Theoretical study on the magnetization reversal of rare-earth magnets at finite temperature

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In viewpoints from both the energy-efficiency and environment problems, the development of high-performance Nd-Fe-B permanent magnets is strongly desired especially for electric vehicles. It has so far been recognized that one of the important issues to be overcome is suppressing the thermal degradation of their coercivity, H_C. As a measure, Dy is currently substituted for part of Nd in Nd-Fe-B sintered magnets. However, this is unfavorable because Dy is expensive and the magnetization decreases owing to the antiparallel coupling between Dy and Fe moments. For these reasons, the microscopic foundations for the magnetization reversal mechanism of Nd-Fe-B magnets are sincerely needed and many theoretical works have been done intensively based on several different approaches.

A direct way to study the hysteresis loop is to employ the Langevin equation so-called stochastic LLG equation which takes into account the thermal fluctuation.[1)] However, the method consumes much computation time to reach the observation time of a few seconds. Alternatively, to handle such a slow relaxation process, usage of the free energy landscape is useful and appropriate. Actually, the magnetization reversal can be interpreted as the transition from metastable magnetic state to a stable state by overcoming the free energy barriers under a reverse magnetic field. The reverse nucleus is formed in this process. To deal with such processes at finite temperature, one needs to evaluate the free energy landscape instead of searching the energy minimum path.[2)]

Recently, we[3)] have succeeded, for the first time, to calculate the free energy $F(T, H_z, M_z)$ of a finite-size particle of $Nd_2Fe_{14}B$ as functions of temperature (T), external magnetic field ($H_z < 0$) and the z-component of the total magnetic moment (M_z) with using replica-exchange Wang-Landau method.[4)] This method enables us to evaluate the $F(T, H_z, M_z)$ with using only the magnetic parameters at zero temperature such as the local magnetic moments (M_i), exchange interactions (J_{ij}) between them and the anisotropy constants (crystal field parameters) all of which can be determined by the first principles calculation.[5)]

Figure 1(a) shows the spatial distribution of the reversed magnetization around the barrier as shown by the arrows in Fig. 1(c). In Fig. 1(b), we show the averaged magnetization density. From these data one can find that the reverse begins at the corner because of the weak exchange field, and then the domain wall propagates toward the center of the particle. Once the $F(T, H_z, M_z)$ is obtained as in Fig. 1 (c), we can calculate, without using any empirical parameter, the energy barrier $F_B(T, H_z)$, activation volume $V_a(T, H_z)$ and viscosity coefficient (fluctuation field) $S_v(T, H_z)$. Taking account of the thermal fluctuation, the coercivity H_C in the observation time of one second can be determined from the relation $F_B(T, H_C) = 25.3k_BT$. Further, we have demonstrated both analytically and numerically that $V_a(T, H_z)$ which is defined as a volume swept out between minimum and maximum energy positions of the domain wall[6)] (corresponding to ΔM_z in Fig. 1(c)) is always given by $-(\partial F_B/\partial H_z)/M_S$, regardless of the form (magnetization reversal model) of $F_B(T, H_z)$. From the data, we found that the $V_a(T, H_z)$ drops sharply with increasing H_z in a low H_z region and goes to a certain constant value as H_z approaches to H_C. This implies that $F_B(T, H_z)$ is approximately proportional to $(1 - H_z/H_0)^n$ with n close to unity when $H_z \simeq H_C$, while, for H_z much smaller than H_C, n is larger than 2. The result $F_B \propto (1 - H_z/H_0)^n$ ($n \simeq 1$) for Nd-Fe-B magnets seems agreeable with the experimental findings by Givord et al.[7)] and Okamoto et al.[8] The physical interpretation for $n \simeq 1$ (V_a is nearly independent of H_z) will be given in the conference.

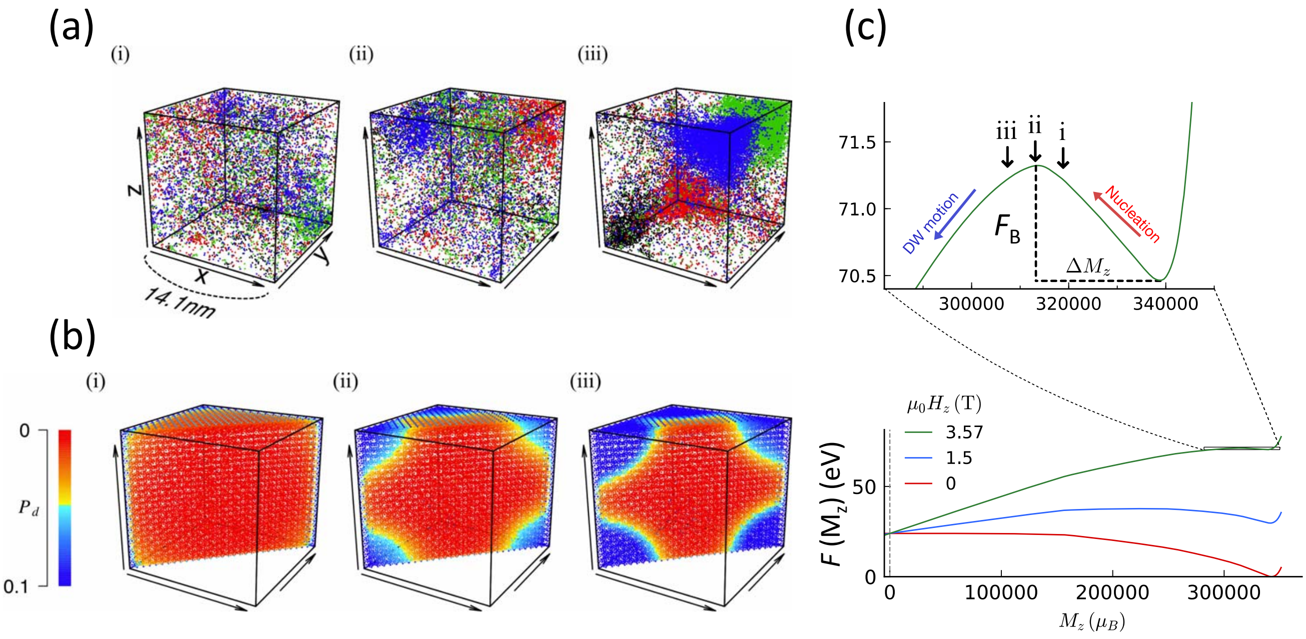

Fig. 1 Free energy landscape simulation of surface nucleation.(a) Snapshots of distributions at the three magnetization points i - iii in the free energy landscape (Fig. 1(c)) simulated by the replica exchange Wang-Landau method for the $Nd_2Fe_{14}B$ isolated particle spin system, whose size is 14.1nm ×14.1nm ×14.6nm (212,536 spins). The dots of each color denote reversed Fe spins in each snapshot. (b) The distributions sliced by (110) plane of the possibility of spin reversal P_d at Fe sites. (c) Free energies as a function of the z-component of the total magnetic moment M_z at $0.46T_C^{cal}$. The blue and green lines are the results of applying reverse magnetic fields H_z along $-z$ direction to the red line.

References

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