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November 6, 1991

Dr. Michael Marron
Materials Division
ONR Code 1141
800 North Quincy St.
Arlington, VA 22217-5000

91-15762

Dear Dr. Marron:

RE: Annual Technical Report for Grant N00014-91-J-1442

Our research has resulted in one paper which is in press as follows:

Role of Monomer Structure and Compressibility on the Properties of Multicomponent Polymer Blends and Solutions: IV. High Molecular Weights, Temperature Dependences, and Phase Diagrams of Binary Polymer Blends. K.F. Freed and J. Dudowicz, Theor. Chim. Acta. (in press).

We have applied the compressible lattice cluster theory of structured polymer blends to studying how the effective interaction parameter χ varies with composition, monomer structure, microscopic interactions, and temperature. We consider a wide variety of different vinyl polymer structures and find that the effective interaction parameter displays a strong dependence on monomer structure. The composition dependence of the effective interaction is generally found to be a parabolic or linear function of composition, in general accord with experimental observations. Strong dependences on the microscopic interaction energies are also present. We have begun studying the influence of monomer structure and interactions upon phase diagrams of compressible binary blends. Firstly, computations of the cloud point curve for PS/PVME blends are in good accord

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with experiments by Han et al. The calculations use the same monomer structures and interaction energies obtained by us previously in fits to the composition dependence of the effective interaction parameter from neutron scattering experiments and to heats and volume changes on mixing. We demonstrate that a polymer blend can in general have both upper and lower solution critical temperatures, although the two critical points may not necessarily be experimentally accessible due to a glass transition or thermal degradation. Calculations also demonstrate the possibility for obtaining closed loop phase diagrams.

We are nearing completion of a study of the influence of monomer structure and compressibility on the angle dependence of neutron scattering from binary blends. The angle dependence in S(k) provides information on the effective interactions and on chain dimensions and correlations in the polymer blend. By combining the lattice cluster theory with our compressible random phase approximation (RPA) for S(k), we are able to deduce the three effective macroscopic interaction parameters that describe the angular dependences in neutron scattering. The effective interaction parameters are obtained as functions of monomer structure, composition, pressure, etc. Computations to date indicate that the standard analysis of experimental data using an incompressible model can lead to the misinterpretation of experimental effects, such as an impuning nonexistent temperature dependence to apparent radii of gyration, because of neglect of blend compressibility. We are studying the detailed experimental data on polystyrene/poly(vinylmethylether) blends where a large composition dependence is observed for both the apparent radius of gyration and the correlation length, both of which are unexplained by the standard theories. The combined lattice cluster theory and compressible RPA explains the general trends for the correlation length, but it is clear that the polystyrene and poly(vinylmethylether) chains cannot have ideal dimensions in the blend. This observation contradicts one of the prime assumptions of the random phase approximation which is used extensively to analyze coherent scattering from concentrated polymer solutions, blends, diblock copolymer systems, etc.

We are in the process of talking with Charles Han's group at NIST to understand what further experimental tests can be made of the lattice cluster theory description of polymer blends.

Reprints of our papers will be sent as they become available.

I anticipate that all funds budgeted for the first year will be spent at the end of the first budget. The one exception is in the funds for the computer system as the University has provided me with additional components that were unanticipated at the beginning of the grant period. Thus, these funds will be used for other peripherals and upgrades of our computer as these become available.

Please let me know if you require any additional information. I understand that under the new regulations the funding for the second grant year will automatically be transferred and that I need not submit a second year budget. Thank you for continued support of my research.

Sincerely,

Karl Freed

Karl F. Freed
Professor of Chemistry

Statement A per telecom
Dr. Michael Marron
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Arlington, VA 22217-5000 NWW 11/27/91