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Coarse-grained Molecular Dynamics Simulations and Analysis of Poly(L-lactic Acid) (PLLA) Melt GAURAV MANIK, HEMANT NANAVATI, Chemical Engg. Department, Indian Institute of Technology Bombay, Mumbai-400076, India, UPENDRA NATARAJAN, Chemical Engg. Department, Indian Institute of Technology Madras, Chennai-600036, India — We present coarse-grained (CG) MD simulations of the melt structure of PLLA, a very useful biodegradable polymer. Our CGMD simulations consider entire repeat unit as a one bead and use IBI scheme. The CG potentials and forces are obtained after performing atomistic MD of 52 PLLA tetramer molecules and employing the probability distributions for the corresponding CG lengths, angles, dihedrals, and the radial distribution function. The initial energy-minimized samples are equilibrated for density in NPT ensemble, followed by structural equilibration. The simulated characteristic ratio (2.13) and density (1.123g/cc) at 450K are in excellent agreement with the expt. values[1] of 2.2 and 1.152g/cc at 413K. The equilibrated structures were analyzed for primitive path properties, tube diameter, a_{pp}, entanglement length, N_e, etc., using Kroger's Z-code[2]. This yields N_e=61.8 and a_{pp}=55.7A^o for longest chains (N=1000) and compare favorably with expt.values.[1], 55 and 47.7A^o (413K).

[1] Dorgan, J R., Janzen, J and Clayton, M.,*J. Rheology*,49,607,**2005**
(a) Kroger, M., *Comput. Phys. Commun.*, 168, 209, **2005**.

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