The visualization of physical properties using the extended Landau energy landscape

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The understanding of the function of real materials in a heterogeneous system, such as magnetic domain and metallographic texture, has been an outstanding issue in materials science. Thus the development of a consistent and fast analysis method that considers the defects, roughness, crystal grain sizes, etc. is of utmost importance.[1)] Here, we are developing a machine learning-based formula that can treat the microscopic morphology and describes the macroscopic properties based on the energy of the system.[2)] The Landau free energy theory is arduous to be implemented in complex applications due to the pinning de-pinning process of the domain walls.[3)] Thus, the description of the physics in inhomogeneous polycrystalline systems considering the metallography texture is necessary for advanced material applications.

In this work, we use micromagnetics simulation (Fig. 1) combined with unsupervised machine learning to produce the energy landscape in the magnetization reversal process for polycrystalline alloys (Fig. 2). The map of the data in the lower dimensional space of the magnetization, in the same direction of the external magnetic field using different sample structures (grain size) and similar parameters, display a correlation of maximum/minimum of feature 1 with coercivity. To elucidate the meaning of feature 2, we kept the same sample structure and we modified the magnetic anisotropic. We could observe a dependence of feature 2 with the magnetic anisotropy (Fig. 2). Our result implies that the magnetic microstructure can be used to extract information of physical properties.

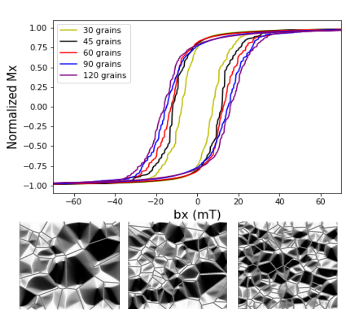

Fig. 1. (Up) magnetization reversal process for different grain sizes, and (down) magnetic domain structures near coercivity for 30, 60, and 120 grains.

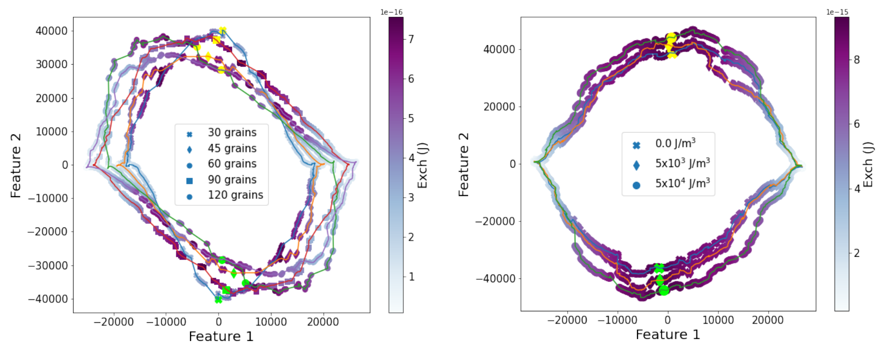

Fig. 2. Extended energy landscape for the magnetization in the x-axis. The green and yellow points correspond to positive and negative coercivity. (Left) Grain number dependence, (right) magnetic anisotropy dependence with fixed grain size.

1) C. Shen, et al., Acta Materialia **179**, 201 (2019).
2) C. H. Chen, et al., J. Appl. Phys. **93**, 7966 (2003)
3) A. Hubert, R. Schäfer "Magnetic Domains: The Analysis of Magnetic Microstructures" (Springer-Verlag, Berlin, Heidelberg, 1998).