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Development of New Kinetic Monte Carlo Simulator for Theoretical Design of MgO Protecting Layer in Plasma Display

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1. Introduction

Plasma display panel (PDP) has gained much attention for a high definition TV, since it is a flat, thin, and large-size display. PDP has been already commercialized for public and individual use. However, in spite of many experimental efforts, the display performances are still unsatisfactory and the lifetime of the PDP is one of the main problems. Sputtering of the protecting layer by the energetic plasma particles during the discharge process is one of the important factors that limit the lifetime of the PDP. Hence, MgO thin film is regularly used for the protecting layer in the PDP because of its high anti-sputtering and secondary electron emission abilities [1-3].

Experimentally it is pointed out that the electric charges accumulated in the MgO surface also degrade the protecting layer under the plasma condition. However, experimental observation of the above effect is very difficult and then theoretical analysis is strongly demanded. Especially, the information on the effect of the MgO surface index on their stability is strongly desired, since this information leads to the design of the best MgO structure having high stability.

Recently, we have succeeded in the development of tight-binding quantum chemical molecular dynamics program and applied it to the investigation of the stability of the MgO surface under the electric field condition [4]. The above works succeeded in proposing new MgO structure having high stability to the electric fields. However, this method can employ only several hundreds of atoms in the simulation cell. Hence, large-scale simulation including more than 10,000 atoms is required to evaluate their stability with high accuracy. Hence, in the present study, we developed new kinetic Monte Carlo simulator, which can realize the large-scale simulation and predict new MgO structure having high stability to the electric fields.

2. Development of New Kinetic Monte Carlo Program for Large Scale Simulation

In the present study, we succeeded in the development of new kinetic Monte Carlo program, which can consider the electric field condition. This program realizes the large-scale simulation employing more than 100,000-1,000,000 atoms and enables us to clarify the destruction process of the MgO protecting layer under the electric field condition.

We employed three different MgO surfaces, (001), (011), and (111). As an example, Fig. 1 shows the model of the MgO(001) surface employed in the present study. This simulation cell is composed of 23,040 atoms. It indicates that our new program realizes large-scale simulation, which cannot be investigated by quantum chemical molecular dynamics approaches.

3. Results and Discussion

New kinetic Monte Carlo program was applied to the destruction process of the MgO(001) surface under 0.1 V/Å electric field condition. Fig. 1 shows the final structure of the MgO(001) surface after the destruction process. This result indicates that the MgO(001) surface was randomly destroyed and the selective evaporation of atoms or clusters was not observed. Fig. 2 shows the final structure of the MgO(111) surface under 0.1 V/Å electric field condition. It is interesting to see that the destruction process of the MgO(111) surface is completely different from that of the MgO(001) surface. The MgO(111) surface was destroyed selectively and nano-dot structure was formed, although MgO(001) surface was destroyed randomly under the electric field condition. From this figure, we confirmed that our new kinetic Monte Carlo program is very effective tool to investigate the stability of the MgO protecting layer and the effect of the surface structures.

We also investigate the stability of the

MgO(011) surface under 0.1 V/Å electric field condition. MgO(011) surface was also destroyed selectively and the formation of nano-dot structure was observed, similarly to that on the MgO(111) surface.

We evaluated the stability of the above three different MgO surfaces by the analysis of the simulation results. The stability is estimated by the number of the evaporated atoms per unit surface area. The results are shown in Table 1. These results indicate that the surface index greatly influences the stability of the MgO surface and the MgO(001) surface was found to have the lowest stability and the MgO(111) surface was found to have the highest stability.

However, it is experimentally well known that the MgO(111) surface has the lowest stability and MgO(001) surface has the highest stability among (001), (011), and (111) surfaces, which is against our present results. Hence, we suggested that the formation of the nano-dot structure under the electric field condition strongly stabilizes the MgO(111) surface. It is noteworthy that the nano-dot structure on the MgO(111) surface is covered by (001) facets. This may be another reason for the high stability of the MgO(111) surface.

The formation process of the nano-dot structure cannot be simulated by the small-scale simulation. Hence, the effectiveness of the large-scale simulation by our new kinetic Monte Carlo simulator is strongly confirmed.

4. Conclusion

Our new kinetic Monte Carlo program enables us to clarify the effect of the surface index on the stability of the MgO protecting layer under the electric field condition. Especially, large-scale simulation was found to be essential for the investigation on the destruction process of the MgO protecting layer. Since large-scale simulation cannot be done by quantum chemical molecular dynamics approaches, we confirmed the effectiveness of our new kinetic Monte Carlo program.

Moreover, we suggested that the MgO(111) surface has the highest stability compared to the MgO(001) and MgO(011) surfaces. Finally, we recommended that MgO(111) surface is most favorable for the protecting layer in the PDP.

References

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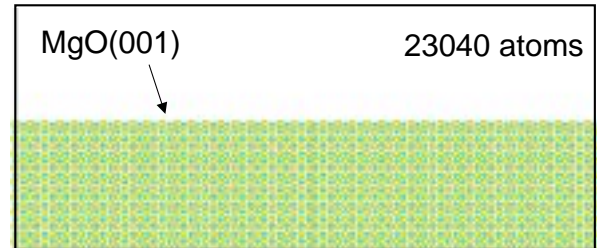
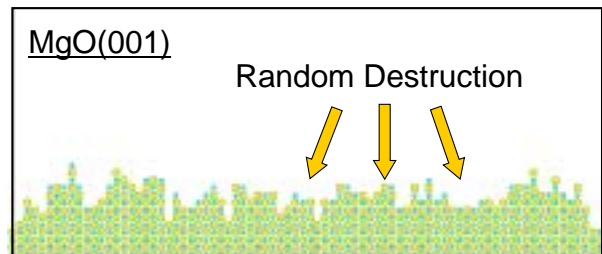Fig. 1 Large-scale simulation model for MgO(001) surface.

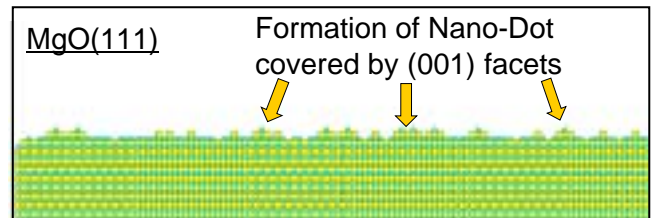Fig. 2 Final structure of MgO(001) surface after the destruction process under the electric field.

Fig. 3 Final structure of MgO(111) surface after the destruction process under the electric field.

Table 1 Effect of the surface index of the MgO surfaces on their stability.

Index	Number of evaporated atoms (A)	Surface area /Å^2 (B)	A/B (Stability)
(001)	13766	5674	2.425
(011)	14479	6019	2.405
(111)	3667	5528	0.663