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A Micromechanical Model for the Elastic Properties of Semi-crystalline Polymers

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Introduction
Elastic moduli of semi-crystalline polymers are important properties and difficult to predict due to their dependence on many factors, such as: molecular weight, cooling rate, annealing, etc. To better design products, it is of significance to accurately predict these properties as a function of the microstructural morphology and crystallinity.

Micromechanical Model
Semi-crystalline polymers can be modeled as two-phase composites, the crystalline phase and the amorphous phase. By using a layered micromechanical model, overall properties can be predicted as a function of crystallinity (figure 1).

Homogenization Methods
Three methods have been used for obtaining the overall properties: Voigt, Reuss and Voigt-Reuss-Hill average.

Results and Discussion
In this section, a two-phase and a three-phase composite inclusion model are used to obtain the effective behavior of HDPE. The spherulitic structure of HDPE is presented by an aggregate of 120 inclusions with random orientation of crystallographic directions and interface normals (figure 3). Monte-Carlo simulation results show that $\delta_r = 1$ to 2 nm (inter-phase thickness) while $\delta_c = 6.8$ nm (crystal thickness) [2].

Conclusions and Future Work
✓ The properties of semi-crystalline polymers can better be predicted if a three-phase composite inclusion model is used.
✓ Hybrid interaction models will be used to form an intermediate approach between the upper bound Voigt and the lower bound Reuss models.

References
[2] T.N. Pham, C.L. Tucker, Polymer processing society 24th annual meeting, 2008, Italy