Visualization of the macroscopic physical properties through the pseudo energy landscape

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1. Introduction

Understanding the function of real materials in heterogeneous system, such as magnetic domain and metallographic structure, has been a outstanding issue in materials science. Thus the development of a consistent and fast analysis method that consider the defects, roughness, crystal sizes, etc. is utmost important.[1)] Here we are developing a machine learning-based formula that can treats the microscopic morphology and describes the macroscopic properties based on the energy of the system. One interesting application is to describe the coercivity based on the structure and micromagnetic properties.[2)] The Landau free energy theory is very hard to be implemented in complex applications due to the pinning de-pinning process of the domain walls.[3)] Thus, the development of pseudo free energy that considers the metallography structure is necessary to describe the physics in inhomogeneous polycrystalline systems.

2. Results and Discussion

In this work, we use micromagnetic simulation to calculate the external field dependence of magnetization in polycrystalline permalloy and analyze it using unsupervised machine learning. The polycrystals were draw using Voronoi tessellation generators. For all simulations, the external magnetic field was set from 0.6T to 0.6T in the x direction. Different grain sizes images (Fig. 1) were used as input to confirm the reproducibility and the accuracy of the method. After, the image data were processed we applied feature extraction dimensional reduction methods to find correlations between the images in the data set.

The energy landscape in magnetization reversal process is successfully visualized as a function of features (Fig. 2). It is observed correlation between the reduced feature space and the hysteresis loop. The map of the data in lower dimension space of the magnetization, in the same direction of the external magnetic field, displays a clearly coercivity dependence. Small grains sizes have smaller components and broader distribution in the feature space, which is inverse proportion to the coercivity. For M_y, the coercivity points are located around the extremities of feature 1 and feature 2. Our result implies that the magnetic microstructure can display information about the macroscale properties which is the building blocks for the development of the pseudo free energy.

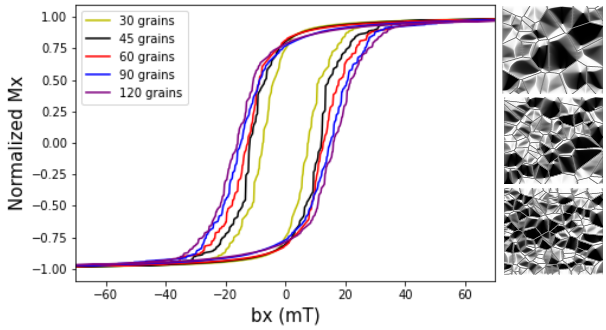

Fig. 1. Hysteresis loop for different grain sizes and magnetic domain structures near coercivity for 30, 60 and 120 grains.

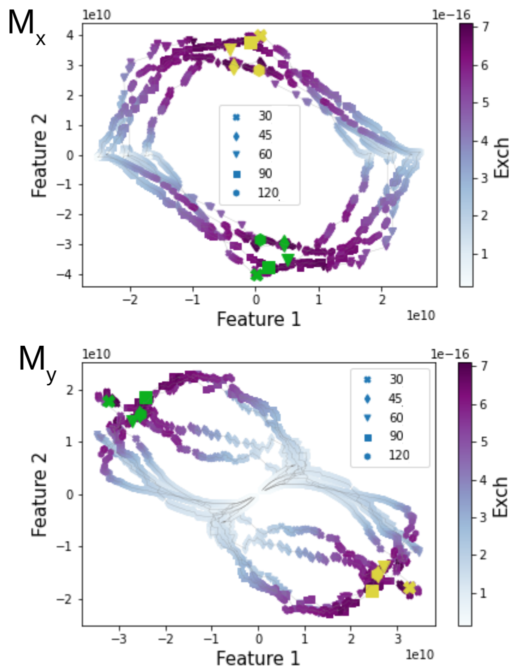

Fig. 2. Reduced feature space of the magnetization reversal process of x and y components. The green an yellow points correspond to the positive and negative coercivity.

References

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