

Report on MERIT Overseas Dispatch Program

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1. Overview

Oversea Stay Period: 2015/8/31~2015/10/20

Research Collaboration Period: 2015/8/31~2015/12/11

Institution: Institut de Physique et de Chimie de Strasbourg (IPCMS)

Supervisor: Prof. Mauro Boero

Research Topic: First Principles Study on Initial Oxidation of SiC [000-1] and [11-20] Surface

2. Research Background

The hosting researcher, Prof. Boero, is one of the main developers of the first principles molecular dynamics (FPMD) code 'CPMD', and is still actively engaged in the method development. FPMD treats electron quantum mechanically so that the method is capable of simulating chemical processes that involve bond formation and breaking, which are not treatable in case of MD with empirical potentials. By using FPMD, we can simulate atomic scale chemical reactions that cannot be observed directly by experiments, and obtain insight for reaction pathways in detail. Since chemical reactions contain processes with high reaction barrier cannot be observed easily in typical simulation time, they are called 'rare events'. In order to explore these reactions, constraint dynamics with bluemoon sampling method and metadynamics, which is a way to explore free energy surface directly, are used.

Last year Prof. Boero visited Oshiyama laboratory, and I started to use bluemoon method to explore the oxidation of SiC. This time, for the first part I visited Strasbourg and for the later part Prof. Boero visited University of Tokyo, and we were in close contact for our research collaboration. The total period was over 3 months. I have used metadynamics to explore complex free energy surface of SiC surface oxidation.

3. More about Research

SiC is a wide-gap semiconductor so that it can operate under severe conditions such as high temperature and high frequency. It is a next generation semiconductor material to replace Si in high power consumption devices. The conventional technology cannot create sophisticated oxide interface so that the devices show significant drop in electronic properties. Especially the electron mobility at the interface is only 10% of that of bulk. The oxide for SiC is SiO₂, and is the native oxide as in case of Si. We can control the SiO₂ thickness with Deal-Grove model, which is a kinetic model. The difference between Si oxidation and SiC oxidation is that in case of SiC, C has to be released from the SiO₂ as CO or CO₂. This brings two new reactions during oxidation, which are the oxidation of C and the desorption of CO or CO₂. Thus, it is natural to

attribute the defects that dramatically damage the interface properties of SiC were introduced during these reactions. Thus understanding the reaction mechanisms for them is critical in improving the interface quality.

In this research, we focus on the emission of C, and calculated the difference in desorption barrier for CO in [000-1] surface (C-face) for different O coverage. We have found that the difference in the next next nearest atom position will effect the energy barrier up to 1 eV. This value is comparable to the effect of the nearest atom position, which is the order of the bond energy. This suggest that the reactions during oxidation is very sensitive to the environment and by adjusting local environment we can dramatically change the reaction pathway.

In case of [11-20] surface, which is the surface that achieve highest electron mobility, the formation of CO or CO₂ is not trivial. I have used density functional theory to search for CO or CO₂ formation in terms of energetics. Then I used FPMD to find the stable/meta-stable structures that can be achieved in dynamics. We have found that in [11-20] surface, there is a CO structure resembling [000-1] surface and also another structure with CO₂-like surface. I am still calculating the desorption barrier in case of [11-20] surface.

4. Life in France

Strasbourg is located at the boundary of France and Germany. It only takes about one hour walk to get to Germany so that the city has a rich culture containing the mix of both France and Germany. The old town was preserved as any typical European city, and the tallest building is the Cathedral of Strasbourg, which used to be the tallest building in the world for more than 150 years. Strasbourg belong to Alsace where is famous for its wine. In autumn, there are many newly released wines in the supermarkets. The city is also famous for its beauty with many flowers in the streets.

5. Acknowledgements

I would like to express my sincere gratitude to MERIT for the financial supports during my stay in France. I really appreciate Prof. Boero for letting me visit his laboratory and also the close research collaboration. I could not survived without his help during my stay since I speak no French. I would also like to thank Prof. Atsushi Oshiyama for contacting Prof. Boero for this collaboration. I thank Dr. Assil Bouzid, Dr. Marwan Deb, Dr. Anatolie Gavriluta, and Mr. Burak Ozdamar for the daily discussions and launch time during my stay at IPCMS.