Mechanisms in Processing:Structure:Property Relationships as a Pathway to Hypothesis Formulation.

Materials Science and Engineering is a field where we endeavor to understand the relationships between Processing, Structure and Properties in order to better engineer the materials' performance. Understanding of these relationships is based on knowing the mechanism of materials structure development as a function processing parameters and on knowing the mechanism by which the materials structure controls the materials properties.

The relationship between an understanding the mechanism of action and an understanding of the materials behavior was once illustrated by John Cahn in the mid-1980s' when confronting an array of materials scientists considering a phenomenon where grain boundaries migrated against curvature during inter-diffusion (DIGM). Several scientists had stated that the phenomenon was associated with a reduction in Free Energy and no other explanation was required. Cahn, who was gifted with clairvoyant physical insight, argued that a mechanism of action of the Free Energy of Mixing change on increasing the grain boundary curvature was required before the phenomenon could actually be understood. To make his point, he made an analogy with the driving of a gasoline powered vehicle up a mountain. The energy required to increase the height of the vehicle obviously comes from the burning of the gasoline. But Cahn pointed out that if you pour the gasoline over the car and light it on fire, the car will not drive to the top of the mountain even though the energy expenditure from the gasoline was equivalent. The only way to understand the process was to understand the engine (the *mechanism*). That is, there has to be some machinery that couples the structure change to the Free Energy change.

Proposing a mechanism of action for the relationship between processing and structure and/or structure and properties will usually involve an application of fundamental theories, such as nucleation theory, transport theory, dislocation theory, magnetic domain theory, band theory etc. These theories are quantitative. That means that you get to work within a rigorous framework, and can avoid any sort of vague, superficial discussion that is so frustrating for other scientists/engineers trying to follow your project presentation. Developing a rigorous framework using fundamental concepts is not an easy task and does require in-depth understanding of the principles of Materials Science. But the pay-off can be significant, not only in developing relevant publishable discussion of experimental results, but also in developing a ***non-trivial, testable hypothesis***.

The fundamental theories of Materials Science applied to develop your mechanism will relate intensive, extensive and length scale variables to the process:structure or structure:property relationships. Some of these variables can be controlled by you and thus lead to predictions of behavior. If you are working on a structure:property relationship, you can think about your materials property as a dependent variable, Y, and the independent variable, X, is a descriptor of the structure (length scale, size distribution, interface band bending, magnetic charge density etc.). The mechanism of action that you propose would then link X and Y through a quantitative function, f(X). That means that now you can make hypothesis statements of "**If** variable X changes, **then** variable Y should change as f(X)". Or, put another way, "**If** variable X increases, **then** variable Y should increase **because** the mechanism of action predicts Y=f(X)". Provided that this statement is original, you now have a ***non-trivial, testable hypothesis.***