Pressures inside a nano-porous medium. The case of a single-phase fluid

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We define the pressure of a porous medium in terms of the grand potential and compute its value in a nano-confined or nano-porous medium, meaning a medium where thermodynamic equations need be adjusted for smallness. On the nano-scale, the pressure depends in a crucial way on the size and shape of the pores. According to Hill [1], two pressures are needed to characterize this situation; the integral pressure and the differential pressure. Using Hill's formalism for a nano-porous medium, we derive an expression for the difference between the integral and the differential pressures in a spherical phase $\alpha$ of radius $p^\alpha$ of radius $\gamma/R$. We recover the law of Young-Laplace for the differential pressure difference across the same curved surface. We discuss the definition of a representative volume element for the nano-porous medium and show that the smallest REV is a unit cell in the direction of the pore in the fcc lattice. We also show, for the first time, how the pressure profile through a nano-porous medium can be defined and computed away from equilibrium.

We test the viability and validity of the pressure expression in the nano-porous medium using molecular dynamics simulations by studying two idealized models for nano-porous media, a single spherical grain and a lattice of spherical grains.

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