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Stretching Helical Macromolecules GUSTAVO A. CARRI, VIKAS VARSHNEY, Department of Polymer Science, The University of Akron, Akron, OH 44325-3909 — We study the elasticity of a homopolypeptide under extension using Monte Carlo simulations based on the Wang-Landau algorithm. The effect of external mechanical forces is described with an extension of a model for helical polymers (V. Varshney *et. al.*, *Macromolecules* **2004**, 37, 8794). We find that the application of a mechanical force first increases the helix-to-coil transition temperature and then decreases it. This non-monotonic behavior is a consequence of a change in the nature of the helix-coil transition which becomes a helix-extended-coil transition for strong forces. We also find that the force-elongation curve at constant temperature displays three different behaviors depending on the temperature of the system. At temperatures below or slightly above the helix-coil transition temperature the force-elongation curve shows one or two coexistence regions, respectively. In these regions helical sequences and random coil domains coexist. At high temperatures our model recovers the elastic behavior of a random coil. We present a quantitative comparison with the theoretical results of Buhot and Halperin, and very good agreement is observed.

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