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A multiscale theory explaining the initial shrinkage of microporous materials upon adsorption

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ABSTRACT

Adsorption-induced deformation is widely observed in porous materials such as cement, coal, clay, aerogel, biopolymers and MOFs. Sorption swelling has been commonly explained by the so-called Bangham effect (Bangham and Fakhoury 1928), i.e. the relaxation of solid-fluid interfacial tension due to adsorption and thus the macroscopic expansion of the porous media. However, experimental studies show that certain microporous materials (pore size less than 2 nm) such as activated carbons contract first at low gas pressure, followed by Bangham's expansion after reaching certain pressure levels (Balzer et al. 2015). Such phenomenon has not been explained and modelled in previous poromechanics theories.

This work extends the recently developed surface poromechanics framework for macro/meso porous media (Zhang 2018) to describe the adsorption-deformation behavior of microporous materials by considering interaction forces in micropores. At distances as small as a few nanometers, short-range intermolecular interactions can give rise to forces that are formerly disregarded in the analysis of macro/meso porous media. The effect of such interactions is considered in this study through an extra work term in the thermodynamics of a single slit pore. As a result of such pore-scale analysis, a pressure known as the disjoining or solvation pressure that acts normal to the pore walls in addition to the bulk fluid pressure is obtained. This effect also modifies the surface tension parallel to the pore walls. The disjoining pressure and the modified surface tension together create a competing effect in determining the shrinkage or expansion of the porous skeleton during adsorption. When the pore size becomes sufficiently large, this new development degenerates to the macro/meso poromechanics theory of Zhang (2018). Through a choice of adsorption and microstructure model, the proposed microporomechanics theory is validated against recent experimental data on activated carbons. To the author's knowledge, this is the first continuum theory that captures the initial shrinkage of microporous solids upon adsorption and is ready to be implemented in FEA or other numerical solvers for IBVP predictions.

REFERENCES

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