Journal of Molecular Liquids
Volume 373, 1 March 2023, 121128

Thermal performance of a phase change material (PCM) microcapsules containing Au nanoparticles in a nanochannel: A molecular dynamics approach

Fengyun Wang [a], Navid Nasajpour-Esfahani [b], As'ad Alizadeh [c], Ghassan Fadhil Smaisim [d e], Azher M. Abed [f], Salema K. Hadrawi [g h], Saman Aminian [i], Roozbeh Sabetvand [j], D. Toghraie [k]

https://doi.org/10.1016/j.molliq.2022.121128

Abstract

This research studied the thermal performance of phase change material (PCM) microcapsules containing gold (Au) nanoparticles (NPs) in a nanochannel (NC) using molecular dynamics (MD) simulations. The MD simulation method is a reliable method for studying at micro and nano scales. In this simulation, the physical equilibrium was studied in the first stage by examining the simulated structure's kinetic and total energies. In the second stage, the thermal performance of simulated structure was surveyed. The thermal performance of structures was studied at different initial temperatures and initial pressure and the number of metal layers in NC shells. The results show that by increasing the initial temperature, the charging and discharging time, the viscosity and phase transition time decrease, and heat flux (HF) and thermal conductivity (TC) increase. Moreover, by changing the initial pressure (from 0 to 5 bar), the simulated samples' charging and discharging time, HF, and TC did not change much. This atomic behavior in the simulated samples shows that the simulated samples could operate without a drop in different initial conditions. The results indicate that by increasing the number of metal layers in the NC shells from 1 to 12, the force on fluid–structure increased, and consequently, the charging and discharging times increase to 2.54 ns and 3.40 ns. On the other hand, increasing the number of metal layers led to decreasing HF and TC of structures to 287.37 W/m^2 and 1.18 W/m.K. Therefore, the dimensions of designed structures in atomic microcapsules to perform the heat transfer process were important. Increasing the shell thickness in these structures will reduce the heat transfer in the structures under study.