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Supplementary information

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1 The model and simulation approaches

1.1 Molecular dynamics calculation

Simulation domain has size $30a_0 \times 10a_0 \times 42a_0$ in *x*,*y*, and *z* directions respectively, where $a_0 = 0.543$ nm is the lattice parameter for Si. Both systems consist of two silicon slabs with a slab of water. For the case of confined water (case i), the slab of water covers all silicon surface, and for the meniscus (case ii) it covers only the central part. All the systems consist of 67800 atoms of Si in total, but with variety of water molecules: 15028 for confined water, 3179 for meniscus with size $6a_0$, 5201 for meniscus with size $10a_0$, and 7225 for meniscus with size $14a_0$. The distance between two silicon slabs is set as $10a_0$.

Silicon was simulated as diamond lattice with lattice parameters of 0.543 nm and its surface is in contact with water with (0,0,1) crystal plane. The interaction between silicon atoms were modeled via the Stillinger-Weber potential¹. Atoms in the bottom and top of silicon slabs ($1.086 < z_1 < 2.172$ nm, $20.634 < z_2 < 21.72$ nm) were fixed with string forces to maintain their position close to the initial. The simple sketch that shows how input parameters are arranged compared to the system is showm in Fig. 1.

Water was simulated in frame of extended simple point charge model, SPC/E^2 . The interaction potential was determined by a combination of the Lennard-Jones, and the Coulombic potentials with cutoff distances $r_c = 1.0$ nm for both of them. For long-range Coulomb forces, each atom is assigned a charge such as q(H) = +0.4238e, and q(O) = -0.8476e. Usage of selected parameters give us a neutral charge for water molecules. To keep the O-H bond length, l = 0.096 nm, and H-O-H angles, 109.46°, sustainable the SHAKE algorithm was applied. For O-O interaction the values of $\varepsilon = 6.736$ meV, and $\sigma = 0.3166$ nm were chosen. In case of O-Si interaction, epsilon varied within 10 – 21 meV, and $\sigma = 0.26305$ nm.

Firstly, the initial system was tempered at temperature T = 1 K by using Gaussian distribution for velocity field. Then the system evolved in the *NVE* ensemble with a gradual temperature

rescaling up to 300 K for 150 ps. (Temperature rescaling to 10 K was applied for 50 ps, to 50 K for 50 ps and finally to 300 K for another 50 ps). Further the systems were equilibrated in *NVT* ensemble for 150 ps.

After equilibration, temperature rescales to 270 K and 330 K were applied to the regions 2.172 < z < 3.801 nm and 19.005 < z < 20.634 nm respectively. Then the simulation was performed for 1 ns. The values of temperature, density, potential and kinetic energy of particles and stress tensors were obtained. The obtained values are averaged from all values calculated every 0.01 ps. The binning of the system was 0.2 nm. In the region with water, calculations were performed with binning 0.1 nm for more precise calculations of water density.

1.2 Usage of FEM procedure

In order to analyze the heat transfer, MD simulations were completed by a model based on the continuum heat diffusion equation. This model makes use of the finite element method (FEM) in COMSOL[®] software to obtain the temperature field in the steady state inside the liquid meniscus and the Si slabs. The boundary conditions considered for the FEM simulations are summarised in Fig. 2. All the boundaries that confined the liquid meniscus and the SI slabs are thermally insulated, excepton at the top and bottom sides of the computational domain where uniform temperatures are imposed. The temperatures of the lower and upper boundaries were set at 330 K and 270 K respectively. A contact thermal resistance is also specified for the interfaces between the liquid and the solid, so that a discontinuity of temperature and heat flux is obtained at these interfaces. As an input, resistance values were taken from the results obtained from MD considering a specific value of ε . The thermal conductivity of silicon and water were chosen equal to 220 and 0.86 W/(m K) respectively to be consistent with MD results. Special care was also taken for the geometry of the liquid meniscus, since the contact angle at the solid/liquid/gas triple junction must be consistent with the value of ε considered for the ITR. Finally, the position and the shape of the meniscus edges in the FEM simulations were adjusted to have a liquid volume that is equal to that considered in the MD simulations. An unstructured triangular mesh is used with elements size around 7.10^{-2} nm. A convergence criterion = 0.001 (or relative tolerance on temperature) was applied to ensure a good accuracy of the results.

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Fig. 1 Representation of the initial systems. Here L_{water} is the size of the initial systems cases i) $30a_0$, and ii) $6a_0$, $10a_0$, $14a_0$, $d_{water} = 10a_0$, $d_{empty} = 2a_0$, $d_{fixed} = 2a_0$, $d_{substrate} = 14a_0$, $d_{therm} = 3a_0$.



Fig. 2 Boundary conditions considered for the FEM modelling

2 A meniscus shape calculation

Curves corresponding to the boundaries of the droplets were obtained based on the circle approximation (see Fig. 3):

$$(x-x_0)^2 + (z-z_0)^2 = R_{\text{circle}}^2$$

where x_0 and z_0 – coordinates of the center of the circle. If *d* is the distance between silicon slabs, and ϕ is the wetting angle:

$$d/2 = R_{\text{circle}} \cos(\phi),$$

$$(x - x_0)^2 + (z - z_0)^2 = R_{\text{circle}}^2,$$

$$(x - x_0)^2 + (z - z_0)^2 = d^2/(4\cos^2(\phi)),$$

$$x = x_0 \pm (d^2/(4\cos^2(\phi) - (z - z_0)^2)^{1/2},$$

where the roots with " \pm " and sign corresponds to a hydropho-

bic (+) and hydrophilic (-) cases respectively. x_0 was calculated based on the fact that the volume v of the droplet for all cases remains constant.

We calculated the volume of the droplet based on the number of water molecules and its density.

$$\frac{v}{2b} = \int_0^{x_0 \pm (d^2/(4\cos^2(\phi)) - (z - z_0)^2)^{1/2}} \int_{-d/2}^{d/2} dx dz$$

b is the thickness of droplet which is not used for curve fitting because we are considering a 2D system. After calculating the



Fig. 3 A simple sketch that shows connection between curves corresponding to the boundaries of the droplets and the system, that we used to obtain curves in Figs.3, 11-13. The input parameters that are shown here are well described in equation above.

integral, we obtain:

$$\frac{v}{2b} = x_0 d \pm \frac{1}{8} \left[\frac{d^2}{\cos^2(\phi)} \cdot \arcsin\left(\frac{(2z_0 + d)\cos(\phi)}{d}\right) - \frac{d^2}{\cos^2(\phi)} \cdot \arcsin\left(\frac{(2z_0 - d)\cos(\phi)}{d}\right) + (d - 2z_0)\sqrt{4z_0(d - z_0) + d^2\tan^2(\phi)} + (d + 2z_0)\sqrt{-4z_0(d + z_0) + d^2\tan^2(\phi)} \right]$$

Thus, we obtained an analytical equation of the curve bounding the drop based on the distance between the silicon slabs and the wetting angle.

3 Temperature profiles of the meniscus with heat fluxes distributions

The same temperature difference between two silicon slabs (60 K) was applied. Fig. 5 shows the temperature profiles with heat fluxes obtained using FEM (left) and MD (right) methods. The central plot shows one-dimensional temperature distributions in the middle of the system obtained from both of these approaches (solid green line represents FEM values and purple dots represents MD values). As it can be seen, the fluxes on the graph for MD are less structured than for FEM. This is expected due to fluctuations of physical quantities that are present in the MD simulation. Distribution for MD was obtained by averaging five simulations, each of them separately gives much more disordered fluxes. Averaging over more simulations would give the more directional fluxes with an increased computational costs.

The increase of the density peak near the surface with increasing ε is represented in Fig. ?? as well. Moreover, from Fig. ??, it can be seen how water penetrates deeper into silicon for high ε . Increasing the ε creates a stronger coupling between water and silicon, which increases the depth of water penetration into the silicon lattice, and the density of the surface layer of water, which in turn reduces the mismatch in the density of vibration states and provides better heat transfer.

4 Effect of surface temperature on temperature jump

In order to make sure that the change in temperature jump, and hence thermal resistance with meniscus size, is not related to the different surface temperature depending on the meniscus size, the dependence of the surface temperature on ε was investigated. The results are presented in Fig. 4.

As can be seen from graphs (a) and (b), the surface temperature depends on the size of the meniscus. However, we considered the thermal jump as the average value between the hotter (T=330K) and colder (T=270K) sides. The averaged values (c) are within errors and the difference between the lowest and the highest value equal to 1 K which can't significantly affect the temperature jump. Therefore, the effect of the surface temperature change on the temperature jump is negligible.



Fig. 4 Surface temperature as a function of ε for the (a) colder, (b) hotter sides and (c) averaged values.



Fig. 5 Temperature profiles of the meniscus with size $6a_0$, ($\varepsilon = 10 - 21$ meV) with heat fluxes distributions obtained from MD simulations.



Fig. 6 Temperature profiles of the meniscus with size $10a_0$, ($\epsilon = 10 - 21$ meV) with heat fluxes distributions obtained from MD simulations.



Fig. 7 Temperature profiles of the meniscus with size 14a₀, ($\varepsilon = 10 - 21$ meV) with heat fluxes distributions obtained from MD simulations.



Fig. 8 Temperature profiles of the meniscus with size $6a_0$, ($\varepsilon = 10$ - 21 meV) with heat fluxes distributions obtained from FEM simulations.



Fig. 9 Temperature profiles of the meniscus with size $10a_0$, ($\varepsilon = 10 - 21$ meV) with heat fluxes distributions obtained from FEM simulations.



Fig. 10 Temperature profiles of the meniscus with size 14a₀, (ϵ = 10 - 21 meV) with heat fluxes distributions obtained from FEM simulations.



Fig. 11 The density profiles of meniscus with size $6a_0$ for different parametrization, ($\varepsilon = 10 - 21$ meV). Values of density are shown in colorbar. The black solid line connects the points where the density of meniscus is equal to the half of the density of confined water. Red lines are the analytically obtained borders of droplet.



Fig. 12 The density profiles of meniscus with size $10a_0$ for different parametrization, ($\varepsilon = 10 - 21$ meV). Values of density are shown in colorbar. The black solid line connects the points where the density of meniscus is equal to the half of the density of confined water. Red lines are the analytically obtained borders of droplet.



Fig. 13 The density profiles of meniscus with size $14a_0$ for different parametrization, ($\epsilon = 10 - 21$ meV). Values of density are shown in colorbar. The black solid line connects the points where the density of meniscus is equal to the half of the density of confined water. Red lines are the analytically obtained borders of droplet.

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