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Molecular Dynamics and Quantum Chemical Molecular Dynamics Approach to Design of MgO Protecting Layer in Plasma Display

Momoji Kubo[1,2], Hiromi Kikuchi[1], Hideyuki Tsuboi[1], Michihisa Koyama[1], Akira Endou[1], Hiromitsu Takaba[1], Carlos A. Del Carpio[1], Hiroshi Kajiyama[3] and Akira Miyamoto[1,4]

[1]Department of Applied Chemistry, Graduate School of Engineering, Tohoku University, 6-6-11-1302 Aoba, Aramaki, Aoba-ku, Sendai 980-8579, Japan.
Phone: +81-22-795-7236 Fax: +81-22-795-7235, E-mail: momoji@aki.che.tohoku.ac.jp
[2]PRESTO, Japan Science and Technology Agency, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan.
[3]Institute of Industrial Science, University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan.
[4]New Industry Creation Hatchery Center, Tohoku University, 6-6-10 Aoba, Aramaki, Aoba-ku, Sendai 980-8579, Japan.

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. Experimentally, it is pointed out that the electric charges accumulated in the MgO protecting layer degrade itself under the plasma condition.

Therefore, we previously applied our original tight-binding quantum chemical molecular dynamics and kinetic Monte Carlo simulators to the destruction process of the MgO protecting layer under the electric field condition [1-3]. Our simulation results suggest that the MgO(111) surface with nano-dot structure has the highest stability to the electric field. In addition to the electric field, sputtering of the MgO protecting layer by the energetic plasma particles during the discharge process is also important factor that limit the lifetime of the PDP.

Hence, in the present study we applied our original molecular dynamics and quantum chemical molecular dynamics programs to the simulations on the destruction process of the MgO protecting layer by Xe irradiation. Especially, the effect of the Miller index on the destruction process of the MgO surface was focused.

2. Method

We employed our original molecular dynamics program “New-RYUDO” to investigate the destruction dynamics of the MgO protecting layer in PDP by Xe irradiation. Moreover, our original tight-binding quantum chemical molecular dynamics program “Colors” was also employed to clarify the electronic states dynamics, electron transfer dynamics, and the second electron emission ability of the MgO protecting layer during its destruction process by Xe irradiation.

3. Results and Discussion

Fig. 1 shows the destruction process of the MgO(001) surface by Xe irradiation simulated by our molecular dynamics program. This figure indicates that our program is very effective to clarify the destruction dynamics of the MgO protecting layer in PDP. Moreover, it is interesting to see the rapid recrystallization of the MgO(001) surface at 10 ps. Previously, researchers in PDP only focus on the stability and destruction of the MgO protecting layer to develop new MgO protecting layer with long life-time. Our simulation results suggest that the recrystallization of the MgO surface after the destruction is very important factor to design new MgO protecting layer in addition to its stablility and destruction. Moreover, the formation of a lot of steps and kinks was observed on the recrystallized MgO(001) surface.

In order to clarify the effect of the Miller index on the destruction process of the MgO protecting layer, we also simulated the destruction process of the MgO(011) surface by Xe irradiation (Fig. 2). Rapid recrystallization of the MgO(011) surface was observed at 10 ps, which is similar to the MgO(001) surface. Moreover, it is interesting to see the formation of nano-dot structure on the MgO(011) surface. This result is completely different from that on the MgO(001) surface. Therefore, we suggest that the Miller index of the MgO surface significantly influences the destrction and stability of the MgO protecting layer.

The destruction process of the MgO(111) surface was also simulated. Rapid recrystallization of the MgO(111) surface was also observed at 10 ps. These results indicate that the recrystallization of the MgO surfaces after the destruction is very important factor to discuss the stability of all the MgO surfaces. Moreover, the formation of nano-dot structure was observed, which is similar to the MgO(011) surface. We discussed the relationship between the stability of the MgO surfaces and the formation of nano-dot structures.

Furthermore, our tight-binding quantum chemical

molecular dynamics program was applied to the investigations on the electronic states dynamics of the MgO surface during its destruction process by Xe irradiation (Fig. 3). The significant electron transfer from Xe to the MgO surface at 190 step was observed. However, at 350 step the electron transfer from Xe is not observed and Xe has a neutral charge. This result suggests that Xe intruded into the MgO surface does not affect the second electron emission ability of the MgO surface.

4. Conclusion

We succeeded to clarify the effect of the Miller index on the destruction process of the MgO protecting layer in PDP by using our molecular dynamics program. Our simulation results clarify that the recrystallization process of the MgO surface is very important to discuss the stability of the MgO protecting layer, in addition to the destruction process. Moreover, it is interesting to see that the self-organized formation of nano-dot structures on the MgO(011) and MgO(111) surfaces, which is not observed on the MgO(001) surface. Furthermore, our quantum chemical molecular dynamics program was found to be very effective to discuss the second electron emission ability of the MgO protecting layer after the destruction.

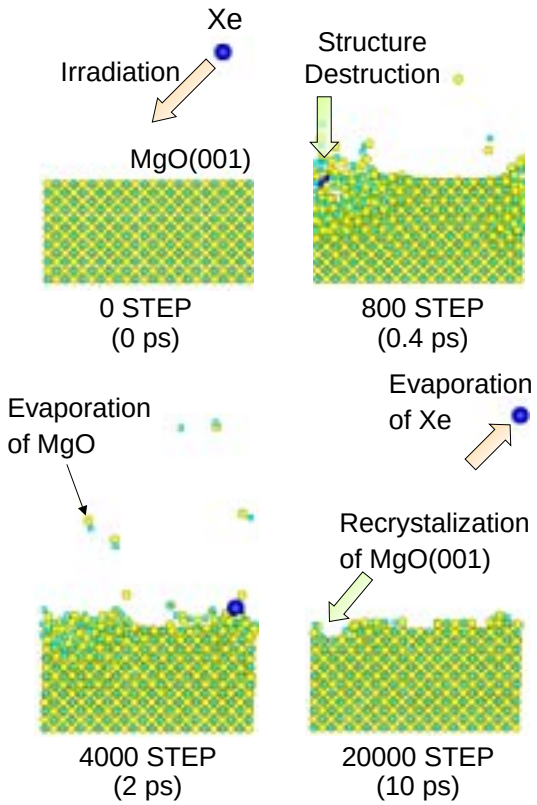

Fig. 1 Destruction process of MgO(001) surface by Xe irradiation simulated by molecular dynamics method

References

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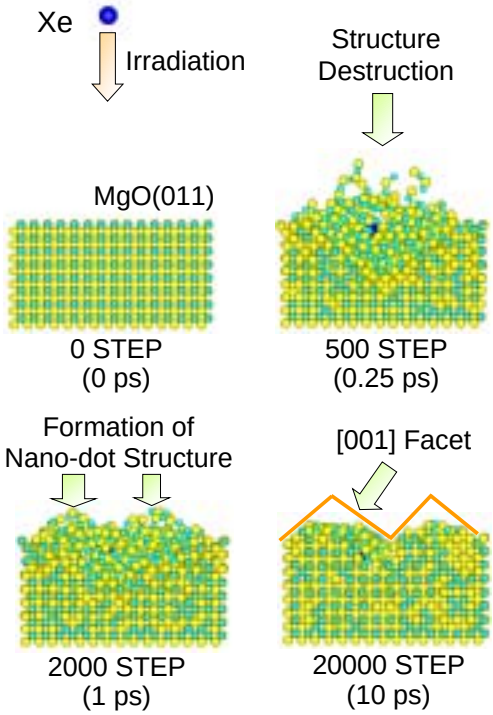

Fig. 2 Destruction process of MgO(001) surface by Xe irradiation simulated by molecular dynamics method

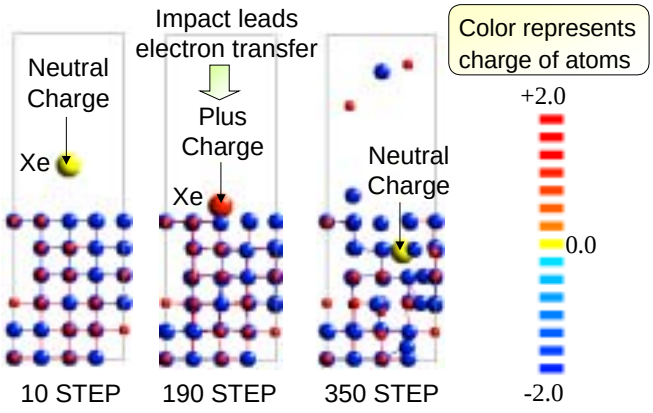

Fig. 3 Destruction process of MgO(001) surface by Xe irradiation by quantum chemical molecular dynamics method