Polymer Nanocomposites : AFM, Interfaces and Data

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Abstract

For polymer composites, nanocomposites and polymer thin film systems, the local properties of polymers can be altered by the chemical and physical interactions with substrates and embedded particles over a length scales exceeding 100nm. In order to better understand and design nanocomposites, polymer coatings and electronic components, it is essential to develop better understanding and robust design strategies. Two key missing links are understanding of altered polymer properties near surfaces/particles and ability to quantitatively leverage prior data for these systems, predictively in a robust manner. Therefore there is great interest in utilizing scanning probe methods to quantify the local property changes in the polymer region near surfaces. Additionally, there is great need to harvest, record and be able to learn from the vast amount of data archived in journal articles.

In the first part of this presentation, we will tackle the challenge to use scanning probe methodologies to generate quantitative measurements of local mechanical properties on polymers and soft materials [1,3,4]. In multiphase soft materials, local changes in the sample modulus and tip-sample interactions impact the acquired force curves. Secondary effects, such as the 'substrate effect', require careful treatment to ensure that measured property gradients are due to changes in polymer structure. Simulations and experiments have been performed to addresses stress field artifacts when indenting near substrates or embedded particles. Simulations of indentations into a rubber interphase demonstrated that structural effects of the particle in an idealized system can be estimated and removed. We developed a 'master curve' that approximates the substrate effect and applied it to AFM indentations of rubber – carbon nanocomposites, demonstrating that substrate effects are well predicted by the 'master curve' and can be differentiated from bound rubber.

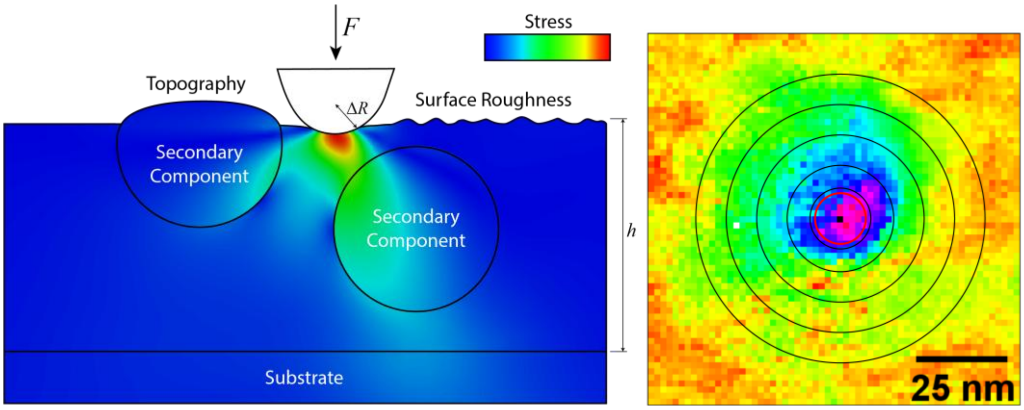

***Fig. 1** – Left: Schematic of complexity of AFM probing of polymer nanocomposite surface [1], highlighting stress field interaction effects. Right: local AFM data around a nanoparticle in PDMS/silica composite showing corrected local interphase property gradient.*

In the second part of this presentation, a new and growing platform for data, analysis tools and simulation portals for polymer nanocomposites will be presented: MaterialsMine (**Fig 2**). MaterialsMine utilizes a robust schema and ontology to hold the data in a software infrastructure with query, visualization and microstructure analysis tools [2]. Case studies are demonstrated which connect the property-structure-property domains through a combination of machine learning and physics-based modeling, demonstrating the ability to identify the most critical features influence properties. Together this work illustrates a new approach to tackle materials design principles for the complex, high dimensional problems inherent in the multi-phase polymer space.

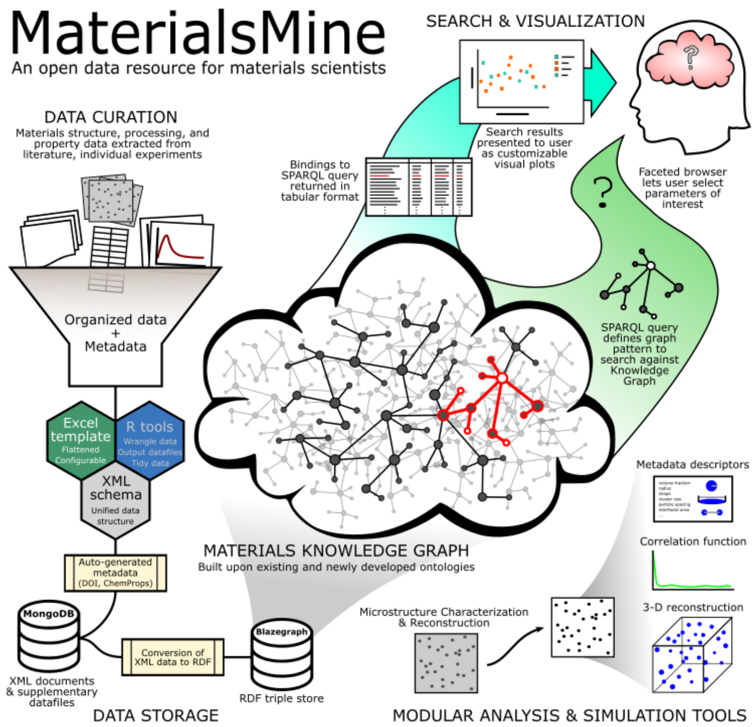

***Fig. 2** – Infographic showing MaterialsMine data resource concept. NanoMine is subode of MaterialsMine focused on polymer nanocomposite data.*

References

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