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Understanding the Time-Dependent Deformation of Microporous Carbons Due to Adsorption

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Equilibrium and kinetic behavior of adsorption-induced deformation attracted much attention in the last decades [1,2]. This phenomenon is ubiquitous but challenging to predict quantitatively due to numerous factors (pore size and geometry, adsorbent/adsorbate combination, temperature, etc.) affecting its manifestation. Time may be considered as one of these factors as many industrial and real-world processes occur far from thermodynamic equilibrium. The theoretical and experimental works cover activated carbons, coals, zeolites, glasses, etc. However, most of the theoretical works are focused only on the equilibrium part of the deformation process or only on the description of the time evolution of the adsorption process. The present contribution [3] aims to cover the existing gap, using the combination of two theoretical frameworks: the diffusion-based description of the time-dependent adsorption process and the osmotic ensemble-based description of adsorption-induced deformation. We obtained self-consistent equations describing equilibrium and out-of-equilibrium adsorption as well as deformation processes. As a next step, we verified the obtained equations on the experimental data [4] of carbon dioxide and methane on activated carbons (AC Chemviron and AC T-3). Our results demonstrate that the model can describe both equilibrium and kinetic adsorption and adsorption-induced deformation data. Also, we considered the possible influence of slow relaxation processes in the adsorbent on the adsorption process. We showed that at low strain relaxation rates, the diffusion process is hindered by deformation. On the other hand, at high strain relaxation rates, the deformation process is defined by the local adsorbate concentration and "follows" the diffusion. The current work helps to interpret experimental data on time-dependent adsorption-induced deformation.

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References

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