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ANOMALOUS THERMOMECHANICAL BEHAVIOUR OF CARBON NANOTUBE BUNDLE

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Abstract. The molecular dynamics method is used to calculate the dependence of pressure on temperature at a constant volume for a bundle of carbon nanotubes (CNTs) considered under plane strain conditions. A chain model with a significantly reduced number of degrees of freedom is used for modeling. The influence of the CNT diameter is analyzed. It was found that for some parameters of the model, the pressure in the CNT bundle can decrease with increasing temperature, which is equivalent to the effect of negative thermal expansion.

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