



Research Paper

Modeling the self-assembly of nanoparticles into branched aggregates from a sessile nanofluid droplet



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HIGHLIGHTS

- A kinetic Monte Carlo model is developed to simulate the drying of a nanofluid droplet.
- A time- and radius-dependent chemical potential function is proposed.
- Branched aggregates from the drying of the nanofluid droplet are predicted.
- Particles distribution and the shrinking of the contact line are investigated.

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ABSTRACT

The drying of sessile nanofluid droplets on a surface can form various patterns and plays important role in micro and nano- manufacture technologies. In this paper, the kinetic Monte Carlo (KMC) approach based on the 2D Ising model is developed to simulate the drying process of a nanofluid droplet in a circular domain. In contrast to assuming a constant chemical potential in previous models, a chemical potential function dependent on time and the radius of the droplet is proposed. This model is used to investigate the formation of branched nanoparticle aggregates resulting from the drying of a nanofluid droplet. The predicted patterns from the drying droplet show a good agreement with the experiments. The distribution of particles and the shrinking of the contact line during the drying process, as well as the effects of the initial boundary chemical potential and the decrease rate of the chemical potential on the drying process have been investigated.

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1. Introduction

Nanofluids are new materials in the industrial production and present some important features, including: enhanced heat transport performance [1,2], high thermal conductivities at low nanoparticle concentrations [3,4], and more stable than many ordinary fluids [5]. With the enhanced heat transfer properties, nanofluids have great potential to be applied in developing highly compact and effective heat transfer equipment [6]. In addition, the drying of nanofluids has gained much audience nowadays due to its important applications in painting, coating, surface patterning, and micro- or nano-fabrication processes. During the drying process of a nanofluid, the dispersed nanoparticles can self-assemble into various complex structures [7–12]. The branch structure pattern was observed in the front of the contact line of the nanofluid during drying process [13–15]. The other structures such as coffee-ring [16,17], networks [18], or worm-like islands were also reported

[19,20]. Numerical models have been developed to study the behavior of the moving drying front and the deposition structures of the dispersed nanoparticles [8,13,15,18,21,22]. The applied models include the hydrodynamic thin film model [21,23], the dynamical-density functional theory [24], and the KMC model [13,15,18]. In these models, the KMC model is a very practical method to simulate the drying-mediated two-dimensional assembly of nanoparticles from nanofluids [8]. It can directly show the drying process of nanofluids and the structures formed by nanoparticles after drying. The previous KMC models adopted different assumptions, such as homogeneous and heterogeneous evaporation [8], full-3D model [25], and pseudo-3D model [15], to explore the drying of thin films and the deposition of nanoparticles. In this paper, a numerical model, which is developed from the 2D lattice-gas KMC method [8], is used to simulate the drying process of a sessile nanofluid droplet. In contrast to assuming the chemical potential as a constant, a linear function, or a nonconstant function depending on the liquid coverage in previous models [13,14,18,26], a chemical potential function dependent on time and the radius of the droplet is proposed to consider the evaporation of a macroscopic droplet with a non-negligible thickness effect. The model is used to investigate the drying of a sessile nanofluid droplet in a circular domain. Branched solid

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aggregates during the drying process are predicted. The distribution of particles and the shrinking of the contact line during the drying process, as well as the effects of the initial boundary chemical potential and the decreased rate of the chemical potential on the drying process have been investigated.

2. Mathematical model

In this section, we describe the 2D lattice-gas KMC model, which is first introduced by Rabani et al. [8]. The model is used to predict the self-assembly process of the nanoparticles and the dynamics of the evaporation during the nanofluid drying.

2.1. Kinetic Monte Carlo model

The main procedures of the simulation program are shown in Fig. 1. In the model, a circular domain instead of a shape of the droplet is used. An empty circular domain is created based on the size of the lattices. The radius of the domain (R) is expressed by an integer number of cells. Then this domain is filled with the liquid phase. In the next step, some spaces are randomly filled with the particles. The total number of particles depends on the global particle coverage ϕ , to be defined in the simulation. After that, the loop of repeating Monte Carlo steps (MCS) starts. In the Monte Carlo model, we introduce two correspondent variables l and n , to represent the status of each cell: particle cells ($l = 0, n = 1$), liquid cells ($l = 1, n = 0$) and vapor cells ($l = 0, n = 0$). In the implementation, the solvent and particles occupy single cells of the lattice. The size of the nanoparticle is not a crucial parameter, which was discussed in the previous studies [8,13].

In the simulation, the total number of the Monte Carlo steps is predefined initially. On each step of the process, two possible moves in the simulation are considered in turn [18]: (1) attempt to convert the solvent phase from liquid to vapor ($l = 1 \rightarrow 0$) or from vapor to liquid ($l = 0 \rightarrow 1$); and (2) attempt to move each nanoparticle by one lattice space in a random lattice direction. Nanoparticles may only move into the wet area of the lattice, that is, in a direction currently occupied by one adjacent liquid cell. This imitates the low nanoparticle mobility on a substrate in the absence of the solvent

[27]. If the nanoparticle moves, the displaced liquid cell is positioned in the nanoparticle's wake to preserve the solvent density.

Each solvent cell is examined in the 2-D pattern, and each attempt is accepted with the Metropolis probability, P_{acc} , given by [8]:

$$P_{acc} = \min[1, \exp(-\Delta E/k_B T)] \tag{1}$$

where ΔE is the system Hamiltonian change, which is the change in energy associated with such a move, k_B is the Boltzmann constant, T is the system temperature, $k_B T$ is the thermal energy of the system. The total system Hamiltonian value E can be calculated at every time moment from Eq. (2) [13], and its change ΔE is the difference between the system energies after and before the affecting moves.

$$E = \frac{-\frac{\epsilon_{nn}}{2} \sum_{\langle ij \rangle} n_i n_j - \frac{\epsilon_{nl}}{2} \sum_{\langle ij \rangle} n_i l_j - \frac{\epsilon_{ll}}{2} \sum_{\langle ij \rangle} l_i l_j}{1 + \sqrt{2}} - \sum_i \mu_i(t) l_i \tag{2}$$

where μ_i is the effective chemical potential of the solvent for position i . ϵ_{nn} , ϵ_{nl} and ϵ_{ll} are the interaction energies for adjacent sites (i, j) filled by (nanoparticle, nanoparticle), (nanoparticle, liquid) and (liquid, liquid), respectively. j is the index of the lattice cells adjacent to the i th cell, and t is the MCS number. The sums $\sum_{\langle ij \rangle}$ are taken for all pairs of the nearest and next-nearest cells. For the next-nearest cells, the interaction coefficients are weighted by a distance factor $1/\sqrt{2}$ [26], and the values of the interaction energies and the chemical potential are nondimensionalized by the ϵ_{ll} factor. In this paper, all the simulations use the value of ϵ_{nl} to be equal to $1.5\epsilon_{ll}$, as discussed in Ref. [8]. However, the value of ϵ_{nn} is less than $1.5\epsilon_{ll}$ in this study compared with that of Vancea et al. [13] in order to reduce the effect of particle aggregation in favor of the particle motion driven by the drying front shrinking. In this way, it can prevent the formation of multiple small separate dot-like islands, and allows the particle aggregation in a larger scale [28].

2.2. The effective chemical potential

In the KMC model, the effective chemical potential μ controls the evaporation and condensation of the liquid [18]. We call $|\mu|$ as

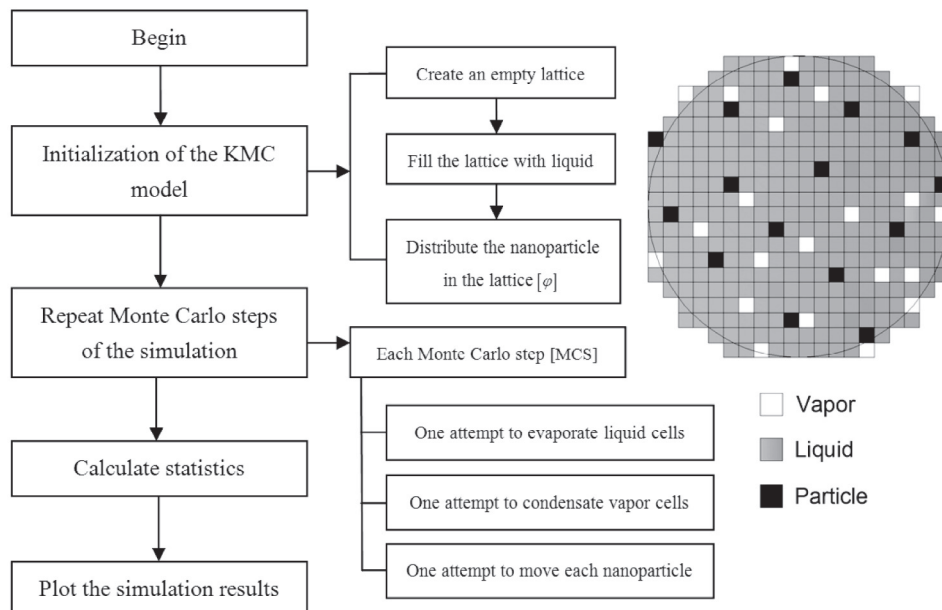


Fig. 1. Schematics of the two-dimensional lattice-gas KMC simulation process in a circular domain.

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