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

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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 [1,2]. 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.

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 [3]. 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 design new atomically-controlled MgO structures with high stability. Hence, more recently, we also developed new kinetic Monte Carlo simulator [4], which can realize the large-scale simulation including more than 10,000 atoms. This new simulator was very effective to investigate the effect of MgO surface index on the stability to the electric field, and succeeded in proposing that MgO(111) surface has the highest stability among various MgO surfaces [4].

In addition to the effect of the surface index, the effect of grain boundary on the stability to the electric field is also important subject in order to propose the atomically-controlled MgO structure with high stability. Hence, in the present study, we applied our new kinetic Monte Carlo program to the simulations on the destruction process of MgO surfaces with grain boundary and investigated the effect of the grain boundary on their stability.

2. Method

We employed our new kinetic Monte Carlo program [4], which can consider the electric field condition. This program realizes the large-scale simulation employing more than 10,000-1,000,000 atoms, which is essential for clarifying the effect of grain boundary on the destruction process of the MgO protecting layer under electric field condition.

We also developed new modeling software to construct the grain boundary structures in the MgO surfaces. We employed three different MgO surfaces, (001), (011), and (111), and various grain boundary structures were constructed on the above MgO surfaces by using the above new software.

3. Results and Discussion

New modeling software for grain boundary was applied to the construction of several grain boundary structures on the MgO(001), (011), and (111) surfaces. As an example, Fig. 1 shows the MgO(011) surface with Σ3 boundary structures. In addition to the Σ3 boundary structures, we also constructed several boundary structures with different Σ values in order to investigate the effect of the boundary structures on their stabilities.

First, we applied our new kinetic Monte Carlo

simulator to the simulation on the destruction process of the MgO(011) surface with Σ3 boundary structure under 1.0 V/Å electric field condition. Fig. 2 shows the initial and final structures of the MgO(011) surfaces with Σ3 boundary structures during the destruction process simulation at 300 K. This figure indicates that the MgO(011) surface was selectively destroyed under the electric field condition and the formation of nano-dot structure was observed at grain boundary position. Here, it is interesting to see that the destruction process of the MgO(011) surface with grain boundary is different from that without grain boundary. Our previous simulation result shows that the MgO(011) surface without grain boundary was randomly destroyed and the selective evaporation of atoms or clusters was not observed. Hence, we confirmed that new kinetic Monte Carlo program is very effective tool to investigate the effect of grain boundary on the stability of MgO surfaces.

Furthermore, we evaluated the stability of the MgO(011) surfaces with and without grain boundary by the analysis of the simulation results. Here, the stability is estimated by the number of the evaporated atoms per unit surface area. The above values were 0.892 and 0.881 for MgO surfaces with and without grain boundary, respectively. These results indicate that the MgO(011) surface with Σ3 grain boundary was found to have the slightly higher stability than that without grain boundary. Hence, the above simulation result suggests that the Σ3 grain boundary increases the stability of the MgO protecting layer in the plasma display. We also clarified that the specific coordination structures of the Mg and O atoms at the grain boundary increase the stability of the MgO surfaces.

Moreover, we also performed the simulation on the destruction process of the MgO(111) surface with and without grain boundary. In this case, we found that the Σ 5 grain boundary increases the stability of the MgO(111) surface. These results suggest that some specific grain boundary structures increase the stability of the MgO surface.

Finally, the effect of grain boundary cannot be simulated by small-scale simulation. Hence, the effectiveness of large-scale simulation by our new kinetic Monte Carlo simulator is strongly confirmed.

4. Conclusion

We succeeded to clarify the effect of the grain boundary on the stability of the MgO protecting layer in the plasma display under the electric field condition by using our new kinetic Monte Carlo simulator. Moreover, we suggested that some specific grain boundary structures increase the stability of the MgO surfaces.

References

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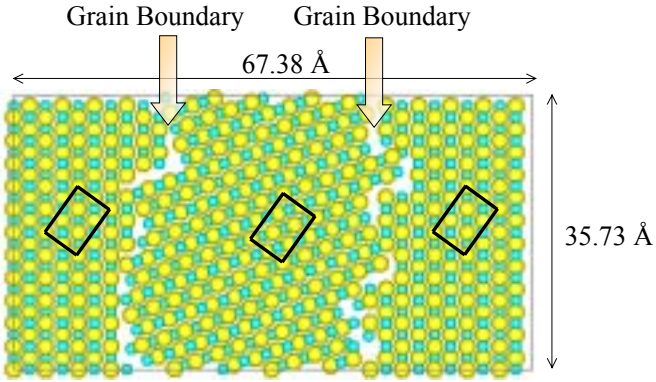

Fig. 1 Large-scale model of MgO(011) surface with Σ3 grain boundary

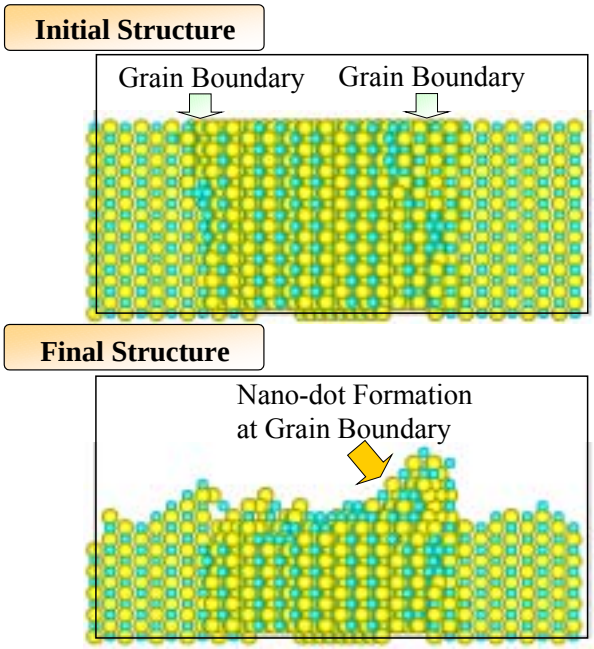

Fig. 2 Initial and final structures of MgO(011) with Σ3 grain boundary during the destruction process under 1.0 V/Å electric field at 300 K.