

# Surface chemistry during atomic layer deposition of Pt studied with vibrational sum-frequency generation

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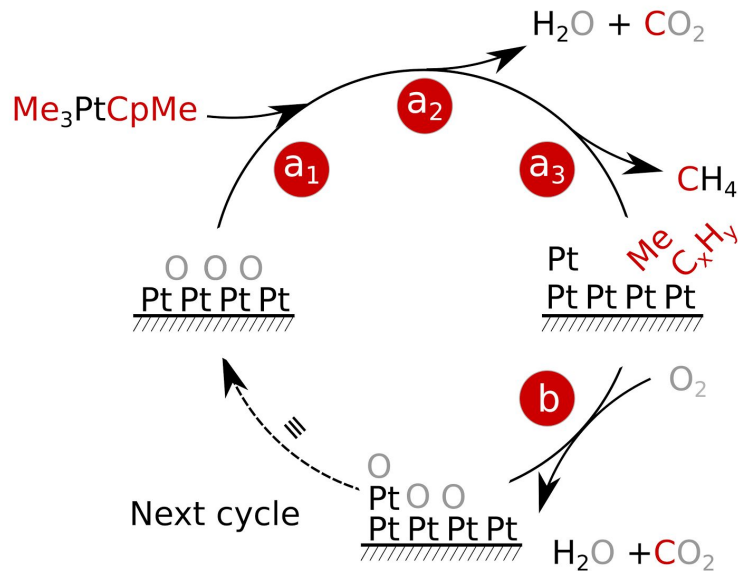


Figure: The key features of the reaction mechanism of Pt ALD using  $\text{MeCpPtMe}_3$  and  $\text{O}_2$  (g) as precursor and co-reactant, respectively. At the beginning of the Pt half-cycle, there is a significant amount of atomic O adsorbed on the Pt surface. (a1) The  $\text{MeCpPtMe}_3$  precursor adsorbs on this surface. (a2) Some of the ligands are combusted to  $\text{CO}_2$  (g) and  $\text{H}_2\text{O}$  (g) by the adsorbed atomic O. Other ligands either remain intact or dehydrogenate to form adsorbed  $\text{C}_x\text{H}_y$  (ads) and H(ads). (a3) Some of the ligands recombine with adsorbed H on the surface to form  $\text{CH}_4$  (g). In the co-reactant half-cycle, molecular  $\text{O}_2$  (g) dissociates on the catalytic Pt surface and reacts with the remaining hydrocarbons groups forming  $\text{CO}_2$  (g) and  $\text{H}_2\text{O}$  (g). Furthermore, the surface is saturated with atomic O adsorbed on the surface.

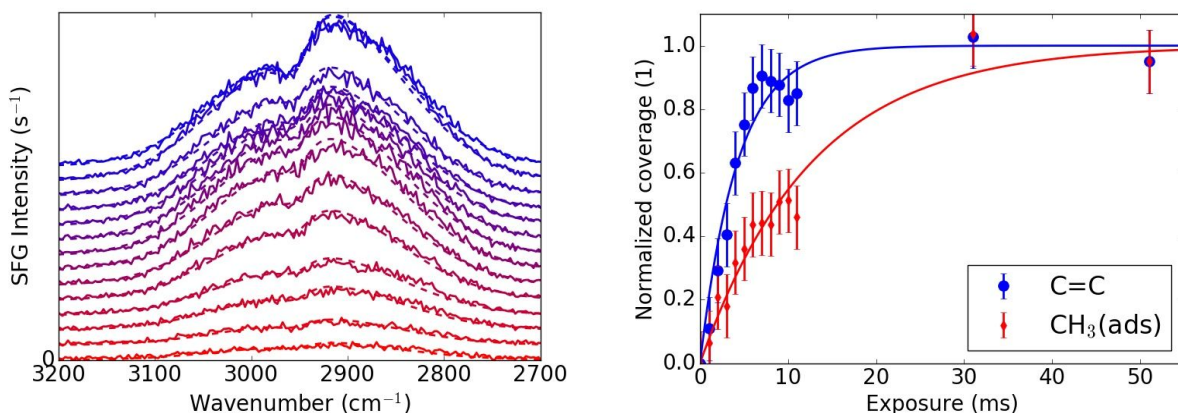


Figure: (left) BB-SFG spectra of the Pt surface as a function of precursor exposure for ALD at 250C, each spectrum has been offset for clarity. The increase in the broad spectral shape is related to coverage of the C=C groups. The dip at  $2950\text{ cm}^{-1}$  is the signature of the  $\text{CH}_3$  groups on the surface. (right) The normalized coverage of the C=C groups and the  $\text{CH}_3$  groups obtained from a fit to the BB-SFG spectra (dashed lines in the left figure). The saturation of the C=C precedes the saturation of the  $\text{CH}_3$  contributions.