

SUPPLEMENTARY MATERIAL

Molecular Dynamics Simulation Study of Heat Transfer Across Solid-Fluid Interfaces in a Simple Model System

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CUMULATIVE KINETIC ENERGY

Fig. S1 shows a typical result for the kinetic energy E added to the hot wall and removed from the cold wall by the thermostats as a function of the simulation time t during the sampling phase of the simulation. The linear dependency indicates a steady-state.

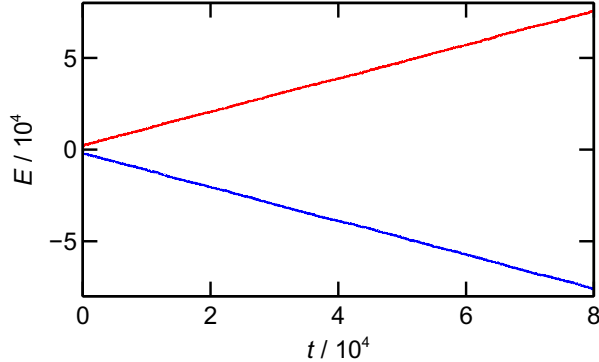


FIG. S1. Cumulative kinetic energy E added to the hot wall (red) and the cold wall (blue) by the thermostats as a function of the simulation time t in the 4 million time steps of the sampling phase. Data taken from simulation 1, cf. Table II in the main text.

INFLUENCE OF THE CHANNEL WIDTH H AND THE WALL TEMPERATURE T_w ON THE KAPITZA LENGTH L_K

The simulations 28 – 62 (cf. Tab. II) were used to study the influence of the channel width on the Kapitza length. As shown in Fig. S2, the Kapitza length L_K is practically independent of the channel width H .

The influence of the temperature difference between the fluid in the center of the channel and the wall ΔT_w was studied by the simulations 63 – 74 (cf. Table II in the main text). The results of these simulations are shown in Fig. S3 and reveal that ΔT_w has no significant influence on L_K in the range of values studied in the present work, i.e. the results scatter around a common mean value.

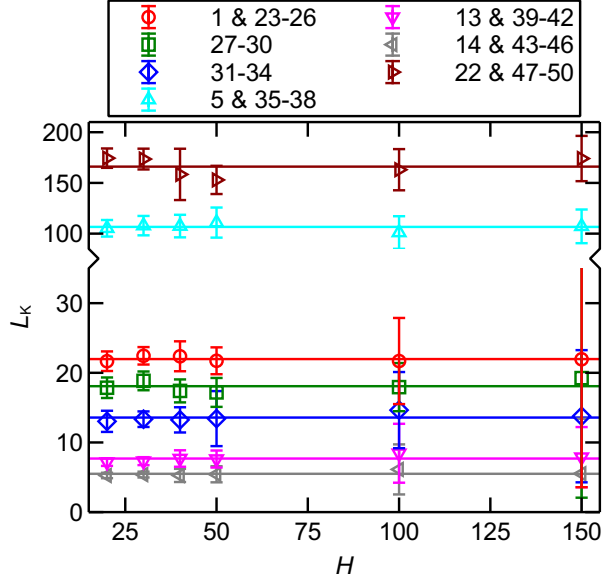


FIG. S2. Influence of the channel width H on the Kapitza length L_K . Results from the simulations (symbols) are indicated in the legend; the numbers correspond to the simulation number given in Table II in the main text. The solid lines represent the mean values of the respective simulations.

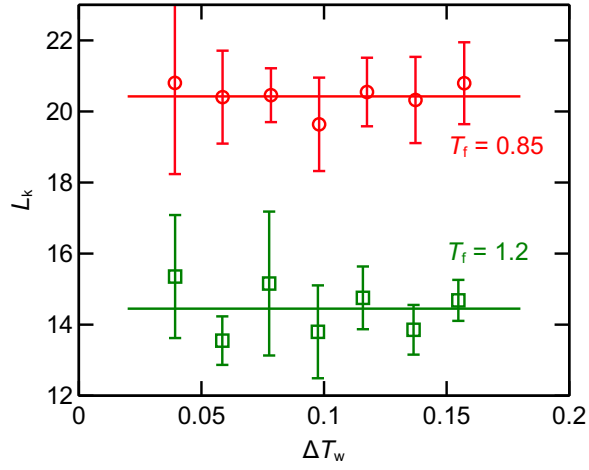


FIG. S3. Dependence of the temperature difference between the fluid in the center of the channel and the wall ΔT_w on the Kapitza length L_K . Results from the simulations 63 – 68 (red symbols) and 69 – 74 (green symbols), cf. Table II in the main text. The red and green solid lines represent the mean value of the respective simulations.

INFLUENCE OF THE SOLID-FLUID INTERACTION ENERGY ε_{sf} , THE FLUID TEMPERATURE T_{f} AND THE FLUID DENSITY ρ_{f} ON THE DENSITY PROFILE NEAR THE SOLID SURFACE

Fig. S4 shows that the solid-fluid interaction energy ε_{sf} has an important influence on the fluid structure at the interface. Not only the width of the maxima depend on ε_{sf} , but also their position. As expected, low numbers of ε_{sf} lead to less ordering. A high ordering in the adsorption layer leads to an increased heat transfer resistance of the interface.

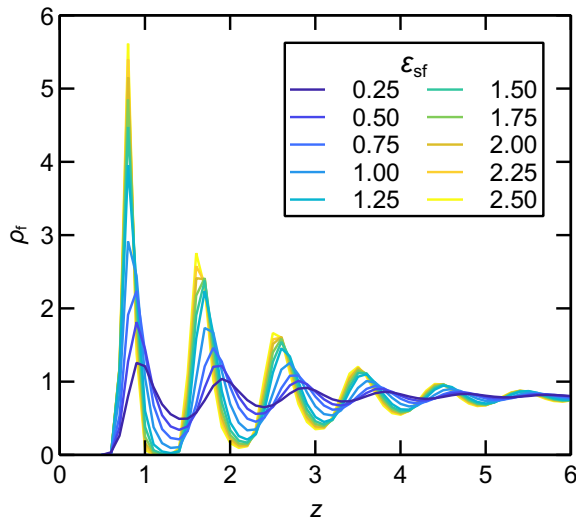


FIG. S4. Density profile of the fluid at the solid-fluid interface for different solid-fluid interaction energies ε_{sf} . The bulk density is $\rho_{\text{bulk}} = 0.8$. Results from the simulations 1 and 10 – 18, cf. Table II in the main text.

Fig. S5 shows the influence of the fluid temperature T_{f} on the structure of the fluid at the interface. Fig. S5 reveals that high temperatures lead to a decrease of the structuring due to a larger fluid particle mobility.

In Fig. S6, the structuring of the fluid is plotted for ten different mean fluid densities along supercritical isotherm $T = 1.3$. It reveals that the number of adsorption layers and thus the structuring of the fluid near the wall increases with increasing density.

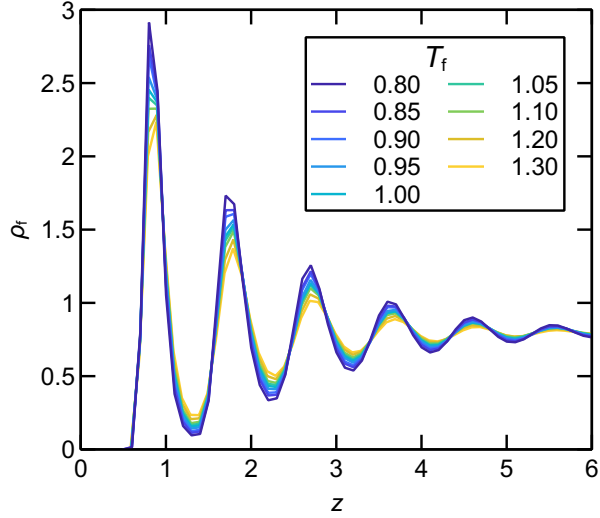


FIG. S5. Density profile of the fluid at the solid-fluid interface for different fluid temperatures T_f . The bulk density is $\rho_{\text{bulk}} = 0.8$. Results from the simulations 1 – 9, cf. Table II in the main text.

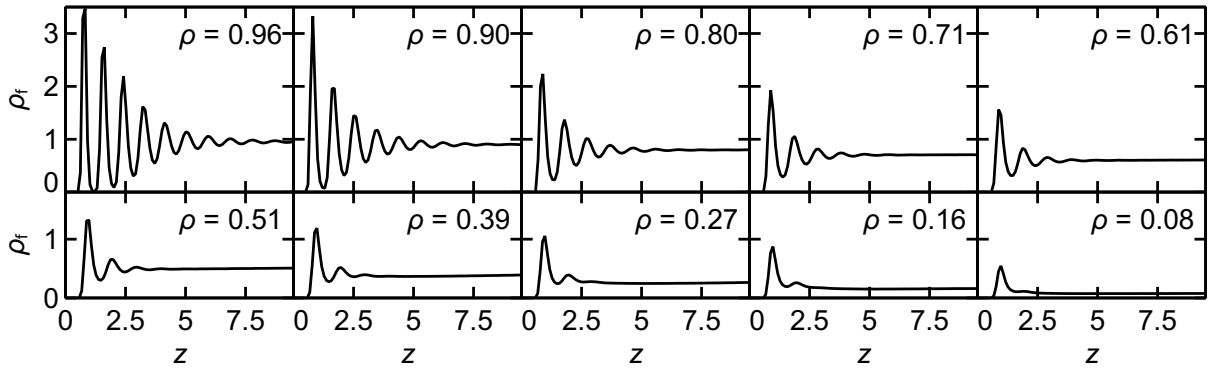


FIG. S6. Density profile of the fluid for ten bulk densities ρ_f at a temperature of $T = 1.3$. The mean bulk fluid density is indicated in each subplot. Results from the simulations 9, 97, 99, 101, 103, 105, 107, 109, 112, and 113, cf. Table II in the main text.