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Predicting Structure-Property Relationship in Segmented Polyurethanes VALERIY GINZBURG, ALAN SCHROCK, CHRISTOPHER CHRISTENSON, The Dow Chemical Company, JOZEF BICERANO, Bicerano & Associates, Inc., ALEXANDER PATASHINSKI, Department of Chemistry, Northwestern University — We develop new theoretical framework to study the relationship between composition and mechanical properties in segmented polyurethanes (PU) and poly(urethane-ureas) (PUU). In particular, we analyze polymer mechanical properties (quasi-static Young's modulus, E, and temperature-dependent storage shear modulus, G') as function of the hard and soft segment chemistry, hard segment weight fraction, soft segment molecular weight, and temperature. It has been known for some time [1] that in many segmented PU and PUU polymers, the hard-soft microphase separation causes the formation of a "percolated hard phase". We propose a new formalism that enables one to predict the onset of the hard phase percolation as function of temperature, soft segment molecular weight, and chemical structures of hard and soft segments. Based on this formalism, we can build micromechanical models to estimate mechanical properties of segmented polyurethanes as function of temperature. We used this theoretical framework to simulate storage moduli of several model compounds, and found very reasonable qualitative agreement with experimental data. [1] See, e.g., A. J. Ryan et al., *Macromolecules,* **24**, 2883 (1991); *Polymer* **32**, 1426 (1991).

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