Materials Science & Engineering Seminar Series

Carnegie Mellon University
Materials Science & Engineering

presents

Data Analytics in Materials Science via Correlation Analysis

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ABSTRACT:
The Materials Genome argues for the use of data science to accelerate materials development. Although there has been much discussion of “big data”, the reality is that materials development will mostly be done with normal, i.e. small data sets. Nevertheless data science has many tools to offer us that can help us analyze and understand our data sets, especially when the number of parameters is more than, say, three (think of the number of columns in a spreadsheet). Seeking correlations between variables is a formal way of asking whether, say, yield stress depends on fraction recrystallized. Finding combinations of variables that can be linked to another variable is another natural analysis, which in traditional metallurgy appears in the form of equations that link, say, martensite start temperature to a combination of composition variables. Such analyses can be performed with the help of standard, open source statistical analysis tools such as Canonical Correlation Analysis and Principal Component Analysis. A convenient framework for such analyses is the open source R package (https://r-project.org). Students are invited to install R on their laptops and come prepared to step through the examples that will be demonstrated in this seminar. Students are further encouraged to bring (email would also work) spreadsheets with their own data that can be analyzed on the spot.

BIOGRAPHY:
Prof. Rollett has been a Professor of Materials Science & Engineering at Carnegie Mellon University since 1995 and before that was with the Los Alamos National Laboratory. His most recent honors were the Member of Honor of the French Society of Materials (SF2M) in 2015, the Edgar C. Bain Award from the Pittsburgh Chapter of ASM International in 2016, and the appointment as US Steel Professor of Metallurgical Engineering & Materials Science at Carnegie Mellon University in 2017. He is a member of the Basic Energy Science Advisory Committee and the Defense Programs Advisory Committee (Dept. of Energy).
Rollett's research focuses on microstructural evolution and microstructure-property relationships in 3D, using both experiments and simulations. Interests include 3D printing of metals, materials for energy conversion systems, strength of materials, constitutive relations, microstructure, texture, anisotropy, grain growth, recrystallization, formability and stereology. Relevant techniques highlight spectral methods in micro-mechanics, Dynamic X-ray Radiography and High Energy Diffraction Microscopy. Important recent results include definition of process windows in 3D printing through characterization of porosity, 3D comparisons of experiment and simulation for plastic deformation in metals, the appearance of new grains during grain growth, and grain size stabilization.
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