

# Development of a kinetic Monte Carlo model for CVD diamond growth

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Due to the range of time-scales spanned by gas-surface reactions occurring during the growth of diamond films using Chemical Vapour Deposition (CVD), variable time-step kinetic Monte Carlo (kMC) allows simulations at time-scales similar to those used experimentally.<sup>1</sup> Previously, the diamond and computational chemistry groups at the University of Bristol have reported a simple cubic kMC growth model that could reproduce many experimental aspects of CVD diamond growth.<sup>2</sup> While such a simplified view of the diamond atomic lattice offers computationally efficient simulations, the geometries of specific adsorption sites or adsorbates thought to be important to growth kinetics cannot be correctly modelled.

The model has been transitioned to a true tetrahedral diamond structure, while remaining on-lattice, allowing a more realistic representation for the diamond lattice and facilitating the implementation and testing of more complicated CVD growth mechanisms. Visualisation of the diamond surface as CVD growth progresses in true tetrahedral co-ordination is also now possible, allowing robust and powerful analysis of implemented reaction schemes and their effect on surface morphology development as a function of time and growth conditions.

Using this new model, we investigate the combined effect of CH<sub>3</sub> flux and energy barrier of preferential etching reactions in order to determine the combination of model parameters which best mimic behaviours seen in experimental literature, primarily using predicted growth rates and surface morphologies.

In addition, the current model's successes and failures in predicting diamond growth will be assessed by investigating how its predictions are affected by changes to growth condition parameters such as substrate temperature, gas temperature and near-surface gas species concentrations.

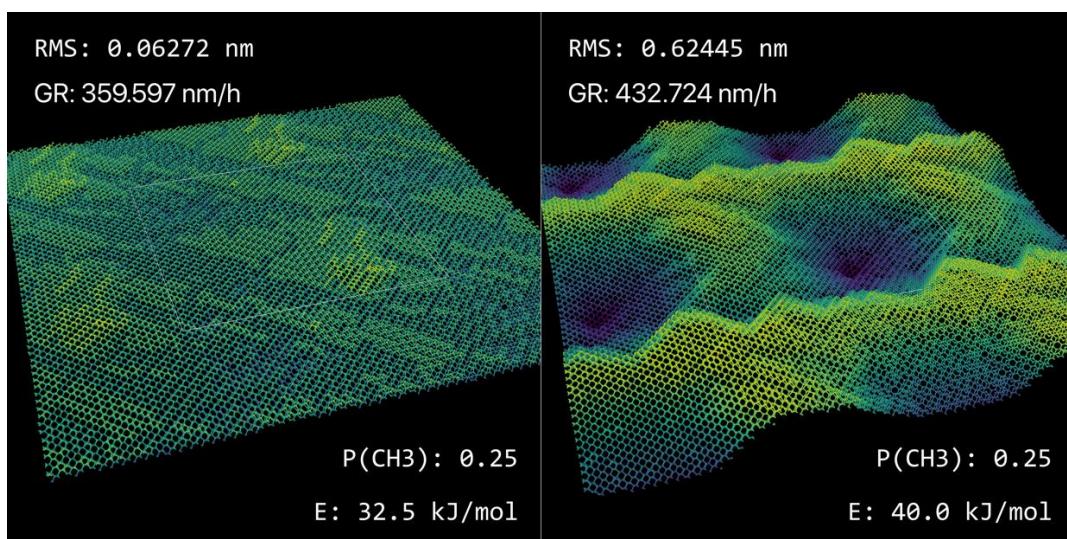


Figure 1: Transition from smooth (left) to rough surface morphologies when the energy barrier to surface species etching is increased from 32.5 to 40 kJ/mol for simulations growth to 120 Å under MCD growth conditions.<sup>3</sup>

## Bibliography

- 1 P. Kratzer, *Multiscale Simul. Methods Mol. Sci.*, 2009, **42**, 51–76.
- 2 W. J. Rodgers, P. W. May, N. L. Allan and J. N. Harvey, *J. Chem. Phys.*, 2015, **142**, 214707.
- 3 P. W. May, J. N. Harvey, N. L. Allan, J. C. Richley and Y. A. Mankelevich, *J. Appl. Phys.*, 2010, **108**, 114909.