Unsupervised Data Mining in Nanoscale X-ray Spectro-Microscopic Study of a NdFeB Magnet

The importance of the rare-earth element based permanent magnet materials can be seen from its wide range of industrial applications, e.g. in MRI scanners [1], Maglev trains [2], and electric vehicles [3]. Materials scientists have been continuously working to improve the performance of this type of magnets, from ease of magnetization to thermal stability and coercivity to corrosion resistance. While considerable attention has been paid to the optimization of the material's bulk composition, the nano/meso scale structural and chemical heterogeneity is one of the areas believed to have a high impact on the overall performance of the material, but is still not well understood.

For many scientific projects including this one, it is essential to have the ability to investigate materials systems that are hierarchically complex and heterogeneously structured. This is because these types of measurements offer the possibility of unraveling the interplay of fine-length-scale factors, which are the origins of the material's macroscopic functionality. While it is often desirable to spatially resolve the fine features within the complex systems, it is usually scientifically even more important to resolve those features with chemical and/or elemental sensitivity. Several recent improvements in resolution, contrast and speed has made synchrotron based nanoscale spectro-microscopy the go-to technique for these types of investigations.

A group of researchers from Wuhan University (China), UCSF, Stanford, HPSTAR (China), and SSRL combined spectroscopic analysis with x-ray based full-field imaging to perform a study of a type of rare-earth element based permanent magnet material, $Nd_2Fe_{14}B$, which is one of the strongest known permanent magnets and has consequently become the most widely used magnet since its discovery in 1982. This study, performed at SSRL Beam Line 6-2, revealed that the magnet material's surface is altered from the desired bulk structure. The observed surface alternation is rich in the precious rare-earth element (Nd), but has a poorer magnetic performance, possibly caused by grain-boundary corrosion.

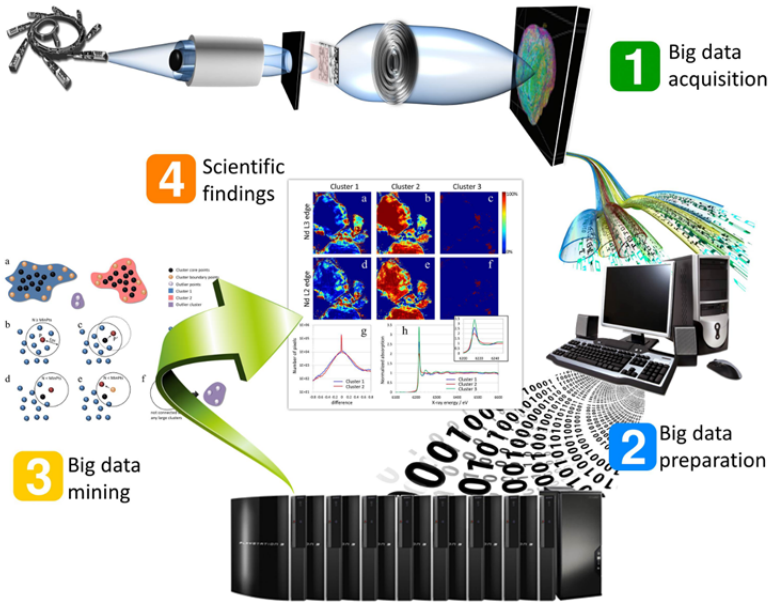

Figure 1. The novel nanoscale spectro-microscopy method is very powerful for studying the hierarchically complex and heterogeneously structured materials. In this study, the researchers combined a novel big data mining method (3) with the existing big data acquisition (1) and preparation (2) capabilities at SSRL to study a type of rare-earth element based permanent magnet material, $Nd_2Fe_{14}B$. The big data mining capability presented in this work greatly accelerated discovery of new scientific findings (4).

It is important to point out that the scientific findings presented in the current study is a result of the

combination of both the state-of-the-art experimental capability at SSRL and novel scientific big data mining methods. The nanoscale spectro-microscopy method is capable of generating large scale data at a rate of about 30,000 spectra per second, posing a major challenge for scientists to analyze and interpret the data. Traditionally, scientists rely heavily on the assumption of complete prior knowledge about the principle chemical species in the system before more quantitative further analysis can be done. In the traditional approach, the data are simply fit to the known spectroscopic signatures of the chemical species that are known to be present in the system, which possibly could have left out some components that were unexpected. In this new study, the researchers utilized an unsupervised data mining method known as the DBSCAN (density-based spatial clustering of applications with noise) [4] to automatically perform big data classification, which efficiently (within a few minutes) extracts the scientifically relevant information with very little human interaction, and to finds out what is actually in the sample.

The presented data analytics approach can also be directly applied to the studies in many other fields, including for catalysts, batteries, fuels cells, and optical devices, in which the rational design of hierarchically complex functional materials plays an important role. Investments in new hardware (from new sources, to new detectors) has resulted in commissioning of exciting new facilities and has driven development of novel experimental techniques, and promised an unprecedented deep understanding of complex materials and devices as they function under real world conditions. However, because of hierarchy of scales in a functioning device, and complexity of the materials, these techniques produce data at an exponentially rising rate; a rate that has far surpassed any human's ability to curate and extract scientific knowledge from it in a comparable time frame. Without development of new data analytics approaches, inspired by advances in unsupervised feature extraction of "big data" over the last decades, minimal-loss data compression, and machining learning that can accurately extract hidden features, trends and high-level scientific information with minimal reliance on humans, from complex high-dimension data sets, the promise of an unprecedented new understanding of the materials world will most likely remain only a dream.

References

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