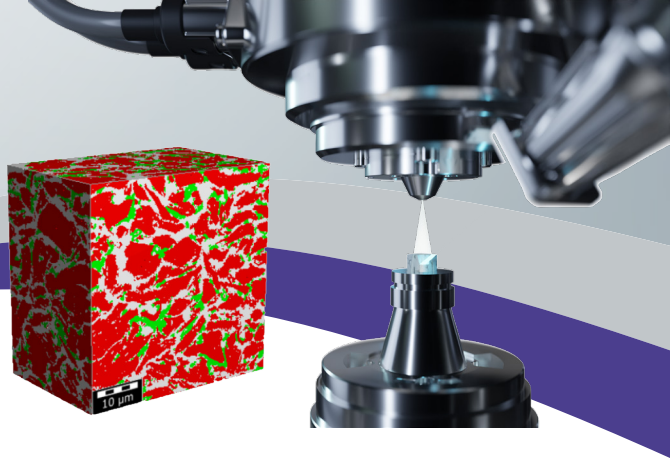
NISSAN ARC, LTD.

Analysis of lithium-ion secondary battery materials and a digital twin concept



Materials technology is one of the indispensable elements for environmentally conscious manufacturing these days. NISSAN ARC, LTD. is a materials analysis company established based on the corporate philosophy of contributing to industries by utilizing the materials analysis technology accumulated over many years in Nissan Motor's R&D department. The company contributes to solving problems not only in the automotive industry, but also in all other industries by providing a variety of material development consulting services. And to complement its advanced analytical technologies and provide more comprehensive services, the company is working to support manufacturing by utilizing digitalization. As one example of its application, this article will introduce 3D structural analysis of lithium-ion secondary battery materials.

Challenges

- Digitize and quantify SEM (Scanning Electron Microscopy) images.
- Enhance results of difficult analyses with simulations.
- Narrow down the optimal conditions through parameter studies.

Mr. Toru Akiba,
General Manager
Analysis Solutions
Planning and
Promotion
Department

Tell us about your business and its focus areas.

We use various in-house analytical instruments to capture characteristics and phenomena related to materials and processes accurately. We provide support for solving complex problems by quantum beam measurements at synchrotron radiation facilities (e.g., SPring-8) and computational science techniques like first-principles calculations on supercomputers. In the automotive sector, challenges arise from the numerous components and diverse environmental conditions, such as temperature and road conditions. Also, these days, with growing electrification, battery analysis is now a key focus in materials research. Nissan Motor Corporation pioneered electric vehicle commercialization, and we have conducted research on analysis technologies alongside their development.

Thanks to our expertise, about 40% of the requests we receive from our business partners are battery analyses. In the case of lithium-ion batteries, expansion due to deterioration is a problem, and it is necessary to analyze the generation of gases that cause this, changes in the properties of the electrolyte that contribute to this, and the condition of the electrodes. Of course, it is also necessary to evaluate whether the battery maintains the required performance, which requires challenging analysis utilizing a variety of devices. Taking these factors into consideration, we support manufacturing through material analysis that incorporates our accumulated experience and knowledge, as well as consideration of a wide range of problem factors.

Was GeoDict introduced to supplement such analysis?

Material analysis sometimes requires digitalization of 3D structures, which is difficult to do with SEM images. To address this, we adopted GeoDict, allowing integrated imaging, digitalization, and simulation.
We have been conducting simulations, such as first-principles and molecular dynamics calculations, for some time. Recently, we have been focusing on materials informatics, and we actively use GeoDict simulations. Figure 1 shows a cross-sectional image obtained by SEM and the 3D visualization of the results obtained with GeoDict. GeoDict makes it possible to understand the distribution of each material component intuitively. We had many requests before for the ability to quantify SEM images, which were previously difficult to analyze. However, with GeoDict, this can now be

done easily, enabling us to provide results that satisfy our customers.

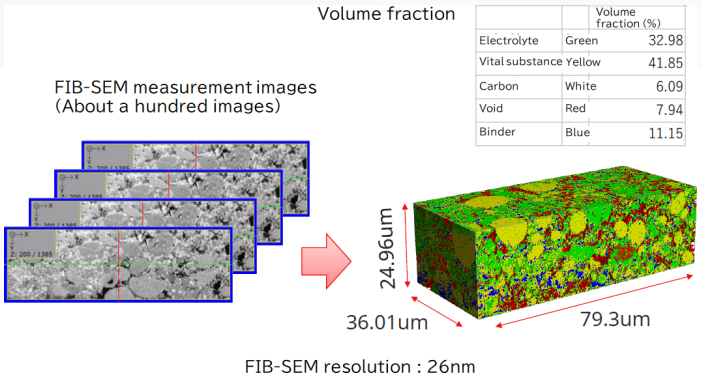


Figure 1 Visualization of 3D distribution of active materials, electrolytes, additives, and binders using GeoDict, from SEM images

This example shows the analysis of a three-layer separator used in lithium-ion batteries, with polyethylene (PE) sandwiched between polypropylene (PP). Figure 2 shows a cross-sectional SEM image of the separator. Pre-treatments like resin embedding or chemical processing improve image contrast, where black indicates pores and light grey represents PE or PP. To examine pore size distribution and the 3D structure of the layers, the data is imported into GeoDict for 3D modeling and quantification. Brightness correction and artifact removal are applied before 3D modeling (see Figure 3). Around 100 images are stacked to create a 3D material model. Figure 4 shows the calculated relative diffusion coefficients.

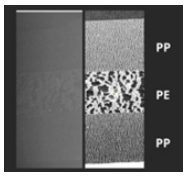


Figure 2 Left: no pre-processing, Right: Pre-processing applied

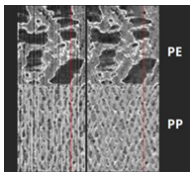


Figure 3 GeoDict image processing. Left: none, Right: applied

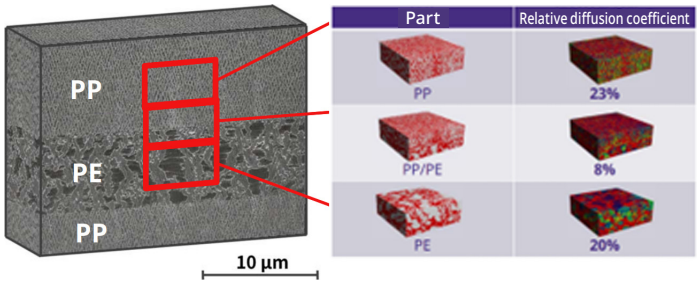


Figure 4 Creating a 3D structure model from a binary image and calculating the relative diffusion coefficient

Furthermore, by analyzing the percolation paths as shown in Figure 5, it is possible to visually capture and quantify the effect of the structure of the PP/PE joint surface on diffusion. The work performed thus far would not have been possible without the combination of the analysis techniques we have cultivated and GeoDict.

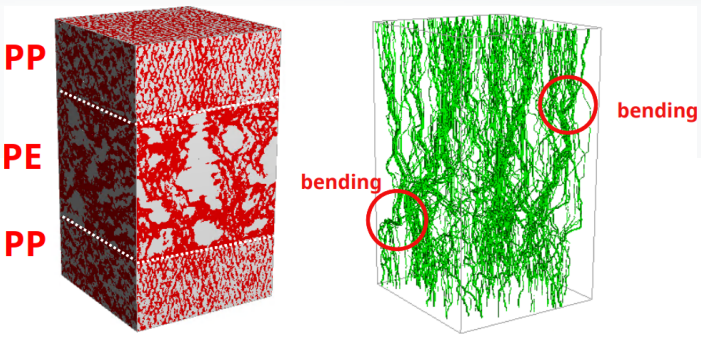


Figure 5 Visualization of network structure by analysis of percolation paths

How effective has GeoDict been in improving operational efficiency and service quality?

Mr. Norio Saito
Nissan Arc Co., Ltd.
Analysis Solutions Planning and Promotion Department

For example, without GeoDict, creating a 3D model of the finished electrode structure would be impossible. We tried other tools, but GeoDict is far more efficient and significantly faster. It is highly user-friendly, with a well-designed GUI and a wide range of integrated functions, like image conversion, make it stand out.
It is also one of the few tools that supports complete end-to-end simulations. When considering alternatives, there is simply no substitute for GeoDict.
New features are added quickly with each version upgrade, and we appreciate that our requests are often included in the next release. GeoDict also supports robust parameter studies, helping us identify optimal conditions and apply them to material design – extending beyond what analysis alone can achieve. This represents the essence of digital twins, and we believe material evaluation using this approach will become increasingly common.

How are you approaching digital twins?

Currently, we begin with observation and analysis, then move to simulation to quantify phenomena. Looking ahead, we aim to support advancements in material development through parameter studies using digital twins. The key point here is realistic modeling using diverse parameters. Actual battery electrodes do not have regular particle shapes, so the challenge lies in how realistically they can be modeled and correlated with actual phenomena.
GeoDict already allows modeling and simulation using specified particle shapes and particle size distributions (Figures 6 and 7), but our goal is to develop models that more closely reflect actual physical properties. Similarly, for 3D structure reconstruction from images, we are optimistic about GeoDict's AI capabilities in producing models that

accurately represent real objects. AI could play a key role in correcting or predicting image discrepancies caused by varying imaging conditions, and we aim to use the latest hardware to make the intensive computations these tasks require practical and efficient.

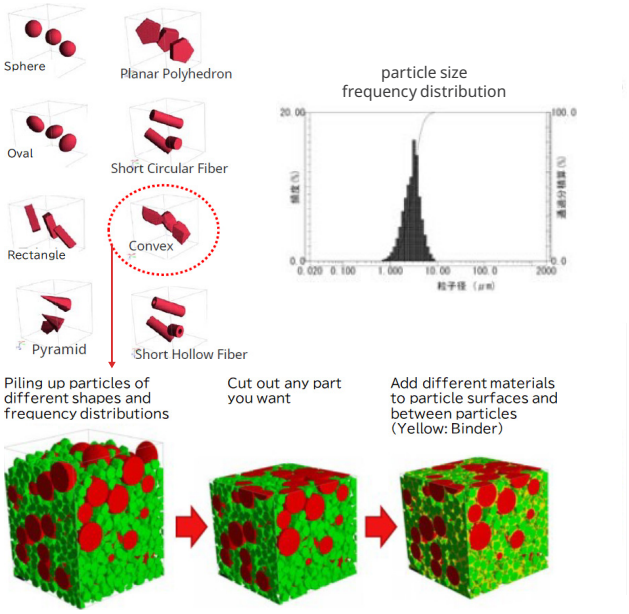


Figure 6 Specifying shape parameters and modeling in GeoDict

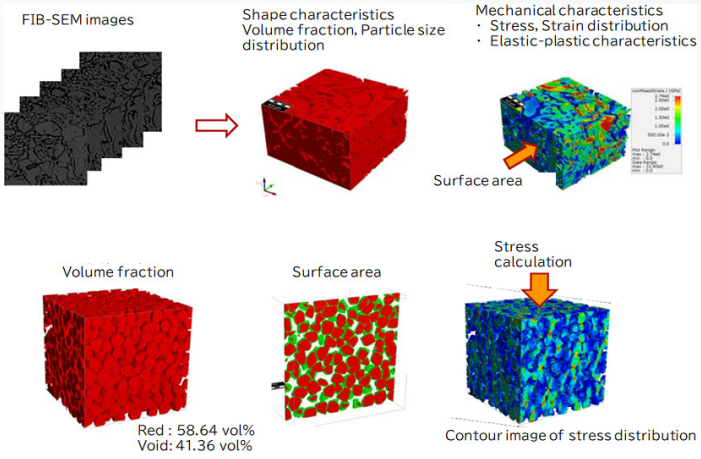


Figure 7 Simulation using 3D image models and virtual models imported into GeoDict

Thank you for introducing GeoDict's use cases. We will strive to provide full support for digital twins of material development.

Customer profile

Nissan Arc Co., Ltd.

Established: December 17, 1990

Business activities: Providing advanced material analysis and analytical technologies to support the understanding of various characteristics and phenomena, as well as problem-solving in materials and processes for Lithium-ion secondary batteries, all-solid-state batteries, fuel cells, metal and organic materials, mechanical properties, degradation, failure, and foreign matter, VOC and odor, power electronics, simulation, and new material development.

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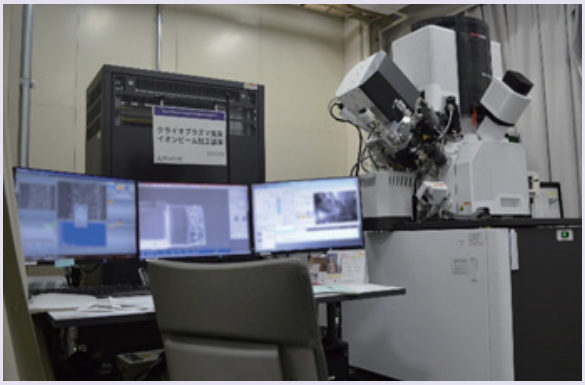
https://www.nissan-arc.co.jp/en/



For more information on GeoDict
▶ https://www.scsk.jp/product/common/geodict

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