

A comparative theoretical study on molecular layer deposition (MLD) of alucone and indicone nanocomposite thin films

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Molecular layer deposition (MLD) is a method for depositing ultrathin organic and organic-inorganic hybrid thin films based on self-limiting surface reactions. Recently we demonstrated fabrication of “alucone (aluminum alkoxide)” thin film by MLD using $\text{Al}(\text{CH}_3)_3$ and hydroquinone (HQ) precursors [1]. Similarly, “indicone (indium alkoxide)” thin film was deposited by MLD using [1,1,1-trimethyl-N-(trimethylsilyl)-silanaminato]indium and HQ. To understand the chemical mechanism of deposition and vibrational characteristics of the thin films, density functional theory (DFT) calculations were used. The precursors were sequentially appended on the $-\text{CH}_3$ moiety on Al or In-terminated surface. It is found that all half reaction of both MLD would be facile and spontaneous, while the reactivity of alucone is higher than indicone. In addition, shifts in the vibrational features in the experimental Fourier-transform infrared (FTIR) spectroscopy of the films are consistently reproduced in our calculations.

[1] Applied Surface Science 458, 864–871, 2018.