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Moisture dependent phonon transport and scattering in nanocellulose

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Heat transport properties in solid materials are driven by the accumulative contributions of phonons spanning a wide range of mean free paths. Porous, hygroscopic, nanocellulose foams exhibit super-insulating properties, highly dependent on their moisture content, and through theoretical estimations and simulations, it has been shown that the heat transfer in such materials is dominated by phonon scattering [1], [2]. Inelastic neutron scattering (INS) is one of the most powerful tools to investigate the vibrational excitation landscape in condensed matter. This work presents an INS study, in which the phonon density of states (DOS) has been extracted for nanocellulose as a function of moisture content and alignment. Through freeze casting, particles have been aligned along the Z-axis and in the XY-plane to carry out direction-dependent measurements in order to detect possible isotropic and anisotropic character of the phonon DOS. We also investigated the effect that particle size and crystallinity have on the phonon DOS; with the longer, thinner, and less crystalline cellulose nanofibrils (CNF) being more prone to moisture sorption than the shorter and more crystalline cellulose nanocrystals (CNC). The preliminary results show that the phonon DOS increases with the moisture content for CNC and CNF aligned along the Z-axis, and a decreasing phonon DOS was observed with increasing moisture content for the particles aligned in the XY plane.

[1] V. Apostolopoulou-Kalkavoura, P. Munier, L. Dlugozima, V.-L. Heuthe, and L. Bergström, 'Effect of density, phonon scattering and nanoporosity on the thermal conductivity of anisotropic cellulose nanocrystal foams', Sci Rep, vol. 11, no. 1, p. 18685, Dec. 2021, doi: 10.1038/s41598-021-98048-y.
[2] V. Apostolopoulou-Kalkavoura et al., 'Humidity-Dependent Thermal Boundary Conductance Controls Heat Transport of Super-Insulating Nanofibrillar Foams', Matter, vol. 4, no. 1, pp. 276–289, Jan. 2021, doi: 10.1016/j.matt.2020.11.007.

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