**First-Principles Study of Ir Desorption from Its Low-index Surfaces**

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Iridium is one of the metals in platinum group. Due to good mechanical properties and chemical inertness especially at high temperature, iridium is broadly used on industries, such as crucibles for single crystal growth, spark plugs in car engines, etc. However iridium has desorption problems[1]. Although iridium has the lowest oxygen permeability, iridium surfaces are oxidized above 1000K, and produce gaseous oxide molecules, such as IrO3[2]. To solve this desorption problem, fundamental understanding of the desorption process is naturally necesarry.

In this study, we investigate oxidation of low index surfaces of iridium such as Ir(110) and Ir(111) to find energetically favorable surface oxides and its IrO3 desorption energy, by using first-principles calculations based on density functional theory. We used OpenMX code, which is based on norm-conserdving pseudopotentials and pseudo-atomic localized basis functions[3]. The GGA-PBE exchange-correlation functional[4] is adopted. Since desorption process is only occurred at high temperture, we used a thermodynamical method, which gives temperature dependence of the free energy or chemical potential by combining DFT calculation with experimental thermodynamic data, particularly useful to gas molecules. This method give us insight of the IrO3 desorption at high temperature, in terms of the temperature dependence of the desorption energy. We find that IrO3 desorption is energetically favorable on some iridium surfaces.

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