

Supplementary Information

Atomistic kinetic Monte Carlo simulation on atomic layer deposition of TiN thin film

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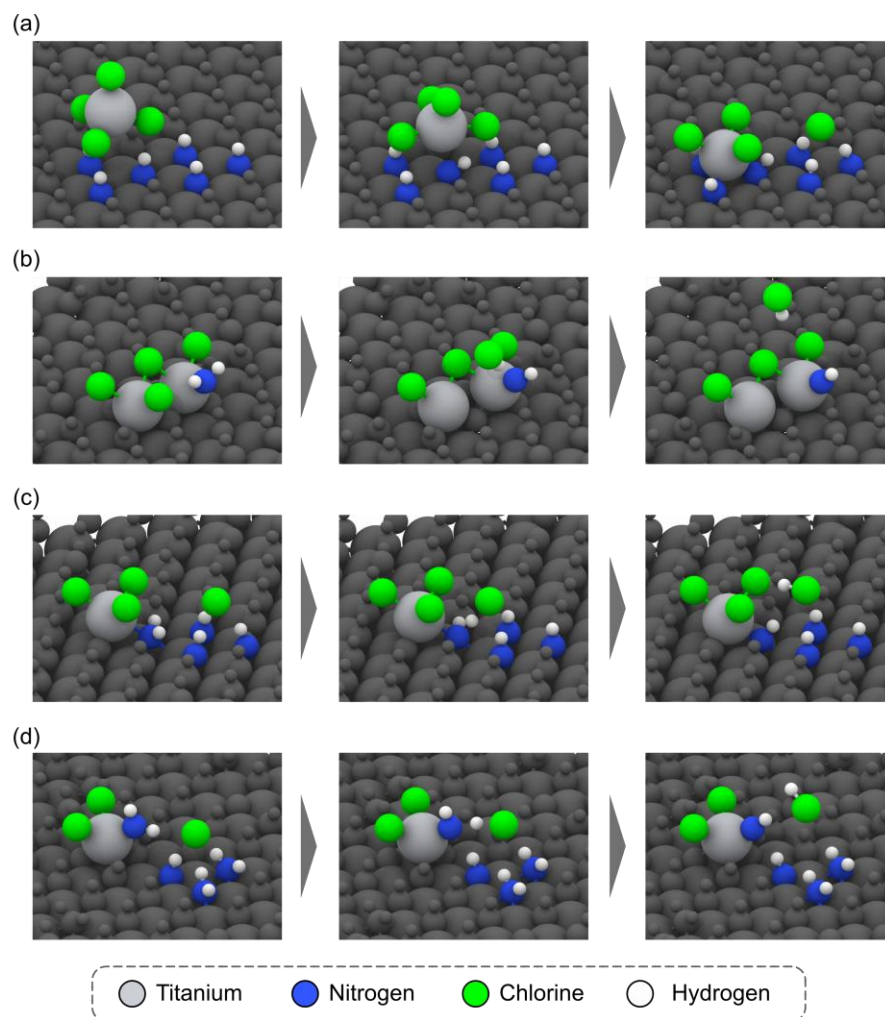


Fig. S1. Reaction mechanism for selected processes. (a) $\text{TiCl}_4 \rightarrow \text{TiCl}_3 + \text{Cl}^*$. (b), (c), and (d) correspond to ①, ②, and ③ in Fig. 2c, respectively. From left, images are the initial, transition, and final states, respectively. For reactions (b) and (d), the middle image is just an intermediate state, as the energy monotonically increases along the reaction path.

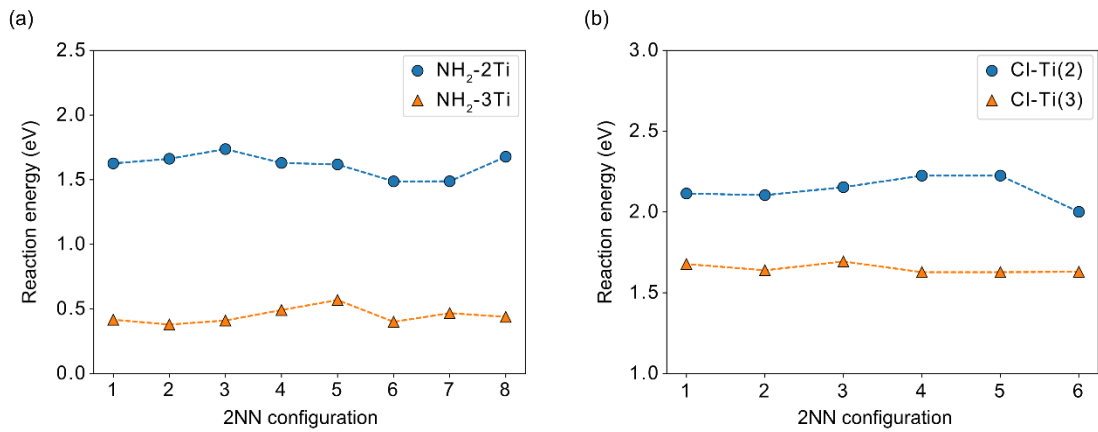


Fig. S2. Reaction energies for $\text{Cl} + \text{NH}_2 \rightarrow \text{NH} + \text{HCl}$. (a) Reaction energies with two different 1NN configurations (2 or 3 Ti atoms) around NH_2 while eight 2NN configurations are chosen randomly. (The other 1NN configurations are the same.) (b) All the 1NN environments are the same but the CN of the Ti atom attached to Cl is either 2 (circle) or 3 (triangle). The other 2NN configurations are chosen randomly for 6 cases.

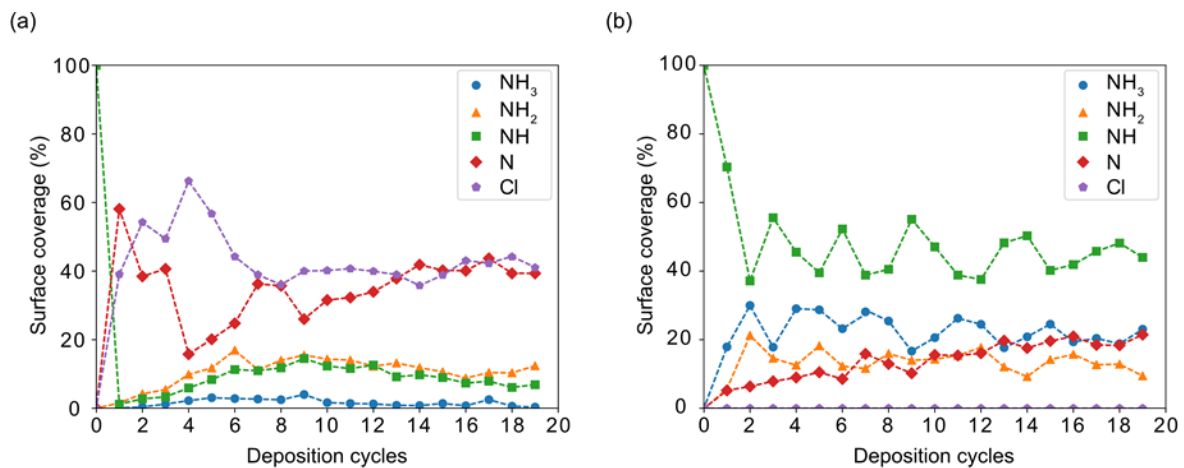


Fig. S3. Coverage of top surface with possible species on surface (NH_3 , NH_2 , NH , N , and Cl) at (a) 300 °C and (b) 400 °C.