Thermal and mechanical attributes and swelling percentage of hydrogels by changing in magnetic field frequency using computer simulation

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Abstract

The thermodynamic, mechanical, and expansion properties of synthetic hydrogels derived from polyacrylamide (PAM) are investigated in this study to the impact of magnetic field frequency (MFF) as an external stimulus. The impact of various MFFs on essential parameters, such as swelling percentage (SP), ultimate strength (US), Young's modulus (YM), heat flux (HF), and thermal conductivity (TC), is assessed using Molecular Dynamics (MD) simulation with LAMMPS software, ranging from 0.01 to 0.05 1/fs. It is important to note that our results indicate that the structural volume decreased from 356,985 to 349,982 Å at 0.05 1/fs as the MFF increased. The alignment of polymer chains in the hydrogel was improved by increasing the MFF, resulting in a more compact structure. Through this compaction, the total structural volume diminished as the chains were drawn closer together, thereby reducing the spaces among them. US experienced a decrease from 0.0325 to 0.0331 MPa, while YM converged to 0.0008 MPa. The alignment and packaging of polymer chains improved, resulting in an increase in the US of hydrogels as the MFF increased. This enhanced alignment resulted in a material that can withstand a larger amount of stress before failing, as a result of the stronger intermolecular interactions. Additionally, the temperature coefficient (TC) increased to 0.56 W/m·K as the MFFs increased. An increase in molecular alignment and a decrease in free volume within the hydrogel can be attributed to the higher MFF. This enhanced alignment enabled the molecules to transfer heat more efficiently, resulting in improved TC and increased HF. These findings illustrate the substantial influence of MFF on hydrogel properties, offering valuable insights for the development of drug delivery systems and responsive materials.