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**Calculation of elastic properties of argon confined in nanopores of various morphologies using grand canonical Monte Carlo** CHRISTOPHER DOBRZANSKI, GENNADY GOR, NJIT — Fluids confined in nanopores exhibit thermo-physical properties that differ from the properties of the same fluids in bulk. Among these properties are the isothermal compressibility or elastic modulus. The modulus of a fluid in nanopores can be extracted from ultrasonic experiments or calculated from molecular simulations. Using grand canonical Monte Carlo simulations, we calculated the modulus for liquid argon at its normal boiling point 87.3 K adsorbed in silica pores of various sizes and morphologies. For both spherical and cylindrical pores above 2 nm, we obtained a logarithmic dependence of fluid modulus on the vapor pressure. Calculation of the modulus of the fluid in spherical pores at saturation displayed a linear function of the reciprocal pore size. The calculation for cylindrical pores shows a similar trend, however, it is hard to make quantitative conclusions from the highly scattered resulting data. With the development of effective medium theories for decoupling properties of nanoporous media and the fluids confined within them, our results set the basis for analysis of the experimentally-measured elastic properties of fluid-saturated nanoporous materials and can enable probing pore size through ultrasonic measurements.

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