Séminaire de Chimie Théorique

Salle conférence, 3eme Est, bat. A12

Lundi 21 Mars à 14:00

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Catalytic Reactions in Crystal Growth and Etching Processes at Semiconductor Interfaces: First-principles Simulations

First-principles molecular dynamics method is a quite powerful tool to elucidate chemical reactions at the atomic level. First, I will discuss on the promotion mechanism of GaN single crystal growth in the Na flux method. The Na flux method is one of very promising techniques to grow large GaN single crystals with high quality. The solubility of N into liquid Ga is quite low and therefore very severe conditions such as high pressure of 1 GPa and high temperature of 1500°C are necessary to grow GaN crystals. On the other hand, the solubility of N into Ga-Na liquid alloy is significantly higher and the required pressure and temperature can be reduced to 2-3 MPa and 750°C. To clarify the microscopic origin for the enhancement of N dissolution and the growth of GaN single crystals by Na, we have carried out first-principles molecular dynamics simulations (1). We also clarified the mechanism of suppression of poly-crystal growth and promotion of single crystal growth by C additives(2,3).

I would like to discuss etching processes of SiC surfaces using Pt catalyst. SiC and GaN are quite stable semiconductors and therefore, it is rather difficult to etch surfaces of these materials. Recently, a quite promising etching method to produce atomically flat SiC and GaN surfaces was proposed by Yamauchi and co-workers using Pt plate as a catalyst. To clarify the reaction mechanisms, we have carried out density functional theoretical simulations (4,5).

References

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