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A Large Scale Quantum Chemistry Study for the High γ MgO Protecting Layer of Plasma Display Panels

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1. Introduction

Plasma display panel (PDP) is one of the most successful flat displays because of its high luminance, contrast and good motion picture resolution. To enhance these advantages, PDPs are expected to become larger area and higher definition. However, these evolutional changes could bring on the increase of its power requirement. Then there is need for low energy operation technologies.

One of solutions to the low power driving of PDP is to fabricate a protecting layer with high ion induced secondary electron emission (IISEE) coefficient (γ value). According to Townsend's discharge theory, a high γ protecting layer can decrease the driving voltage of PDP. From the report by Uchiike *et al.*[1], MgO has been used as the protecting layer material. However, in spite of its long history, MgO has not constantly performed their full γ potential yet, because of the lack of theoretical knowledge to the origin of the high γ value. Therefore, to suggest a direction for designing the high γ protecting layer, we estimated the γ values of flat, irregular, and water contamination MgO surfaces based on quantum chemistry.

2. Method

2.1 MgO Surface Modeling

To construct surface models, we used a molecular dynamics (MD) simulation program "NEW-RYUDO". For the modeling of water contamination surface, a grand canonical monte carlo (GCMC) simulation program "MONTA" was employed. In the GCMC calculation, we assumed the density of water was 1 H_2O molecular / nm^2 for simplification.

2.2 Estimation of Electronic Structure and γ value

To estimate the γ value of constructed models, we used the following equation reported by Motoyama *et al.* [2]:

$$\gamma = \int_{MAX\{0,\varepsilon_{\min}\}}^{\varepsilon_{\max}} P_e(\varepsilon)\rho_{unocc}(\varepsilon)T(\varepsilon)\mathrm{d}\varepsilon \Big/ \int_{MAX\{\varepsilon_{unocc}^{bottom},\varepsilon_{\min}\}}^{\varepsilon_{\max}} \rho_{unocc}(\varepsilon)T(\varepsilon)\mathrm{d}\varepsilon \quad (1)$$

where, ε, T, ρ_{unocc} and P_e are the electron energy, the function corresponding to the occupied band, the density of states in unoccupied levels, and the escape probability of one excited electron respectively. In equation (1), T and ρ_{unocc} are expressed by using the ionization potential of Ne or Xe, and the following band parameters; $\varepsilon_{unocc}^{bottom}$, ε_{occ}^{top} and $\varepsilon_{occ}^{bottom}$ stand for the lowest energy level of unoccupied levels, the highest and the lowest energy level of the occupied band respectively. In the present study, we determined these band parameters from the electronic structure calculation by our original tight binding quantum chemistry calculation program "New-Colors".

3. Results and discussion

3.1 Structure of MgO Surface

First, we made the ideally flat (111) surface shown in figure 1a. Then to obtain the more realistic surface structure, we simulated the surface reconstruction of <111> orientation MgO by NEW-RYUDO. Figure 1b shows the constructed surface. As shown in Figure 1b, this irregular surface has (110) faces and {100} facets. Moreover, we simulated the chemisorption of water on this irregular surface by MONTA. Figure 1c shows the water contamination surface. Shown in figure 1c, OH derives from water mainly covered the low coordination Mg atoms on the surface, and H covered the low coordination O atoms.

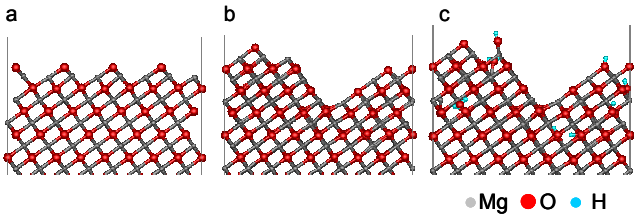

Figure 1 <111> orientation MgO surface models; i. e. a) ideally flat (111), b) irregular, and c) water contamination surfaces.

3.2 Electronic structure of MgO surface

The electronic structure of each surface was computed by New-Colors. Figure 2 shows the density of states (DOS) for each surface. From figure 2, there is no significant difference in the valence band of each structure. On the other hand, surface levels greatly depended on its surface condition.

Figure 3 shows the molecular orbital (MO) at the bottom of surface levels in the case of the flat surface and

the irregular surface. As shown in figure 3a, flat surface hardly keep electrons in surface levels because an electron diffuses away somewhere via this spreading and low energy MO. Contrastingly, the MO shown in figure 3b is localized around the low coordination surface Mg atoms. This MO can be electron traps on the surface like an oxygen defect site. Therefore, compared with ideally flat surface, irregular and water contamination surface have some electron trap levels around the lower side of surface levels shown in figure 2. Densities of trap levels for flat, clean irregular and water contamination surfaces are 0, $8.8*10^{-15}$ and $6.9*10^{-15}$ (5 GCMC calculation sample average) cm^{-2} respectively. The water contamination decreased the trap density by generating the end OH bonds on the low coordination surface Mg atoms which are the origin of trap levels. Moreover, the water contamination surface has lower energy electrons relative to the valence band. These low levels also derived from surface OH.

3.3 γ value for Ne^+ and Xe^+

Figure 4 shows the estimated γ value of each surface and the energy diagram of MgO surface and noble gas ions; Ne^+ and Xe^+. In the IISEE process, a secondary electron is emitted through the neutralization of noble gas ion. Namely, the recombination of one surface electron and ion occurs and simultaneously, another surface electron goes upto the excited state by using the recombination energy. This excited electron should be emitted as a secondary electron in a certain probability.

For Ne^+, the γ value of clean irregular surface is higher than that of flat surface because of electron trap levels. Despite water contamination surface also has some trap levels, this surface has the lowest γ value because of low energy electrons in surface OHs.

For Xe^+, the γ value of flat surface was estimated to be 0. The flat surface doesn't have any traps so the highest energy electron is at the top of valence band. Here, the recombination energy, which would be used for the excitation of another surface electron, is no more than 4 eV. Because of such small excitation energy, no electron can get out from the flat surface. On the other hand, irregular surfaces have positive γ values because they have trap levels which are higher energy relative to the valence band. The water contamination surface has lower γ value than that of the clean irregular surface. Water contaminations decrease the density of trap levels which are the origin of positive γ values for Xe^+.

As above, the γ value especially for Xe^+ is very sensitive to the surface condition. Therefore, the management of surface condition should be the key to the high γ protecting layer,

4. Conclusion

We constructed flat, clean irregular, and water contamination MgO <111> orientation surface, and estimated the γ values based on quantum chemistry. From our study, we can suggest following two theoretical knowledge for the fabrication of better protecting layer; firstly, the introduction of the atomistic scale surface roughness to produce low coordination Mg atom increases the γ value; secondary, the water contamination over the MgO surface decreases the γ value.

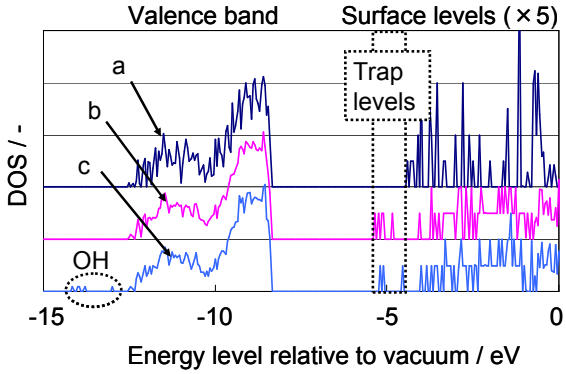

Figure 2 Electronic structures of a) ideally flat, b) irregular, and c) water contamination surface.

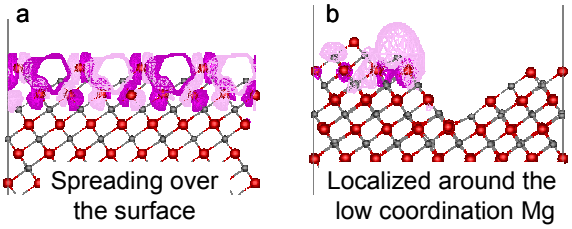

Figure 3 Schematic illustration of MO; a) the lowest surface level in ideally flat surface and b) one example around the lower side of surface levels in the irregular or water contamination surface.

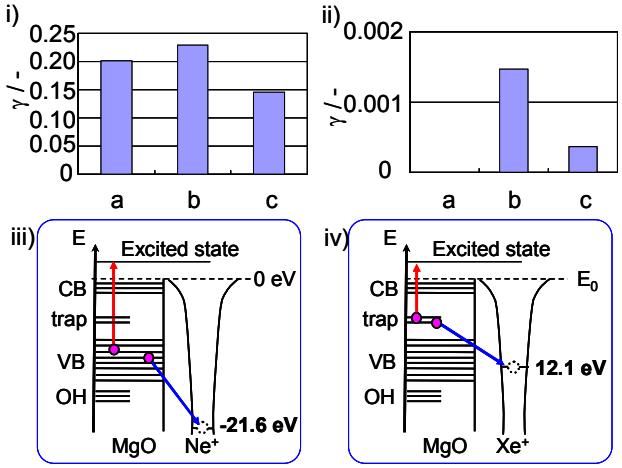

Figure 4 Estimated γ value for i) Ne^+ and ii) Xe^+; a) ideally flat, b) irregular, and c) water contamination surfaces: Energy diagram of MgO surface and iii) Ne^+ and iv) Xe^+.

References

[1] H. Uchiike, K. Miura, N. Nakayama, T. Shinoda and Y. Fukushima, IEEE Trans. Electron Devices, 23, (1976) 1211.

[2] Y. Motoyama and F. Sato, IEEE Trans. Plasma Sci., 34, (2006) 336.