# Development of Material Data Resource and Analysis for Polymer Nanocomposites

## ICME 2016

**He Zhao[1], Xiaolin Li[2], Wei Chen[2], Linda S. Schadler[3], L. Catherine Brinson[1*]**

[1]Department of Mechanical Engineering
Department of Material Science and Engineering
Northwestern University
Evanston, IL, 60208, USA
e-mail: cbrinson@northwestern.edu, web page: http://brinson.mech.northwestern.edu

[2]Department of Mechanical Engineering
Northwestern University
Evanston, IL, 60208, USA
e-mail: weichen@northwestern.edu, web page: http://ideal.mech.northwestern.edu

[3]Department of Material Science and Engineering
Rensselaer Polytechnic Institute
Troy, NY, 12180, USA
e-mail: schadl@rpi.edu, web page: http://homepages.rpi.edu/~schadl/

## ABSTRACT

Material science is founded on a processing-structure-properties (p-s-p) diagram with a vast array of material data collected over the decades along with understanding of mechanisms. While systematic approaches and databases for archiving and reusing materials data have been developed in some areas such as metallic alloy systems, the realm of polymer composites and nanocomposites are much less developed due to the complexity of polymer behavior, unknown properties at the matrix-filler interphase, and high sensitivity of microstructure and composite response to small changes in processing conditions and constituents. Despite numerous examples of property enhancement in nano-reinforced polymeric materials, a fundamental understanding across p-s-p domains, which is critical to understand composite behaviour and assist material design, is still missing.

In this work, we present a data-centric methodology for property prediction and material design of polymer nanocomposites using a nascent polymer composite data resource (NanoMine). In order to standardize terminology and structure of parameters across p-s-p domains, we created a data template using hierarchical XML schema by curating 30 recent papers and experimental data. Current template contains six major sections: data source information, material compositions, processing conditions, characterization methods, sample microstructure, and reported material properties. This template serves as a comprehensive collection of parameters to account for a single nanocomposite sample.

Using the XML schema as data template, we developed a prototype web-based system for nanocomposite material data curation, exploration and analysis with the Material Data Curator System (NIST) as the backbone of database and interface infrastructure. Current database contains more than 300 data points from experiments and nanocomposite literature. We focused our initial curation process on samples with surface treated spherical inorganic nanofillers with explicit reports of nanophase dispersion, well documented processing and experimental procedures, and functional data of viscoelastic and/or dielectric properties. While the schemas developed are robust and have been tested with the initial curation, significant effort will be devoted toward continuous data curation, addition of data quality metrics, and development of simple and rapid methods for users to self-curate data.

## REFERENCES

[1] H. Zhao, X. Li, Y. Zhang, L.S. Schadler, W. Chen and L.C. Brinson, *NanoMine: a material genome approach for polymer nanocomposites analysis and design.* To appear in APL Materials