Kinetic Monte Carlo Simulation Study of The Early Stages of Epitaxial SiC (0001) Growth

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INRODUCTION: SiC epitaxial growth is usually performed by step-flow growth on the Si face of off-axis substrates. However, homoepitaxy on off-axis substrates has several disadvantages such as the propagation of basal plane dislocations (BPDs) and so on[1,2]. On the other hand, on-axis epitaxial growth would avoid these problems. In this work, a detailed two-component kMC simulation with a cluster-multiple labeling technique is developed to study the early stages of on-axis epitaxial growth of SiC. Using conditions similar to experiments, the formation of submonolayer islands on SiC(0001) surface is studied. The role of the Si:C flux ratio, deposition flux and temperature on the island sizes and shapes is also explored. Finally, the detailed statistics of the island size distribution is analyzed.

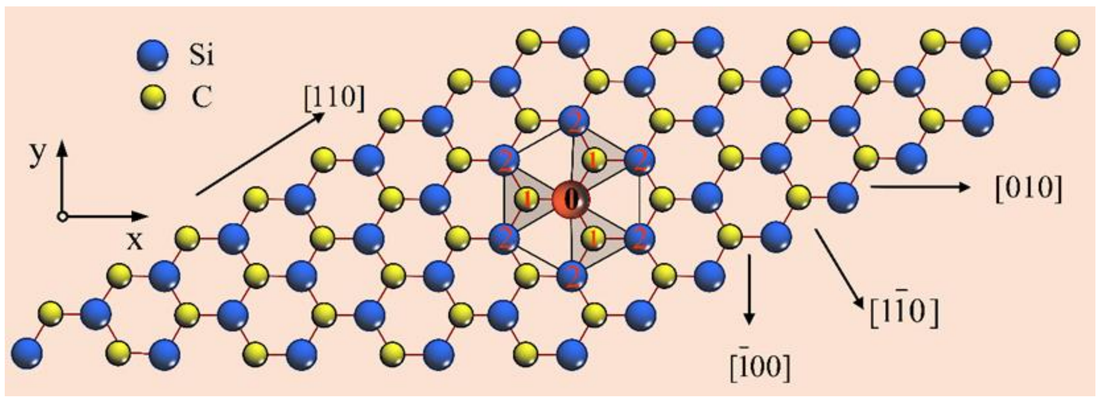

Figure 1. Top view of a SiC(0001) surface

COMPUTATIONAL METHODS: A two-component kMC model with the wurtzite crystal structure has been constructed to simulate the epitaxial growth of SiC(0001). A projection view of the Si-C bilayer is shown in Fig.1. the kMC model is essentially governed by three fundamental processes: the deposition, the diffusion and the desorption on the substrate surface. The diffusion rate is given by the Arrhenius equation:

$$R_d = \nu_0 \exp\left(-\frac{\Delta E + E_{diff}}{kT}\right)$$

where:

ν_0: hopping frequency k: Boltzmann constant T: temperature

E_{diff}: diffusion barrier $\Delta E = \begin{cases} E_i - E_f & \text{if } E_i - E_f > 0 \\ 0 & \text{otherwise.} \end{cases}$

The initial E_i and final E_f energy of jumping atom can be calculated by

$$E_{i(f)} = E_{\mathrm{SiC}} \sum_{j=1}^{NN_{i(f)}} N_j + E_{\mathrm{Si\text{-}Si}} \sum_{k=1}^{NNN_{i(f)}} N_k + E_{\mathrm{C\text{-}C}} \sum_{m=1}^{NNN_{i(f)}} N_m$$

where:

E_{SiC}=0.75 eV, $E_{\mathrm{Si\text{-}Si}}$=0.35 eV, and $E_{\mathrm{C\text{-}C}}$=0.65 eV respectively.

RESULTS:

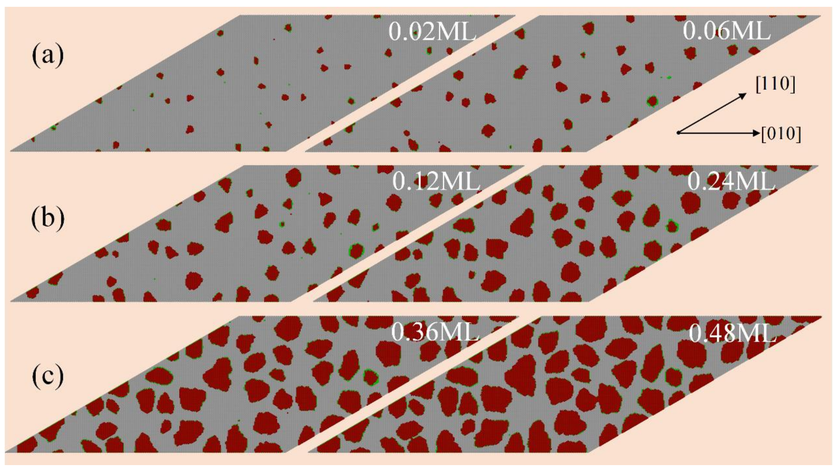

Figure 2. Snapshots of a growing surface as a function of increasing coverage.

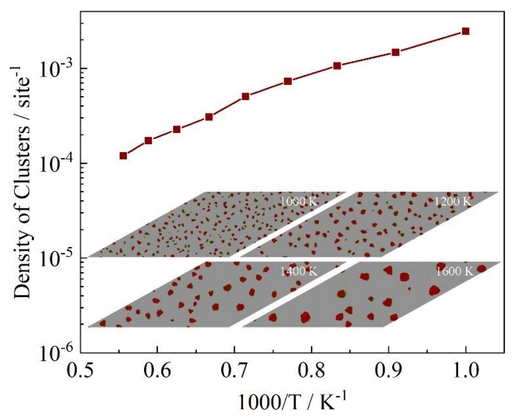

Figure 3. Semilog plot of cluster density as a function of growth temperature.

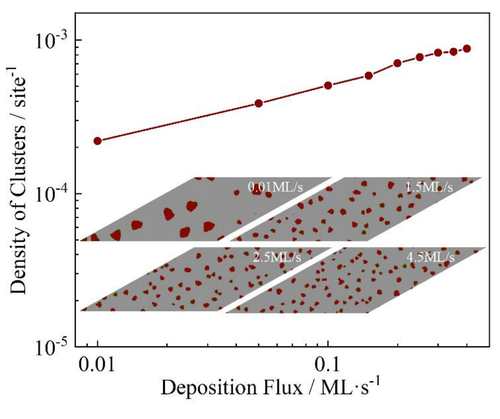

Figure 4. Semilog plot of cluster density as a function of flux rate.

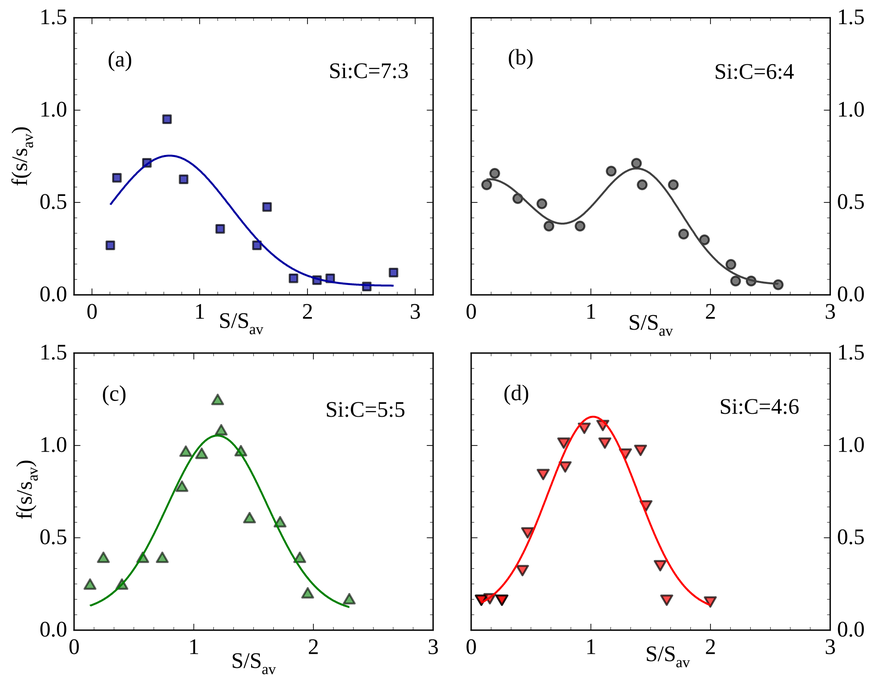

Figure 5. Scatter plot of scaled island-size distributions at different values of Si:C ratios

CONCLUSIONS: The dynamic behavior of Si-C clusters at the early stage of SiC(0001) surface epitaxial growth is investigated by the kMC methods. The simulation results showed that the number of Si-C clusters gradually decreases with increasing substrate temperature and decreasing deposition rate, and that the average size of Si-C clusters at high temperature is much larger than that at low temperature. Furthermore, The Si/C ratio on the growing surface has a significant effect on surface morphologies.

REFERENCES:

1. K. Masumoto, K. Kojima, H. Yamaguchi, Investigation of Factors Influencing the Occurrence of 3C-Inclusions for the Thick Growth of on-Axis C-Face 4H-SiC Epitaxial Layers, Materials, 13 (2020) 4818.
2. T. Kimoto, High-voltage SiC power devices for improved energy efficiency, Proceedings of the Japan Academy, Series B, 98 (2022) 161-189.