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Surface morphology of InAs considering entropy effects

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Epitaxial growth of Ⅲ-Ⅴ compound semiconductors on Si(001) substrates is important to incorporate Ⅲ-Ⅴ materials with outstanding electrical and optical property into the conventional silicon base technology. The epitaxial growth is conducted at a high-temperature and low-pressure conditions where entropy effects become nontrivial. However, the theoretical study of the surface science has usually been conducted on 0 K assuming that the results may not be significantly different from the experimental condition. Therefore, in this study, the thermodynamic effects on the InAs growth was investigated by density functional theory (DFT) calculations including the entropy terms. As the atomic vibrational motion was allowed and configuration was considered, the entropy was found to be important in calculating the high-temperature surface energy. Then, the thermodynamic equilibrium morphology of InAs was determined by Wulff shape as a function of T and P in the region relevant to the experimental growth chamber. By doing so, the change of the surface morphology which is usual process to control the surface properties in experiments could be predicted.