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Ultra Accelerated QCMD Study on Secondary Electron Emission Properties of MgO Protecting Layer for Plasma Display Panels

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1. Introduction

Plasma Display Panel (PDP) is expected to become a high definition and large area display. Therefore, the development of low power driving technique is required. In spite of many experimental efforts, the power requirement of PDP is still high. For the decrease of power requirement, it is very effective to increase the secondary electron emission (SEE) coefficient (γ value) of the protecting layer in the luminescence cells shown in Fig. 1 [1]. High γ protecting layer helps to create and to sustain plasma and achieves high luminescence efficiency. Here, this SEE phenomena occur with Auger neutralization of noble gas ions which come close to the surface of protecting layer. MgO has been used as the protecting layer since the suggestion of Uchiike et al [2].

For the creation of higher γ protecting layer, many researchers measured and estimated γ values. However, the γ values obtained by experimental method were not constant because of its sensitivity to experimental condition. Therefore, γ value was calculated theoretically [3]. But the effect of noble gas ions collision on γ value was not considered yet. To make higher γ protecting layer, it is necessary to understand the properties of γ value. Therefore, to clarify the collision effect on γ value, we estimated γ value of MgO based on quantum chemical calculation.

2. Calculation method

We employed the ultra accelerated quantum chemical molecular dynamics (UAQCMD) method to estimate the γ value of MgO. The UAQCMD method can treat large scale molecular dynamics (MD) because of its low calculation cost. This method is composed of tight binding quantum chemical simulator "Colors" [4] and MD simulator "NEW-RYUDO" [5]. Colors was used for setting up inter atomic potential. By using this potential, MD simulation was performed by NEW-RYUDO.

Figure 2 shows the calculation model consisted of Ne ion and MgO (100) surface. We first carried out geometry optimization of MgO surface. With the geometry optimized structure, the collision of Ne ion was simulated. In this study, we assumed that the acceleration voltage of Ne ion is in the range from 30 V to 600 V. The bottom layer of MgO was fixed during the simulation. γ values for each acceleration voltage was calculated by equation (1) [3]. In this calculation, density of state (DOS) obtained from this simulation was applied.

$$\gamma = \int P_e(\varepsilon)\rho_c(\varepsilon)\rho_v(\varepsilon)\mathrm{d}\varepsilon \Big/ \int \rho_c(\varepsilon)\rho_v(\varepsilon)\mathrm{d}\varepsilon \qquad (1)$$

Here, ε, ρ_c and ρ_v and P_e are the electron energy, DOS of conduction band and valence band and the expulsion probability of one exited electron, respectively.

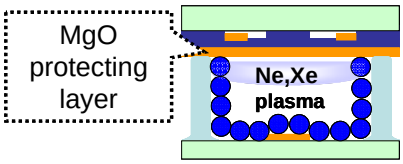

Fig. 1 Schematic of luminescence cell

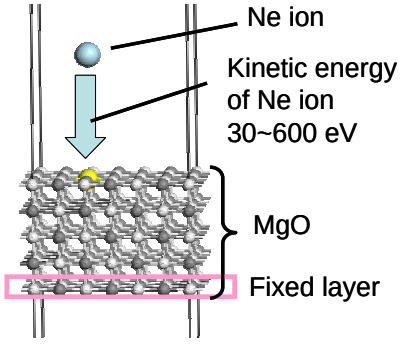

Fig. 2 Calculation model

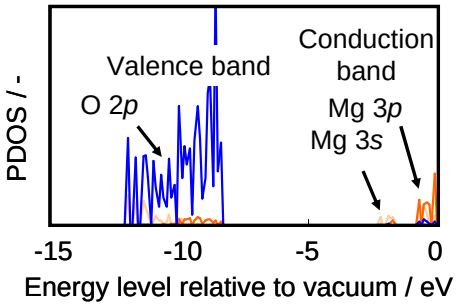

Fig. 3 PDOS of geometry optimized MgO surface

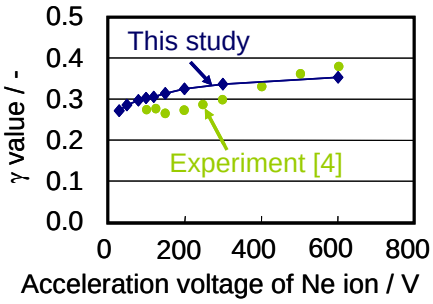

Fig. 4 Relationship between γ value and acceleration voltage of Ne ions

3. Results and discussion

Electronic Structure of MgO Surface

The electronic states of MgO surface were calculated and partial density of states (PDOS) were obtained. Figure 3 shows the PDOS of MgO surfaces. From Fig. 3, we can find that the valence band of MgO surface and the bottom of conduction band are mainly composed by O 2*p* orbital and Mg 3*s* orbital, respectively.

γ value of MgO for Ne ions

γ values were calculated by equation (1) and DOS obtained by our Colors code. Calculated and experimental [6] γ values are shown in Fig. 4. From Fig. 4, the increase in γ value with respect to acceleration voltage is shown theoretically and experimentally.

Effect of collision on γ value

To consider the effect of collision on γ value, PDOS are shown in Fig. 5 when Ne ion accelerated (a) at 50 V and (b) at 300 V come close to the surface. Compared with Fig. 3, a destabilized molecular orbital (MO) was formed in both (a) and (b). Moreover, the destabilized MO in (b) had higher energy than that of (a). Fig. 6 shows the destabilized MO for the acceleration voltage of 300 V. From Fig. 6, we can find that this MO consists of two anti-bonding interactions. One is the interaction between Ne 2*p* orbital and collided O 2*p* orbital. The other is the interaction between collided O 2*p* orbital and O 2*p* orbital around the collided O. Here, the energy of this MO increases with the increase of anti-bonding interaction. Therefore, the collision of highly accelerated Ne ion push up the energy of this MO higher because the collision of Ne ion with surface O atom decrease the Ne-O distance shoter and pushes the surface O at closer distance with subsurface O atoms. This has the

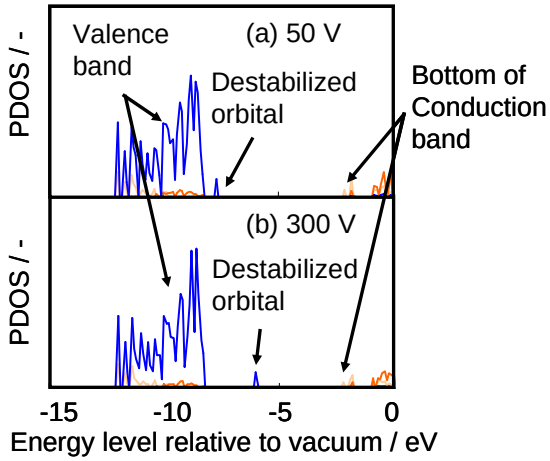

Fig. 5 PDOS when Ne ion accelerated at (a) 50 V and (b) 300 V comes closest to MgO surface.

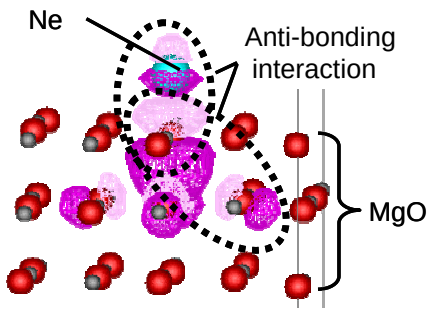

Fig. 6 Molecular orbital destabilized by the collision

effect of the increasing of the energy of this MO. The electron in high energy level can be emitted easily. Therefore, it is suggested that γ value becomes higher with the increase of acceleration voltage.

4. Conclusion

In this study, the relationship between γ value of MgO and acceleration voltage of Ne ion is clarified. It is shown that the effect of collision is important factor to study SEE phenomena.

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