SYSTAT Application Notes

Statistical Analysis in Materials Science & Engineering Using SYSTAT

Introduction

Without new materials and their efficient production, our world of modem devices, machines, computers, automobiles, aircraft, communication equipment, and structural products could not exist. Materials scientists and engineers will continue to be at the forefront of these and other areas of science and engineering in the service of society as they achieve new levels of understanding and control of the basic building blocks of materials: atoms, molecules, crystals, and non-crystalline arrays.

Analysis and Modeling

There are some recent theoretical and computational developments that are changing the very nature of materials science and engineering. Two complementary forces are driving these changes. First, there is the unprecedented speed, capacity, and accessibility of computers. Problems in mathematics, data analysis, and communication that seemed untouchable just a few years ago now can be solved quickly and reliably.

Second, there is the growing complexity of materials research. The latter change has occurred in large part because we now have instruments with which to make highly detailed and quantitative measurements and we have the computational and analytical ability to deal with the resulting wealth of data using Systat.

Complementing these technology push factors is the pulling force of the technological demand for increasingly complex materials. Underlying all of these developments are advances in our theoretical understanding of the properties of materials and in our mathematical ability to devise accurate numerical simulations.

In short, materials research is evolving into a truly quantitative science. Analysis and modeling in materials research traditionally has been divided into roughly three different areas of activity-areas that can be characterized by the length scales at which the properties of materials are being considered.

The most fundamental models, those used primarily by condensed-matter physicists and quantum chemists, deal with microscopic length scales, where the atomic structure of materials plays an explicit role. At a more phenomenological level, much of the most sophisticated analysis is carried out at intermediate length scales, where continuum models are appropriate.

Finally, there is work at macroscopic length scales, in which the bulk properties of materials are used as inputs to models of manufacturing processes and performance.

Historically, research in each of these three areas has been carried out by separate communities of scientists applied mathematicians, physicists, chemists, metallurgists, ceramists, mechanical engineers, manufacturing engineers and so on.

Applications

In submerged arc welding (SAW), selecting appropriate values for process variables is essential in order to control heat-affected zone (HAZ) dimensions and get the required bead size and quality.

Also, conditions must be selected that will ensure a predictable and reproducible weld bead, which is critical for obtaining high quality. In this kind of investigation by Gunaraj and Murugan (2002), mathematical models were developed to study the effects of process variables and heat input on various metallurgical aspects, namely, the widths of the HAZ, weld interface, and grain growth and grain refinement regions of the HAZ.

The color metallography technique and response surface methodology were also used. Direct and interaction effects of the process variables and heat input on the characteristics of the HAZ were presented in graphical forms. The study revealed:

1) heat input and wire feed rate have a positive effect, but welding speed has a negative effect on all HAZ characteristics;

2) width of grain growth and grain refinement zones increased and weld interface decreased with an increase in arc voltage; and

3) width of HAZ is maximum (about 2.2 mm) when wire-feed rate and welding speed are at their minimum
limits.

Regression analysis was used to evaluate the coefficients of the model. The adequacy of the models was then tested by the analysis of variance technique (ANOVA). Significance of the coefficients was tested using the Systat software package. The software's step backward option was used to eliminate insignificant coefficients and to recalculate the values of significant coefficients.

Reduced models with significant coefficients were developed. It was found the reduced models were better than the full models because they have higher values of R^2 (adjusted) and lesser values of standard error estimates.

Wang et al. (2001) study the use of Raman spectral features to characterize the structural and compositional characteristics of different types of pyroxene from rocks as might be car-

ried out using a portable field spectrometer or by planetary on-surface exploration. Samples studied include lunar rocks, martian meteorites, and terrestrial rocks. The major structural types of quadrilateral pyroxene can be identified using their Raman spectral pattern and peak positions. Values of Mg/(Mg + Fe + Ca) of pyroxene in the (Mg, Fe, Ca) quadrilateral can be determined within an accuracy of +/- 0.1.

The precision for Ca/(Mg + Fe + Ca) values derived from Raman data is about the same, except that corrections must be made for very low-Ca and very high-Ca samples. Pyroxenes from basalts can be distinguished from those in plutonic equivalents from the distribution of their Mg' [Mg/(Mg + Fe)] and Wo values, and this can be readily done using point counting Raman measurements on unprepared rock samples.

The correlation of Raman peak positions and spectral pattern provides criteria to distinguish pyroxenes with high proportions of non-quadrilateral components from (Mg,Fe,Ca) quadrilateral pyroxenes.

The correlation between pyroxene composition and Raman peak positions were obtained using the multiple linear regression program of Systat.

Conclusions

The description above just gave a bird's eye view of Systat's capabilities. But Systat provides a powerful statistical and graphical analysis system in a graphical environment using descriptive menus and simple dialog boxes.

Systat's command language provides functionality not available in the dialog box interface in addition to complete coverage of menu-based functionality. Robust algorithms from leading statisticians give meaningful results even with extreme data.

Create missing value estimates using regression based point estimation or an EM algorithm. Obtain complete distributions and standard errors using Systat's bootstrapping capability implemented globally across 21 statistical procedures even when normality assumptions are violated and no model is available.

Matrix procedure allows you to use matrix algebra to specify statistical analyses and perform data management tasks.

Systat offers more scientific and technical graphing options than any other desktop statistics package. Compare subgroups, overlay charts, and transform coordinates, change colors, symbols and more to create insightful presentations.

Speed up your analysis by rotating your 3-D graphs to visually determine the perfect power or log transformation to normalize your data using the Dynamic Explorer to speed up your analysis. Create compelling reports by combining formatted statistical output with publication-quality graphs in Systat's rich text output window.

References (in order of appearance)

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ALIAN WANG, BRAD L. JOLLIFF, LARRY A. HASKIN, KARLA E. KUEBLER, & KAREN M.VISKUPIC (2001). Characterization and comparison of structural and compositional features of planetary quadrilateral pyroxenes by Raman spectroscopy. American Mineralogist, Vol.86, pp.790-806.