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Coupling mechanism of sorption and deformation in amorphous cellulose with hierarchical porous structure

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Wood, as natural adsorbent and significant building material, features complex biopolymer composition and hierarchical porous structure, endowing it with distinguished sorption properties accompanied by sorption-induced deformation. In former studies, sorption, deformation and sorption-deformation interactions have been studied for single-scale materials, but not for materials where micropores and mesopores coexist. This work, establishing a mesoscopic slit pore between two slabs of amorphous cellulose with micropores, aims to provide a first attempt at modeling sorption and sorption-induced deformation in hierarchical porous structure. Specifically, the atomic system is numerically modeled by a hybrid workflow synthesizing molecular dynamics (MD) and grand canonical Monte Carlo (GCMC) simulation. Based on the simulation, sorption/deformation mechanisms in porous materials with different slit size are clarified. In microscopic pores prevailing in the cellulose slab, pore filling happens throughout the full relative humidity (RH) range. Under low RH, adsorption happens mainly by filling existing voids. At high RH, adsorption continues via imposing a sorption stress, leading to a swelling and additional sorption of the microporous material. In the mesoscopic slit pore between the two cellulose slabs, surface sorption takes place, with negligible amount initially but remarkable thickness with increasing RH. Meanwhile, increasing surface roughness is observed, in response to the varying surface energy caused by the multilayer adsorption. At a certain RH, the water molecules residing on the opposite cellulose slabs undergo capillary condensation, which exerts a negative hydrostatic pressure perpendicular to the slab surface on the structure, resulting in an increase in slab volume, a decrease in distance between the center of mass (COM) of the slabs and thus a thinning of the slit pore.

Participation

In-Person

References

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