.65	3.8	5.3

On the other hand, in the secondary electron emission yield γ_m by a metastable atom, this γ^D is considered to be the main component, namely, $\gamma_m = \gamma^D$.

Similarly to the procedure for obtaining γ^N , the energy distribution, $N_i'(\varepsilon)$, of the excited electron is given by

$$\begin{aligned} N_i'(\varepsilon) &\propto \rho_0 \int_0^{\varepsilon_v} n(\varepsilon_2) \delta(\varepsilon_2 + E_m' - \varepsilon) d\varepsilon_2 \\ &= \rho_0(\varepsilon) n(\varepsilon - E_m'). \end{aligned} \quad (7)$$

Also, in Auger deexcitation, by adopting the same escape probability as in Auger neutralization and the excitation energy E_m' at $s = s_m$, γ^D is obtained as follows:

$$\begin{aligned} \gamma^D &= \int_{\max\{E_m', \varepsilon_0\}}^{E_m' - \xi + \varepsilon_0} P_e(\varepsilon) \sqrt{\varepsilon - \varepsilon_c} n(\varepsilon - E_m') d\varepsilon \\ &\quad \Bigg/ \quad \int_{\max\{E_m', \varepsilon_c\}}^{E_m' - \xi + \varepsilon_0} \sqrt{\varepsilon - \varepsilon_c} n(\varepsilon - E_m') d\varepsilon. \end{aligned} \quad (8)$$

Here, as in Auger neutralization, assuming $\rho(\varepsilon)$ is a flatband, and putting $x \equiv \varepsilon/\varepsilon_0$ and $\sigma \equiv \varepsilon_c/\varepsilon_0$, we obtain

$$\begin{aligned} \gamma^D &= \int_{\max\{\alpha_m, 1\}}^{\beta_m} P_e^*(x) \sqrt{x - \sigma} n^*(x) dx \\ &\quad \Bigg/ \quad \int_{\max\{\alpha_m, \sigma\}}^{\beta_m} \sqrt{x - \sigma} n^*(x) dx \end{aligned} \quad (9)$$

where $\alpha_m \equiv E_m'/\varepsilon_0$, and $\beta_m \equiv (E_m' - \xi)/\varepsilon_0 + 1$. The function $n^*(x)$, which is finite only when $\alpha_m < x < \beta_m$, is given as follows, depending on the state density assumed for flatband

$$n^*(x) = 1, \quad \alpha_m < x < \beta_m. \quad (10)$$

TABLE III
CALCULATED γ VALUES BASED ON AUGER NEUTRALIZATION BETWEEN THE VALENCE BAND AND THE F AND F^+ BANDS OF MgO FOR RARE-GAS IONS

E'_i (eV)	γ_{ff}	γ_{f+f}	γ_{f^+}	γ_{f^+f}	γ_{fv}	γ_{vf}	γ_{f+v}	γ_{vf^+}	γ_{vv}
He ⁺ 23.27	0.472	0.469	0.460	0.456	0.420	0.459	0.413	0.441	0.329
He ₂ ⁺ 22.23	0.470	0.467	0.457	0.453	0.415	0.455	0.407	0.435	0.307
Ne ⁺ 20.36	0.466	0.462	0.451	0.446	0.405	0.446	0.395	0.421	0.257
Ne ₂ ⁺ 20.33	0.466	0.462	0.451	0.445	0.405	0.446	0.394	0.420	0.256
Ar ⁺ 14.80	0.445	0.435	0.419	0.401	0.346	0.357	0.226	0.234	0
Ar ₂ ⁺ 14.50	0.444	0.432	0.416	0.396	0.334	0.344	0.206	0.215	0
Kr ⁺ 14.00	0.440	0.427	0.410	0.387	0.299	0.311	0.165	0.174	0
Kr ₂ ⁺ 12.87	0.431	0.412	0.394	0.358	0.197	0.220	0	0	0
Xe ⁺ 11.33	0.411	0.377	0.357	0.258	0	0	0	0	0
Xe ₂ ⁺ 11.02	0.406	0.366	0.345	0.165	0	0	0	0	0

III. DERIVATION OF SECONDARY ELECTRON EMISSION YIELD γ OF MgO WITH DEFECT STATES

In order to include the effects of the F and F^+ bands in γ^N , we have to consider Auger transitions between the valence band, and the F and F^+ bands. Fig. 2(a) shows a schematic diagram of Auger neutralization of an ion at the MgO surface that possesses the F and F^+ bands. The notions of physical parameters used in Fig. 2 are also defined in Table I. The secondary electron emission yields γ^N derived from these transitions were calculated using (4). The band parameters of MgO used in these calculations are shown in Table II, where $\varepsilon_v = 5.0$ eV, $\varepsilon_g = 6.8$ eV, and $\chi = 0.85$ eV [2]. In general, it is not easy to determine the values of ε_f and ε_{f^+} using CL, due to the Stokes shifts. Therefore, the values of $\varepsilon_f = 3.8$ eV and $\varepsilon_{f^+} = 5.3$ eV, as shown in Table II, were assumed, based on the results of the calculations which were made using the embedded cluster method [14]. Table III shows the calculated γ^N values, based on Auger neutralization between the valence band, and the F and F^+ bands of MgO for He, Ne, Ar, Kr, and Xe ions of atoms and molecules. Here, as in Fig. 2(a), when an electron 1 in the valence band moves to the ground state and an electron 2 in the F^+ band is excited at the same time, the symbol for this secondary electron emission yield is assigned as γ_{vf^+} , for example. The symbols for the other secondary electron emission yields are also represented by similar procedures. In practical calculations, the estimated values of E'_i for He, Ne, Ar, and Xe ions are 23.27, 20.36, 14.80, and 11.33 eV, respectively, [7], [15]. As for Kr, He₂, Ne₂, Ar₂, Kr₂, and Xe₂ ions, the values of E'_i are 14.00, 22.23, 20.33, 14.50, 12.87, and 11.02 eV, respectively [16], [17] on the assumption that the values of E'_i are equal to those of E_i (free space ionization energy). The widths of the F and F^+ bands are assumed to be 0.3 eV. For Xe and Xe₂ ions, the values of γ_{fv} , γ_{vf} , γ_{f+v} , γ_{vf^+} , and γ_{vv} fall to zero because of the conditions $E'_i < \xi + \varepsilon_f$, $E'_i < \xi + \varepsilon_{f^+}$, $E'_i < \xi + \varepsilon_{f^+}$, $E'_i < \xi + \varepsilon_{f^+}$, and $E'_i < 2\xi$, respectively, as shown in Table III. The values of γ_{vv} for Ar, Kr, Ar₂, and Kr₂ ions are also zero because of the condition $E'_i < 2\xi$. The values of γ_{f+v} , γ_{vf^+} for Kr₂ ions are similarly zero because of the condition $E'_i < \xi + \varepsilon_{f^+}$.

Fig. 2(b) shows a schematic diagram of Auger deexcitation of an excited atom or molecule at the MgO surface that includes

TABLE IV
CALCULATED γ VALUES BASED ON AUGER DEEXCITATION FOR THE VALENCE BAND AND THE F AND F^+ BANDS OF MgO FOR EXCITED RARE-GAS ATOMS AND MOLECULES

	(eV)	γ_f	γ_{f^+}	γ_v
He E'_m	19.81	0.472	0.461	0.406
He ₂ E'_m	17.79	0.469	0.456	0.392
Ne E'_m	16.61	0.466	0.452	0.382
Ne ₂ E'_m	16.07	0.465	0.450	0.376
Ar E'_m	11.55	0.449	0.425	0.276
Ar ₂ E'_m	10.86	0.445	0.419	0.259
Kr E'_m	9.91	0.439	0.409	0.226
Kr ₂ E'_m	8.49	0.426	0.386	0.133
Kr ₂ E'_m	9.34	0.435	0.401	0.198
Xe E'_m	8.31	0.424	0.382	0.112
Xe ₂ E'_m	7.17	0.408	0.349	0
Xe ₂ E'_m	8.16	0.422	0.379	0.092

the F and F^+ bands. The secondary electron emission yields γ^D derived from these transitions were calculated using (9). Table IV shows the calculated γ^D values, based on Auger deexcitation between the valence band, and the F and F^+ bands of MgO for metastable He, Ne, Ar, Kr, Xe atoms and He₂, Ne₂, Ar₂, Kr₂, Xe₂ excimers. Here, as in Fig. 2(b), when an electron 1 in the excited state of atoms or molecules moves to the ground state and an electron 2 in the F^+ band is excited at the same time, the symbol of this secondary electron emission yield is represented by γ_{f^+} , for example. The symbols of the other secondary electron emission yields are also represented by similar procedures. As for the Kr₂ and Xe₂ excimers, not only the values of γ^D for E'_m (energy of the central wavelength in the lowest continuous spectrum at a distance s from the MgO surface), but also those of γ^D for E'_m (energy of the central wavelength in the second-lowest continuous spectrum at a distance s from the MgO surface) were calculated. The calculations of γ^D were made on the assumption that the values of E'_m , E'_m , and E'_m are equal to those of energy in free space. The values of E'_m for metastable He, Ne, Ar, Kr, and Xe atoms

TABLE V
CALCULATED γ VALUES BASE D ON AUGER NEUTRALIZATION OF MgO FOR RARE-GAS IONS

Gas	He	He ₂	Ne	Ne ₂	Ar	Ar ₂	Kr	Kr ₂	Xe	Xe ₂
γ_{\min}^N	0.329	0.307	0.257	0.256	0	0	0	0	0	0
γ_{\max}^N	0.349	0.330	0.287	0.286	0.0484	0.0448	0.0371	0.00563	0.00292	0.00198

TABLE VI
CALCULATED γ VALUES BASE D ON AUGER DEEXCITATION OF MgO FOR EXCITED RARE-GAS ATOMS AND MOLECULES

Gas	He	He ₂	Ne	Ne ₂	Ar	Ar ₂	Kr	Kr ₂		Xe	Xe ₂	
								E_m^*	E_m^{**}		E_m^*	E_m^{**}
γ_{\min}^D	0.406	0.392	0.382	0.376	0.276	0.259	0.226	0.133	0.198	0.112	0	0.092
γ_{\max}^D	0.412	0.399	0.389	0.384	0.292	0.276	0.245	0.160	0.219	0.140	0.0367	0.122

are 19.81, 16.61, 11.55, 9.91, and 8.31 eV, respectively [6]. The values of $E_m'^*$ for He₂, Ne₂, Ar₂, Kr₂, and Xe₂ excimers are 17.79, 16.07, 10.86, 8.49, and 7.17 eV, respectively [17], [18]. The values of $E_m'^{**}$ for Kr₂ and Xe₂ excimers are 9.34 and 8.16 eV, respectively. As for $E_m'^*$ of Xe₂ excimer, the value of γ_v falls to zero because of the condition $E_m'^* < \xi$, as shown in Table IV.

According to time-dependent perturbation theory [3], the probabilities of transitions are expected to be proportional to the density of states [7]. Therefore, the densities of the F and F^+ bands for MgO are assumed to be proportional to the CL intensities from the F and F^+ bands. Based on this assumption, the γ^N and γ^D values of MgO, which include the F and F^+ centers, are respectively obtained as follows:

$$\begin{aligned} \gamma^N = & (P_f R_f)^2 \gamma_{ff} + (P_{f+} R_{f+})^2 \gamma_{f+f+} + P_v^2 \gamma_{vv} \\ & + (P_f R_f P_{f+} R_{f+}) (\gamma_{ff+} + \gamma_{f+f+}) + (P_f R_f P_v) (\gamma_{fv} \\ & + \gamma_{vf}) + (P_{f+} R_{f+} P_v) (\gamma_{f+v} \gamma_{vf+}) \end{aligned} \quad (11)$$

$$\gamma^D = P_f R_f \gamma_f + P_{f+} R_{f+} \gamma_{f+} + P_v \gamma_v \quad (12)$$

where $P_f R_f + P_{f+} R_{f+} + P_v = 1$; R_f and R_{f+} represent, respectively, normalized density of the F and F^+ bands for MgO; P_v , P_f , and P_{f+} represent the density ratios of the valence band, R_f and R_{f+} , to the total density.

IV. RESULTS AND DISCUSSION

The γ^N values of He, Ne, Ar, Kr, and Xe ions of atoms and molecules for an MgO film, deposited under the optimum conditions for the highest γ values, were calculated using (11) and the calculated values in Table III. In this calculation, it was determined that the values of R_f , R_{f+} , P_f , and P_{f+} were 0.45, 1, 0.01, and 0.1, respectively, by adjusting to fit the experimental results from CL spectra [10]. These calculated γ^N values are probably the highest γ_{\max}^N values of MgO. Table V shows the results obtained. Here, γ^N values of MgO without defect states also shown; these γ^N values are equal to γ_{vv} values in Table III. These calculated γ^N values are probably the lowest γ_{\min}^N values of MgO.

The γ^D values of metastable He, Ne, Ar, Kr, Xe atoms and He₂, Ne₂, Ar₂, Kr₂, Xe₂ excimers for MgO film deposited under

the optimum conditions for the highest γ values were also calculated using (12) and the calculated values in Table IV. These calculated γ^D values are probably the highest γ_{\max}^D values of MgO. Table VI shows the results obtained. Here, γ^D values for MgO without defect states also shown; these γ^D values are equal to γ_v values in Table IV. These calculated γ^D values are probably the lowest γ_{\min}^D values of MgO.

As mentioned above, we also have to consider the electron emission process: resonance neutralization + Auger deexcitation. The resonance neutralization cannot occur with the combinations of the band parameters for MgO (see Table II) and rare-gases shown in Tables III and IV, except for Ne and Xe₂ ions. Therefore, the γ_i values of MgO for rare-gas ions, except Ne and Xe₂ ions, are determined by Auger neutralization only, namely $\gamma_i = \gamma^N$ in Table V. The resonance neutralization for Ne and Xe₂ ions can occur because of the conditions $\varepsilon_f \leq E_i' - E_m' \leq \varepsilon_f + 0.3$ and $\varepsilon_f \leq E_i' - E_m'^* \leq \varepsilon_f + 0.3$, respectively. The γ_i values for Ne and Xe₂ ions were calculated using (6) on the assumption that $1 - g = (1/2)R_f P_f$. The calculated γ_i values for Ne and Xe₂ ions are 0.287 and 0.00206; the calculated γ^N values for Ne and Xe₂ ions are 0.287 and 0.00198. Therefore, γ values of the MgO for Ne and Xe₂ ions are also almost completely determined by Auger neutralization only.

On the other hand, in the secondary electron emission yield γ_m by metastable atoms or excimers, this γ^D is considered to be the main component, namely, $\gamma_m = \gamma^D$ in Table VI.

The γ_{\min}^N values of Ar, Kr, and Xe ions of atoms and molecules for MgO fall to zero because of the condition $E_i' < 2\xi$. The γ_{\min}^D value of the Xe₂ excimer ($E_m'^*$) for MgO falls to zero because of the condition $E_m'^* < \xi$. The difference between γ_{\max}^N and γ_{\min}^N values decreased with increasing E_i' values of ions, because the γ^N values for large E_i' values of ions are determined by the Auger transitions, which occur principally in the valence band. On the other hand, the difference between γ_{\max}^D and γ_{\min}^D values also decreased with increasing E_m' values of metastable atoms and excimers, because the γ^D values for large E_m' values of metastable atoms and excimers are determined by the Auger transitions, which occur principally in the valence band.

TABLE VII
COMPARISONS OF THE THEORETICALLY CALCULATED γ_i VALUES OF MgO
WITH EXPERIMENTAL γ_i VALUES FROM THE LITERATURE

Gas	He	Ne	Ar	Kr	Xe
$\gamma_{i \min}$	0.329	0.257	0	0	0
$\gamma_{i \max}$	0.349	0.287	0.0484	0.0371	0.00292
Ref. 19	-	0.45	0.05	-	-
Ref. 20	-	0.25	-	-	0.035
Ref. 21	0.17-0.35	0.06-0.17	≤ 0.05	≤ 0.015	≤ 0.007
Ref. 22	0.13	0.3	0.009	0.009	0.002
Ref. 23	-	0.5	0.03	-	0.003
Ref. 24	0.14	0.12	0.06	-	0.04

The γ^N values of ions of atoms are a little larger than those of molecules, as shown in Table V. The γ^D values of metastable atoms are also a little larger than those of excimers, as shown in Table VI.

As for rare-gas ions of atoms, the experimental γ_i values of MgO have been previously reported. Table VII shows the comparisons between our results and the experimental results. The results of six experiments are shown in Table VII; in three of those the γ_i values were measured using an ion beam [19], [21], [24]; the rest were estimated from breakdown voltages in gas [20], [22], [23]. In general, measurement of γ_i for MgO is not always easy because of the possible difficulties due to the charge-up effect and adsorption on a surface of a sample. Here, although the measured γ_i values are not always the same between the experiments, their tendency to vary, depending on the kind of gas ion, agrees well with our results.

V. CONCLUSION

The γ^N values of He, Ne, Ar, Kr, and Xe ions of atoms and molecules for an MgO film, deposited under the optimum conditions, were calculated, assuming Auger transitions between the valence band, and the F and F^+ centers in the MgO surface. The γ^D values of metastable He, Ne, Ar, Kr, Xe atoms and He₂, Ne₂, Ar₂, Kr₂, Xe₂ excimers for an MgO film deposited under the optimum conditions were also calculated. These calculated γ^N and γ^D values are probably the same as those used for MgO in practice. All the calculated γ values fall to nonzero with combinations of MgO and these rare-gas particles, whereas the γ^N values of Ar, Kr, and Xe ions of atoms and molecules for MgO without defect states fall to zero. The γ^D value of Xe₂ excimer (E_m^*) for MgO without defect states also falls to zero. These calculated γ^N and γ^D values for MgO without defect states are probably the lowest values theoretically.

Resonance neutralization cannot occur with the combinations of MgO deposited under the optimum conditions and these rare-gas particles, with the exception of Ne and Xe₂ ions. For Ne and Xe₂ ions, the difference between the calculated values of γ_i and γ^N was small. Therefore, γ values of the MgO

for Ne and Xe₂ ions are also almost completely determined by Auger neutralization only, namely $\gamma_i = \gamma^N$.

The difference between γ^N values of MgO deposited under the optimum conditions and those of MgO without defect states decreases with increasing ionization energy of ions because the γ^N values for ions possessing large ionization energy are determined by Auger transitions, which occur principally in the valence band. On the other hand, the difference between the γ^D values of MgO deposited under the optimum conditions and those of MgO without defect states also decreases with increasing excitation energy of metastable atoms and excimers because the γ^D values for metastable atoms and excimers which have large excitation energy are determined by Auger transitions which occur principally in the valence band.

The γ^N values of ions of atoms are a little larger than those of molecules. The γ^D values of metastable atoms are also a little larger than those of excimers.

As for rare-gas ions of atoms, the calculated γ_i values were compared with experimental results reported previously. Here, although the measured γ_i values are not always the same between the experiments, their tendency to vary, depending on the kind of gas ion, agrees well with our results.

These results will be useful for investigating the mechanism of discharge of PDPs in further detail.

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