Learning about material integrity from statistical data

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With chemical imaging data, scientists can better predict the molecular behavior of materials that must handle harsh environments, such as those found in space or in nuclear reactors.

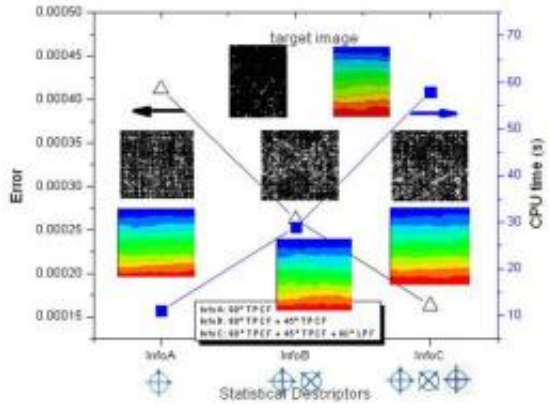
Whether it protects space satellites or sequesters nuclear waste, scientists want to understand tiny features that could significantly alter how a material behaves. Locating microscopic defects can be done with powerful microscopes, but scientists want more. They want to use the microscopes to locate and understand the very molecules involved in the defects. Describing the location of the molecules and atoms in images often relies on statistics that can be inaccurate and expensive. The trick is to pick the statistical approach that accurately and economically

describes the situation. Pick the wrong one, and the mathematical description won't match the microscope's image.

At Pacific Northwest National Laboratory, a team of scientists analyzed several statistical descriptors, different mathematical options that explain the distribution of items in an image, to help researchers select the right statistical information. They found that the simpler descriptions were inexpensive, but inaccurate. The more detailed, mathematically complex approaches gave higher accuracy, but used more computational time at greater cost.

"Get the right descriptor and you get the right, accurate, and true information," said Dr. Louis Terminello, Director of the Chemical Imaging Initiative at Pacific Northwest National Laboratory. "Next, the challenge is to make that accurate, expensive version more accurate and less expensive."

Using accurate and effective statistical descriptors lets scientists gather complex data from images. With this data, scientists can better predict the behavior of materials at the molecular level. If they know how a material will respond, they can select the properties they want and design the materials for them, reducing the need for expensive and time-consuming trial and error.



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The structural information of some materials can be obtained from micrographs alone, but obtaining a representative image of complex and heterogeneous materials can be challenging. The team used two statistical descriptors to investigate microscopic images of the glass form and determined which gave the most accurate representation. They used the two-point correlation function, a statistic used to describe the distribution of particles in a microstructure, and lineal path functions.

"Our findings will enable scientists to predict the behavior of complex material systems," said Dr. Dongsheng Li, the PNNL scientist who led the study for the Laboratory's Chemical Imaging Initiative. "Scientists will be able to predict properties based on the 'whole picture,' not just a small 'typical' part anymore," Li added.

The next steps will be to integrate this work into computer models that predict material properties based on multiple scale modeling and microstructure reconstruction. Data fusion and image enhancement will be combined with microstructure reconstruction to integrate different chemical imaging instrumentation.

More information: Li DS, et al. 2012. "Comparison of Reconstructed Spatial Microstructure Images Using Different Statistical Descriptors." *Computational Materials Science* 51(1):437-444. doi:10.1016/j.commatsci.2011.07.056