On the description of multilayer argon adsorption on graphite surface below the bulk triple point

This study explores the adsorption isotherm of argon on graphite at temperatures below the bulk triple point temperature using Monte Carlo simulations. Two different models are employed, the first model (S-model) has a planar surface of infinite extent in the two directions parallel to the surface, and the second is a finite surface called (2D-Patch model). Both models have been compared with experimental data. The 2D-Patch model accurately mimics the experimental isotherm better than S-model. The results obtained lead to a comprehensive description of the adsorption isotherm of simple gases on graphite at various temperature, which has not been widely documented in the literature.

Abstract

Monte Carlos Simulation was employed to investigate the adsorption of argon on graphite at temperatures below the triple point temperature, $T_{tr(bulk)} = 83.8K$. Two surface models were used: a planar surface (S-model) with periodic boundary conditions parallel to the surface, and a finite surface 2D-Patch model to examine the effect of boundary conditions on the adsorption isotherm. While both models were compared against experimental data, the 2D patch model provided a more accurate representation of the experimental isotherm and condensation pressure during the first-order transition. In contrast, the S-model exhibited numerous sub-steps in the adsorbate layer, leading to a poor description of higher adsorbate layers. These findings support the interpretation of boundary growth and the mismatch between the lattice of the adsorbed phase and the box dimensions.

By combining the outcomes of simulation conducted at temperatures lower than the bulk triple point temperature with published literature findings at higher temperatures $T_{tr(bulk)}$, and incorporating experimental data, we have developed a generic model that characterizes the adsorption isotherm of basic gases on graphite. This model encloses a wide temperature range, from significantly below the bulk triple point temperature and extending up to the bulk critical temperature. It is worth noting that this comprehensive depiction of adsorption isotherms on graphite is not commonly acknowledged in the existing literature.

Keywords: 2D-critical; Steele surface; 2D surface; Adsorption; Graphite