動的モンテカルロ法とニューラルネットワークポテンシャルを用いたトリメチルアルミニウムによる Al_2O_3-ALD プロセスの解析

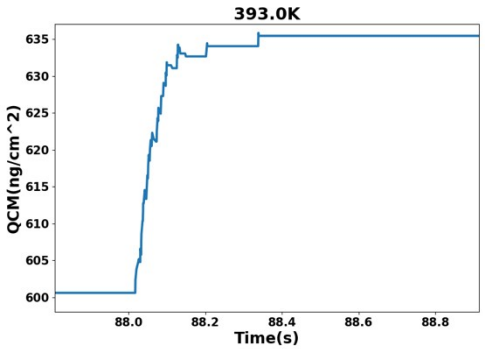
Computation of Al_2O_3 ALD by trimethylaluminum with Kinetic Monte Carlo and neural network potential

東大院工○(M1) 鄒 逸宸 (D) 呉 宇軒, (P) 山口 潤, (P) 佐藤 登, 筑根 敦弘, 霜垣 幸浩

The Univ. Tokyo [1] ○(M1) Y. Zou, (D) Y. Wu, (P) J. Yamaguchi, (P) N. Sato, A. Tsukune, and Y. Shimogaki

E-mail: shimo@dpe.mm.t.u-tokyo.ac.jp

Atomic Layer Deposition (ALD) is widely utilized in semiconductor manufacturing due to its method of alternately introducing precursor and reaction gases, which relies on surface saturation adsorption of the precursor. This approach ensures excellent uniformity in thickness controlling against variations in processing conditions but is challenged by its growth rate compared with other deposition methods. Investigation into the growth rate of ALD draws tremendous attraction in the experiments but could be facilitated by the emerging computation methods which cut the cost. Traditional computational methods, such as Density Functional Theory (DFT), offering insights into surface adsorption and reactions, are time-intensive when predicting growth rate per cycle for ALD applications—particularly for large metalorganic compounds. To overcome these challenges, we are leveraging Kinetics Monte Carlo (KMC, a emerging time-scale reaction simulation method) and Matlantis™ (a cutting-edge atomic-level simulator that utilizes neural network potentials) to investigate the adsorption of Trimethylaluminum (TMA) during Al_2O_3 ALD using H_2O as the reactant. The powerful Matlantis™ calculates energies accurately and efficiently for multiple TMA molecules adsorption and reaction on the surface, and energies are introduced into KMC to predict the growth rate for Al_2O_3 in each cycle. In the following figures, we successfully predict the adsorption kinetics for TMA during the TMA supply step, which shows a mass increase of 36 ng/cm^2 in about 0.3 seconds. Our TMA adsorption and growth simulations show strong alignment with previous DFT calculations and Quartz Crystal Microbalance (QCM) experimental results.



Monte Carlo simulation

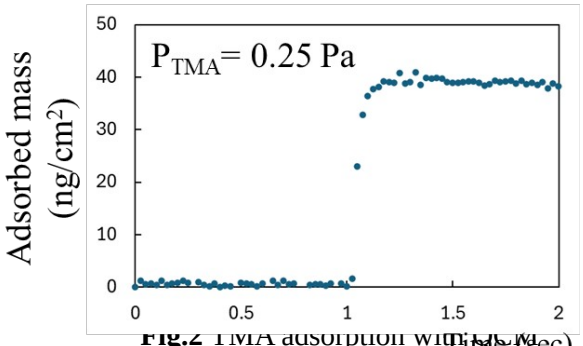


Fig.2 TMA adsorption with QCM experimental