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Relation of dynamics and local structure to glass-formability in a crystallizable bead-spring polymer model HONG NGUYEN, TYLER SMITH, ROBERT HOY, Univ of South Florida, NIKOS KARAYIANNIS, Universidad Politecnica de Madrid, Madrid, Spain — We relate the dynamics and local structure of equilibrium and supercooled polymer melts using a model wherein a single parameter (bending stiffness) controls the morphology of the equilibrium, low-temperature crystal. The dynamical slowing down in strongly glassforming systems correlates directly to the increasing presence of microstructural features that are incompatible both with each other and with crystalline order. Systems which more readily crystallize also exhibit rich behavior since their solid-state morphology can be varied from nearly amorphous to highly crystalline by varying their thermal preparation protocol. We tie the “critical” cooling rates, across which this behavior varies, to the lifetimes of structural features such as small crystalline nuclei and stable liquid-like clusters. The role such structures play is analogous to that recently demonstrated for colloidal systems [S. R. Williams, arXiv:0705.0203, 2007], but is considerably enriched both by the dynamical constraints imposed by covalent connectivity and by the presence of a second characteristic length scale (the polymer Kuhn length) controlled by chain bending stiffness.

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