

Accelerating the Development of Magnetic Materials with Digital Twins

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Target audience:

Graduate students and researchers dedicated to materials science as well as companies interested in advanced simulations for their R&D.

Online Seminar: 14:00 - 15:00, January 14th (Tue), 2025

Remarkable advances in microstructure characterization, high-throughput data accumulation and processing have stimulated the development of digital twins for various materials – accurate in-silico representations of the material microstructure and its functional response. These digital twins are a powerful tool for establishing the correlations between material properties and its microstructural features, including the rich diversity of defects. They help to optimize material performance toward the physical limit and to design on-demand materials for specific applications.

This talk will demonstrate digital twins of some magnetic materials (Fig. 1), such as FePt nanogranular media for data storage [1,2], anisotropic thin films of prospective SmFe_{12} -based alloys [3], and ultrafine grained Nd-Fe-B permanent magnets [4]. The approaches used to develop the large-scale finite element models based on different microscopy data (TEM and FIB-SEM) will be discussed along with the insights into magnetic properties revealed with simulations.

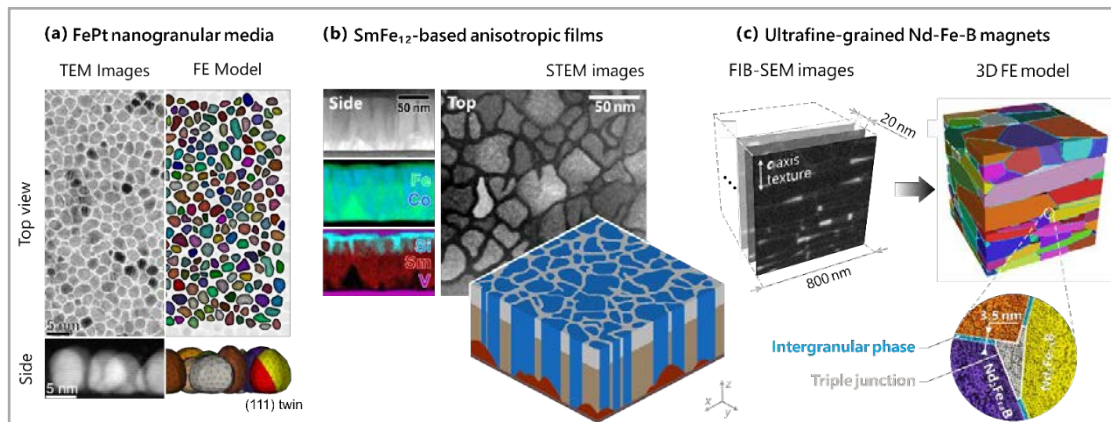


Figure 1. Digital twins of different magnetic materials: (a) TEM image-based models of FePt nanogranular media with reproduced defects such as $\{111\}$ twins [1,2], (b) TEM image-based models of $\text{Sm}(\text{Fe},\text{Co})_{12}\text{B}_{0.5}$ films [3], (c) large-scale models of ultrafine grained Nd-Fe-B magnets constructed based on FIB-SEM tomography [4].

References:

- [1] A. Bolyachkin, H. Sepehri-Amin, I. Suzuki, H. Tajiri, *et al.*, Acta Mater. 227 (2022) 117744.
- [2] E. Dengina, A. Bolyachkin, H. Sepehri-Amin, and K. Hono, Scripta Mater. 218 (2022) 114797.
- [3] A. Bolyachkin, H. Sepehri-Amin, M. Kambayashi, Y. Mori, *et al.*, Acta Mater. 227 (2022) 117716.
- [4] A. Bolyachkin, E. Dengina, N. Kulesh, Xin Tang, *et al.*, npj Comput. Mater. 10 (2024) 34.

✳️Pre-registration for the online seminar (zoom)

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