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Modeling of Polymer Melting JIANING ZHANG, University of Massachusetts, Amherst, MURUGAPPAN MUTHUKUMAR, University of Massachusetts, Amherst — We have employed modified Potts model with anisotropic interaction to simulate melting of polymer crystals. Using this coarse-grained model with fixed lamellar thickness, we have successfully reproduced many experimental results. A broad melting transition is found and becomes broader with decreasing crystallization temperature T_c, increasing heating rate β or crystallization time t_c. The melting temperature T_m depends on β, t_c and T_c as follows: $T_m \propto \beta^{0.5}$; $T_m \propto \log t_c$ for intermediate t_c values; T_m is constant in low-T_c region and gradually increases with T_c in high-T_c region, in contradiction with Hoffman- Weeks plot but consistent with experimental observations over a wide T_c range. A new relation for T_m is proposed: $T_m = T_m(\beta = 0) + const\sqrt{\beta}\log R$, where R is the average lamellar diameter following the law $R \propto t_c^{1/3}$.

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