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Guest Editorial

Bridging Microstructure, Properties, and Processing of Polymer Based Advanced Materials

Advancement on modeling, microstructure characterization, property measurement, and processing in polymer based advanced materials raised interest to integrated computational materials engineering. How to advance computational materials science to guide the processing of advanced materials is an emerging field, reflected in the mission of Materials Genome Initiative recently announced by White House.

The papers collected in this special issue emphasize significant challenges, current approaches, and future strategies necessary to advance the development of polymer based materials. They were partly presented at the symposium of "Bridging microstructure, properties, and processing of polymer based advanced materials" in the TMS 2011 annual conference meeting, which was held in San Diego, US, on February 28 to March 3, 2011. This symposium was organized by the Pacific Northwest National Laboratory (USA) and the Institute of Mechanics of Fluids and Solids of the University of Strasbourg (France). The organizers were D.S. Li, S. Ahzi, and M. Khaleel.

The first paper by Li, Sun, and Khaleel is a lead paper that presents an example on how theoretical modeling can guide material processing to achieve desired properties by tailoring the microstructure. The mechanical properties of cellulose nanowhisker enforced all-cellulose composite is predicted by microstructure based finite element analysis. Orientation of cellulose nanowhisker in the composite is achieved by magnetic alignment. The microstructure based finite element method demonstrates how the microstructure descriptors, such as nanowhisker volume fraction, orientation distribution, whisker size, and aspect ratio can determine the mechanical properties. A similar approach is demonstrated in paper by Deuerling, Vitter, Converse, and Roeder. The biomaterials system studied is also a whisker enforced composite. A micromechanical model was proposed to simulate the elastic properties based on the orientation distribution of the reinforcement, hydroxyapatite whisker, in polyetheretherketone composites. This model was used to bridge microstructure measured by X-ray diffraction, mechanical properties and compressive molding to tailor the orientation distribution.

Microstructure enhancement is also achieved by magnetic alignment in the study by Tehrani and Al-Haik. Low magnetic field used in the study makes this technique applicable in industry. The orientation distribution of epoxy molecular chain was characterized and the creep properties were measured by nanoindentation. The results revealed that under low magnetic fields both the quasi-static and viscoelastic mechanical properties of the epoxy were improved. Similar framework was also applied on structure materials, neutron detector materials, and biomaterials, demonstrated in the other papers from this special issue. Generally, the following topics were addressed: microstructure sensitive materials design, microstructure enhancement, micromechanics and homogenization approaches, and molecular dynamics modeling.

Finally, we would like to thank the reviewers for providing constructive comments and suggestions.

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