Kinetic Monte Carlo Simulation of Deposition of Zircona Coating

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Background

An extension to the Kinetic Monte Carlo(KMC) technique was developed to study the column grain deposition. By comparing other atomic three-dimensional simulations of deposition, such as molecular dynamics (MD) simulation, KMC could conduct a larger time-scale and system size. Through this method, it could show the deposition process through atomic scale, and the effects on the shape and height of deposition layers were also studied by varying the incident angles, temperatures, and substrates.

Model details

KMC simulation was performed for various incident angles and environment temperatures ZrO_2 deposition systems. A cylinder substrate with a radius of 25 atoms and thick of 4 atoms. A cylinder simulation box is chosen because the influence of the rotating substrate will be evaluated. A cubic lattice with unit-less spacings of 1.0 served as a medium for atoms to propagate. The energy set for this system is defined with bond energy. The energy between Zr-Zr, Zr-O, and O-O are 1.3, 1.6 and 0.6[1]. As the ratio of Zr and O in ZrO_2 is 1:2, the rates of deposition for Zr and O are set to 10 and 20 atoms/deposition cycle, respectively. The temperature was defined by thermal energy KT. The KT was specified as 0.0257, which corresponds to room temperature (T=300K). The modified version of software SPPARKS(Stochastic Parallel Particle Kinetic Simulator) was used for KMC simulation[2,3]. The values the barrier command takes on represent the self-diffusion barriers of each atom in their host crystal in the modified version. To realize the rotation of the substrate, the neighbor command was modified to obtain the neighbor information, and Python scripts were used to rotate the substrate and make a loop between rotation and deposition.

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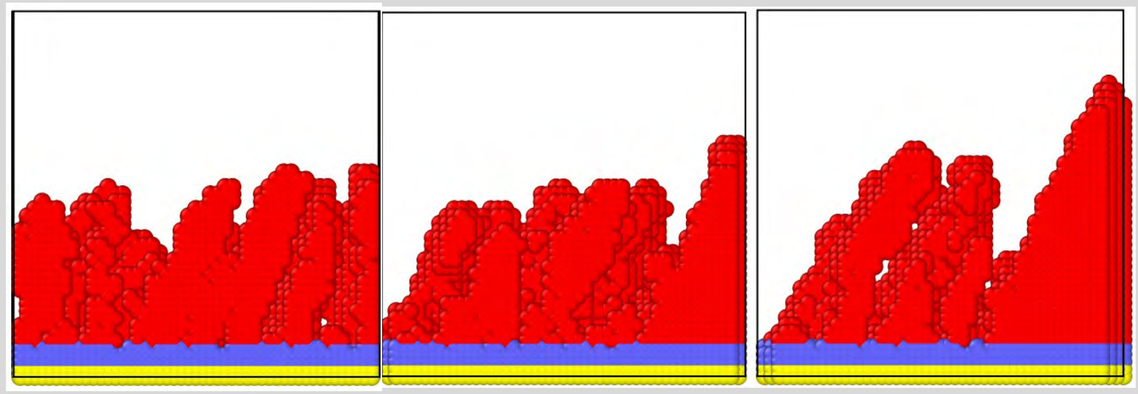
Results and discussion

- Different incident angles

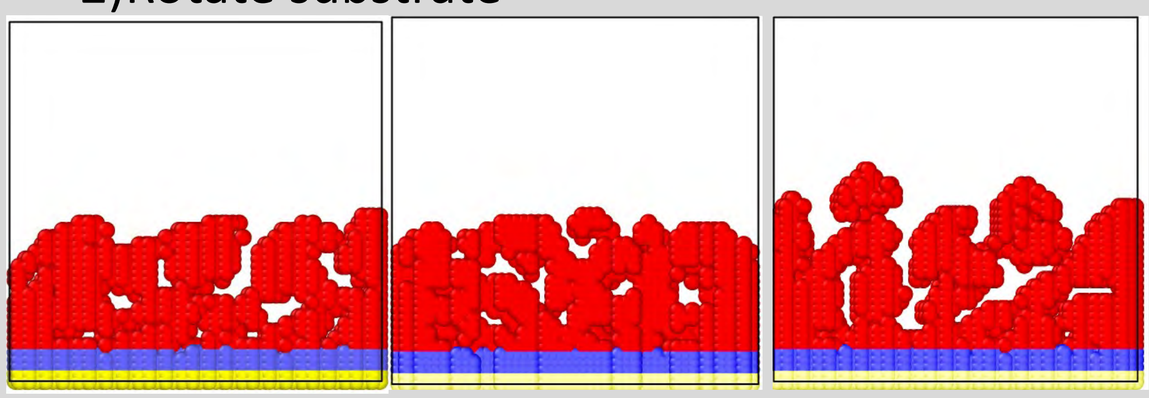
1)Fixed substrate



30° 45° 60°

The angles between the deposition layer and substrate increase with the increase of incident angles. The shadowing effect becomes obvious for the models with the incident angles of 45° and 60°.

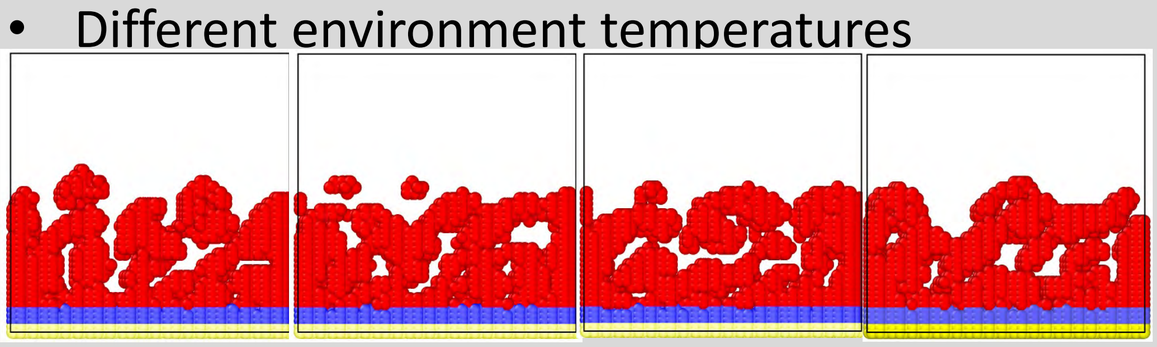
2)Rotate substrate



30° 45° 60°

The deposition layers are dense for the model with the rotating substrate. The shape deposition layers are not like column grains with fixed angles, and it has some wave columns instead.

- Different environment temperatures



300K 500K 1000K 2000K

The waves' shape is more obvious at low temperatures. The hole spaces inside the column grains are relatively higher under low temperatures.

Conclusions

1) KMC model successfully simulates the ZrO2 deposition process. The deposition layers show the obvious structure of column grain.
2) The shadowing effect is obvious with the fixed substrate.
3) The column grain becomes fluctuating with the rotating substrate.
4) The deposition layer becomes dense with higher environmental temperatures.

Acknowledgment
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