Effect of interfacial dipole on heterogeneous ice nucleation

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Received 2 May 2021, revised 18 June 2021
Accepted for publication 28 June 2021
Published 14 July 2021

Abstract
In this work, we performed molecular dynamics simulations of ice nucleation on a rigid surface model of cubic zinc blend structure with different surface dipole strength and orientation. Our results show that, although substrates are excellently lattice-matched to cubic ice, ice nucleation merely occurred as the interfacial water molecules (IW) show identical or similar orientations to that of water molecules in cubic ice. Free energy landscapes revealed that, as substrates have non-suitable dipole strength/orientation, there exist large free energy barriers for rotating dipole IWs to the right orientation to trigger ice formation. This study stresses that, beyond the traditional view of lattice match and the similarity of lattice length between the substrate and new-formed crystal, the similarity between molecular orientations of interfacial component and component in the specific new-formed crystalline face is also critical for promoting ice nucleation.

Keywords: heterogeneous ice nucleation, interfacial water molecules, interfacial dipole

Supplementary material for this article is available online
(Some figures may appear in colour only in the online journal)

1. Introduction

Ice nucleation is important in many ways, such as climate, microbiology, and atmospheric science [1–5]. Due to the lower free energy barrier of heterogeneous nucleation, in practice, the freezing process of water is commonly dominated by heterogeneous nucleation caused by external medium. The external medium is called ice nucleating particle (INP), and there are many substrates that have been identified as effective heterogeneous INPs, such as dust [6], cholesterol [7, 8], silver iodide [1, 2, 9–11], kaolinite [12–15], etc.

From perspective of classical nucleation theory (CNT), lattice match between INPs and ice is the main reason for promoting ice nucleation in traditional views [1, 16–19]. Kaolinite and silver iodide are effective INPs in ice nucleation because the Al-surface of kaolinite and γ-AgI show crystallographic match with hexagonal and cubic ice, respectively [14, 17]. However, recent researches reported that, only with lattice match, it is insufficient to predict the ability of INPs in ice nucleation [1, 2, 20–24]. Zielke et al [17] found that ice nucleation occurs only when silver ions are exposed on the AgI surface, rather than iodide ions exposed on the surface of AgI. There are differences in the icing temperatures between Ag+ enriched side and I− enriched side [25]. Furthermore, ice nucleation events do not occur in any base plane of barium fluoride (BaF2), although there is a good crystallographic match between BaF2 and ice crystals [26, 27]. Beyond lattice match in the process of ice nucleation, hydrophobicity [22, 28] and external electric field [16, 29] should be taken into consideration. Shao et al [26] revealed that the combination of the
oxygen lattice order and the hydrogen disorder of interfacial water molecules (IWs) on substrates can effectively facilitate the freezing of top water.

In this work, a substrate model of cubic zinc blende structure with different surface dipole strength and orientation, which is finely crystallographic matched to ice, was adopted to reveal the role of interfacial dipole on heterogeneous ice nucleation. Free energy landscapes of dipole orientation of IWs were calculated to reveal the ability of substrates in promoting ice nucleation. In the subsequent simulation with restricting IWs, we identified that molecular orientation of IWs is the key to unlock the secret of ice nucleation.

2. Simulation details

As is known, there are many materials with crystalline structure similar to cubic zinc blende, e.g. cadmium sulfide (CdS) [30], γ-AgI [31], who have ability in promoting ice formation [17]. Thus, in this study, crystalline γ-AgI was taken as substrate model to investigate heterogeneous ice nucleation. The lattice parameters of γ-AgI ($a = b = c = 6.50 \text{ Å}$, $\alpha = \beta = \gamma = 90^\circ$) show lattice mismatch of 2.36% to cubic ice ($a = b = c = 6.35 \text{ Å}$, $\alpha = \beta = \gamma = 90^\circ$) [32, 33]. The simulation cell consisted of two mirrored substrate slabs to eliminate the long-range electric field produced by lattice truncation [17, 34, 35]. The slabs were placed with a gap of 4.80 nm for placing 4032 water molecules, and a 3.00 nm vacuum outside the two slabs. The dimension of simulation box was set to be $5.20 \times 5.20 \times 13.000 \text{ nm}^3$ (see the supplementary material (https://stacks.iop.org/JPCM/33/375001/mmedia), figure S1). Periodic boundary conditions were applied in all directions.

All molecular dynamics (MD) simulations were carried out under NVT ensemble using the GROMACS 4.6.7 package [36]. The TIP4P/Ice [37] water model (melting point 270 ± 3 K) was adopted to describe water molecules. The substrate slabs were positioned rigid during the simulations. The Lennard-Jones parameters of substrates are taken from earlier work of Hale and Kiefer (cations-oxygen: $\varepsilon = 2.289 \text{ kJ mol}^{-1}, \sigma = 0.317 \text{ nm}$, anions-oxygen: $\varepsilon = 2.602 \text{ kJ mol}^{-1}, \sigma = 0.334 \text{ nm}$) [17, 38]. LINCS algorithm was employed to restrict hydrogen bond lengths [39]. A time step of 2 fs was employed. The particle-mesh Ewald [40] method was used to calculate the long-range Coulomb interactions, with a cutoff of 1.3 nm for the separation of the direct and reciprocal space summation. The cutoff distances for vdW interactions were set to 1.3 nm. Nose–Hoover thermostat was used to maintain the temperature [41, 42].

Ice Formation on Different Substrates. The temperature in the simulations was performed at 300 K for 1 ns and then decreased to 250 K, with 20 K below the TIP4P/Ice water model melting point, for the rest of the simulation time. Surface dipole strength was adjusted by the partial charges of cations/anions, ranging from 0.0 to 1.0 e (refer to table 1 for more details). For each system, $10 \times 200$ ns MD trajectories were carried out.

| Partial charges | 0.1 e | 0.2 e | 0.3 e | 0.4 e | 0.5 e | 0.6 e | 0.7 e | 0.8 e | 0.9 e | 1.0 e |
|-----------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Cation          | -     | ✓     | ✓     | ✓     | ✓     | ✓     | -     | -     | -     | -     |
| Anion           | -     | -     | -     | -     | -     | -     | -     | ✓     | ✓     | ✓     |

3. Results and discussion

Figure 1 shows the snapshots of water-substrate systems with cation-exposed (+0.4 e, figures 1(A) and (B)) and anion-exposed surface (−0.4 e, figures 1(C) and (D)) at different simulation times. The freezing of water molecules on the cation-exposed surface only takes a short time (about 15 ns) (see the supplementary material, movie 1). However, the water molecules on the anion-exposed surface maintain the liquid state even after 200 ns (figure 1(D)) (see the supplementary material, figure S3 and movie 2). The substrates, with almost perfect lattice match with ice, exhibit completely different promotion capacity on heterogeneous ice nucleation. Therefore, the surface dipole, as the only difference between the two substrates, deserves additional consideration.

To explore how the interfacial dipole affects ice nucleation, $10 \times 200$ ns MD trajectories were performed for all the systems with different anion/cation partial charges. As listed in table 1, the partial charges of cations/anions varied from 0.0 e to 1.0 e with an interval of 0.1 e. Systems that show freezing events are marked with ‘✓’. The cation-exposed surface with the partial charges of cations ranging from $+0.2 \text{ e}$ to $+0.6 \text{ e}$ can nucleate ice in all the 10 MD trajectories, which is consistent with previous reports [17]. However, there were
no ice nucleation events observed when the partial charges of exposed cations/anions outside of $+0.2 \, \text{e}$ to $+0.6 \, \text{e}$. From these results, it can be concluded that the interfacial electrostatics can significantly alter the promotion effect of substrate on heterogeneous ice nucleation.

As is mentioned above, the interfacial electrostatics can severely alter the heterogeneous ice nucleation. Moreover, it has been reported that the configurational behavior of IWs played a key role on heterogeneous ice nucleation [26, 46–50]. Given the strong dipole of water molecules, it is reasonable to believe that, in our MD simulations, the configuration of IWs was altered by the interfacial electrostatics on different substrates, thereby affecting heterogeneous ice nucleation. To explore the mechanisms underlying how interfacial electrostatics affects heterogeneous ice nucleation, the density distribution profiles (along $z$-axis) of hydrogen and oxygen atoms in IWs were extracted and shown in figure 2. The detailed configurational snapshots of the IWs are shown in figures 2(D)–(F).

As shown in figures 2(A) and (C), the density distribution profiles of hydrogen/oxygen atoms in IWs are significantly different from those in ice. For the IWs configurations shown in figure 2(D) and (F), the dipole orientations of IWs are parallel to the $z$-axis. For these two systems, there was no ice nucleation event observed even in $10 \times 200 \, \text{ns}$ trajectories. Whereas, in figure 2(B), the density distribution profiles of hydrogen/oxygen atoms in IWs are almost identical to those in the substrate-induced ice (formed in the system of $+0.4 \, \text{e}$ system at 250 K). For the IWs configurations shown in figure 2(E), one of the H–O bonds in IWs is parallel to the $z$-axis, making an angle of 1.19 rad between the $z$-axis and dipole orientation of IWs, which is almost identical as the water molecules in the substrate-induced ice. Within 15 ns, the number of water molecules freezing to ice reached the maximum value. Thus, the different configurational behaviors of IWs shown in figures 2(D)–(F) result in totally different ice formation processes. The heterogeneous ice nucleation process can be roughly divided into two steps: (i) the formation of ice-like structure (figure 2(E)) on the substrate; (ii) the accumulation of other water molecules around the ice-like structure to form ice [16]. In the cubic zinc blende structure, the distances between two neighboring cations/anions (in $x$-$y$-axis directions) are 6.50 Å, which are almost identical to the O–O distances between two neighboring water molecules in (001)
The free energy barrier is found to be 13.4 kJ mol$^{-1}$, which is far from 1.19 rad. Moreover, the free energy (figure 3(B)), the 2D free energy minima locate at the angle of 1.19 rad. In panels (E)–(G), cations, anions, hydrogen atoms, and oxygen atoms are colored by purple, grey, white, and red, respectively. Panel (G) is the configurations of exposed cations/anions on the surface and water molecules in (001) face of Ic. In panels (E)–(G), cations, anions, hydrogen atoms, and oxygen atoms are colored by purple, grey, white, and red, respectively.

To quantitatively investigate the impact of IWs configurations on heterogeneous ice nucleation, 2D free energy landscape of IWs’ dipole orientation was calculated (figure 3). As shown in figure 3, the 2D free energy landscape of IWs’ dipole orientation exhibits a periodic structure along the x-axis, with the maxima corresponding to the surface cations/anions and the minima corresponding to the adsorption sites (see figures 2(D)–(F)). For the 2D free energy landscapes of system $+0.4$ e (figure 3(A)), the 2D free energy minima locate at the angle (between z-axis and dipole orientation of water molecules) of 1.19 rad, which is almost identical to that of IWs in substrate-induced ice (1.15 rad). The free energy barrier is about 1.3 kJ mol$^{-1}$ for the adsorbed IWs rotating to an ice-like structure ((001) face in Ic). Whereas, for the system of $-0.4$ e (figure 3(B)), the 2D free energy minima locate at the angle of 2.14 rad, which is far from 1.19 rad. Moreover, the free energy barrier is found to be 13.4 kJ mol$^{-1}$ for the adsorbed IWs changing into an ice-like structure, making the ice nucleation process on the substrate much more difficult, which is consistent with the results of ice formation simulations for the $-0.4$ e system in which ice nucleation events were not observed in 10 × 200 ns trajectories. These results indicate that the interfacial electrostatics of substrates can severely alter the behavior of IWs, thereby affecting heterogeneous ice nucleation.

It should be pointed out that although the substrates cannot nucleate ice in 200 ns (15 out of 20 systems in table 1), it does not mean that they never nucleate ice. For these substrates, ice could nucleate under a much larger supercooling or in a much longer time. For instance, the free energy barrier of $-0.4$ e system is 12.1 kJ mol$^{-1}$ larger than that of $+0.4$ system (about 5.82 k$T$ at 250 K), which will result in an about 337 (e$^{82}$) times smaller heterogeneous ice nucleation rate. Besides, in a previous experimental study [25], it was found that the icing temperature of Ag$^{+}$ side of poled wurtzite AgI is $-2.7 \pm 0.4 ^\circ$C, while the icing temperature is $-4.2 \pm 0.4 ^\circ$C for that I$^{-}$ side of poled wurtzite AgI.

According to CNT, the heterogeneous promotion effect of a substrate depends on the interfacial correlation factor $f (m, R')$ (equation (1)), which is due to the fact that the substrate-crystal interface can reduce the interfacial free energy penalty caused by liquid-crystal interface during the nucleation stage [5]:

$$f (m, R') = \frac{\Delta G_{\text{hete}}^s}{\Delta G_{\text{homo}}^s}, \quad (1)$$

where $\Delta G_{\text{homo}}^s$ and $\Delta G_{\text{hete}}^s$ are the homogeneous and heterogeneous nucleation barriers, respectively. The interfacial correlation factor $f (m, R')$ indicates how much the nucleation barrier is reduced with respect to the presence of foreign bodies/substrates. The parameter $m$ can be written as:

$$m = (\gamma_{\text{sf}} - \gamma_{\text{ic}})/\gamma_{\text{cf}}, \quad (2)$$

Figure 2. Density distribution profiles of hydrogen/oxygen atoms in water molecules on the surface of substrates along z-axis. The partial charges of the exposed cations/anions on the surface in panels (A)–(C) are $+0.7$ e, $+0.4$ e, and $-0.4$ e, respectively. The profiles of hydrogen atoms and oxygen atoms are black and red. The dot lines of the density distribution of hydrogen/oxygen atoms in substrate-induced ice (formed in the system of $+0.4$ e system at 250 K) in panels (A)–(C) are black and red, respectively. The vertical green dotted line coincides with the position of the outermost cations/anions on the surface. Panels (D)–(F) are configuration snapshots of IWs corresponding to panels (A)–(C).
where $\gamma_{sf}$, $\gamma_{sc}$, and $\gamma_{cf}$ are the interfacial free energy between the substrate and the fluid phase, the substrate and the crystal phase, and the crystal phase and the fluid phase, respectively. For a solid crystalline, the interfacial free energy between the crystalline phase and substrate $\gamma_{cs}$ is highly dependent on the misorientation angle $\varphi$ [5]:

$$\gamma_{cs}(\varphi) \approx \gamma_{cs}(\alpha_0) + \frac{\varepsilon b \varphi}{4\pi(1-\nu)} \left( 1 - \frac{\varphi - \varphi_{max}}{\varphi_{max}} \right), \quad (3)$$

where $\gamma_{cs}(\alpha_0)$ is the minimum specific interfacial free energy at a given orientation $\alpha_0$; $\varepsilon$ is the elastic modulus; $\nu$ is the Poisson constant; $b$ is the Burgers vector; and $\varphi$ is the misorientation angle from the given orientation $\alpha_0$.

For a monoelemental crystal, e.g. metal systems, there is no orientation issue for the incorporation of one crystalline unit into the crystal phase. Thus, the interfacial free energy between the substrate and crystal phase is largely dependent on the size match of substrate and crystal lattices. However, for a molecular crystal, despite the size match of substrate and crystal lattices, the orientation of interfacial molecules can also change the substrate/crystal interfacial free energy, thereby altering the heterogeneous nucleation barrier and the nucleation rate of the molecular crystalline system. Thus, to predict the heterogeneous nucleation promotion effect of substrate for a molecular crystalline system, the concept of lattice match should be extended to structure match, including the lattice match and molecular orientation match between the interfacial component of substrate and the new-formed crystalline face on the substrate.

Based on the results of ice formation simulations, IWs adsorbing configurations and 2D free energy landscapes, it is emphasized that, with a suitable interfacial dipole strength and orientation, the substrate can guide water molecules at the interface to adjust their adsorption configurations to form an ice-like structure, and then the formation of bulk ice is promoted. In a previous report, it was also found that the behavior of IWs is greatly affected by charged graphene [55]. With the increase of the charge value, the IWs on charged graphene experience electromelting (first-order ice-to-liquid), and then electrofreezing (liquid-to-ice) phase transitions. This indicates that the surface charge induced change of the orientations of IWs is critical to the phenomenon of electromelting and electrofreezing in a system, which is consistent with the simulation results in this work. To further verify this point, the equilibrium adsorption configuration of IWs (before freezing) in $+0.4$ e system was extracted, fixed and applied to the systems of $-0.4$, $-0.2$, $0$, and $+0.7$ e.

With non-fixed IWs on the substrates, for systems of $-0.4$ e, $-0.2$ e, $0$ e, and $+0.7$ e, there was no ice formation observed in $10 \times 200$ ns MD simulation trajectories (table 1 and figures 4(A)–(F)). Whereas with fixed IWs on the substrates, ice formation was observed in all $10 \times 200$ ns MD simulation trajectories for all the systems motioned above, regardless of the partial charges of the exposed cations/anions. The snapshots of ice formation trajectories at 15 ns in all systems are shown in figures 4(a)–(f). For the systems of $+0.2$ e and $+0.4$ e (see the supplementary material, movie 3), there are more frozen water molecules than that in systems of $-0.4$ e (see the supplementary material, movie 4), $-0.2$ e, $0$ e, and
Figure 4. Ice formation events in several systems with different substrate dipole strength and orientation. IWs were not fixed in panels (A)–(F). While, IWs were fixed in panels (a)–(f). For clarity, only oxygen atoms are visible in TIP4P/Ice water molecules. The partial charges of cations/anions and simulation time are shown in the bottom of each panel. Cations, anions, and oxygen atoms are colored by purple, grey, and red, respectively.

+0.7 e, illustrating that, with the fixed IWs, the partial charges of the exposed cations/anions can only slightly alter the speed of ice formation, instead of preventing the formation of ice. Thus, the interfacial electrostatics indirectly affects the heterogeneous nucleation of ice by regulating the adsorption behavior of IWs.

4. Conclusions

We performed MD simulations of ice nucleation on a rigid surface model of cubic zinc blende structure with different surface dipole strength and orientation. Results demonstrated that the substrate dipole (strength and orientation) guides the behavior of water molecules at the interface, thereby affecting ice nucleation. We revealed that ice nucleation on substrate with well lattice match to ice cannot be effectively promoted, breaking down the traditional view of lattice match. Effective promotion of ice nucleation on substrate occurs as the crystalline lattice between the substrate and formed crystal, and the orientation of interfacial component and formed crystalline face are both well matched. Thus, to predict the heterogeneous promotion effect of a substrate on ice nucleation, the concept of lattice match should be extended to structure match, which also includes the matching between the orientation of interfacial component and new-formed crystalline face.

See the supplementary material for simulation details and partial simulation trajectories.

Acknowledgments

This work was financially supported by the National Natural Science Foundation of China (Grant Nos. 11904300, 11772278 and 11502221), the Jiangxi Provincial Outstanding Young Talents Program (Grant No. 20192BCBL23029), the Fundamental Research Funds for the Central Universities
The data that support the findings of this study are available upon reasonable request from the authors.

Data availability statement

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