

# Computer Simulation of Switching in Stoner-Wohlfarth Colloids

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*Abstract*— We have developed a method for the inclusion of transverse magnetization into a computer simulation of a magnetic ink, a colloidal suspension of acicular particles. Previous simulations have assumed a fixed longitudinal magnetic moment. We determine the magnetization (assumed uniform) by minimizing the Stoner-Wohlfarth energy, so the moment can point in any direction relative to the particle axis. The particle-magnetization changes and particle rotations occurring during a hysteresis loop will be shown in the form of a video. This method can be used to simulate particle orientation during the magnetic-tape coating process.

## I. SIMULATION TECHNIQUE

As in other molecular-dynamics type simulations, we follow the trajectories of a large number (100 or more) of particles in a periodically replicated box. The force and torque on each particle are sums of contributions from steric, magnetic, viscous drag, and Brownian forces and torques. The steric force has contributions only from nearest neighbors. It models the forces between the polymer coatings on the particles, by a potential which is proportional to the square of the minimum distance between two particle axes [1]. We have chosen the coefficient of this force so that the effective thickness of the polymer coating is 0.15 times the radius of the particle. The effective shape of the particle is a sphero-cylinder (a cylinder with a spherical cap.) The magnetic force (described further below) has contributions from all neighbors, as well as from an infinite number of images (in other copies of the periodic box) of each neighbor. The infinite sum is performed using a Fourier transform technique, and the computation is speeded up by using a PPPM (Particle-Particle Particle-Mesh) method [2][3].

We did calculations with solid fractions of 3% and 6% by volume, appropriate for a let-down dispersion being coated onto a tape. We prepared an initial condition by

placing particles randomly in a large box (volume fraction < 1%) and then shrinking the box to the desired volume fraction [4].

## II. SIMULATED SYSTEM

We have used particles with an aspect ratio (the ratio of the axial length to the diameter) of 6.5, an axial length of 0.06  $\mu\text{m}$  and a magnetization of 148 emu/gm.

## III. MAGNETIC FORCES

We assume a single-domain Stoner-Wohlfarth particle, i.e., the magnetization is uniform and varies only in direction (its magnitude is fixed at its saturation value). The principal improvements in our treatment of the problem lie in the way we handle the magnetic interaction. Previous simulations have assumed in addition that the direction of the magnetic moment is fixed in the particle along the easy axis. The uniform longitudinal magnetization creates a surface pole density at each cap. This has been approximated in the past [1][4][5], by two oppositely charged point poles at the centers of the spherical caps (see Fig. 1(a)).

In our present calculation, we consider a particle whose magnetization can be in any direction, determined by a Stoner-Wohlfarth energy criterion. Thus the magnetization will in general have a transverse as well as a longitudinal component. The magnetic pole densities due to the longitudinal and transverse component of the magnetization are treated separately. The longitudinal component is approximated by two poles as before. The transverse component of the magnetization creates long strips of surface pole density along the flanks of the particle, which we represent by lines of equally spaced monopoles as shown for the transversely magnetized particle in Fig. 1(b). In general, both components of the magnetization may be nonzero, so the poles are as shown in Fig. 1(c).

## IV. RESULTS

We have simulated a hysteresis loop. Because the initial condition was obtained by shrinking the box to the correct size at zero magnetic field, it has nearly zero magnetization. From zero, the magnetic field  $H$  was increased

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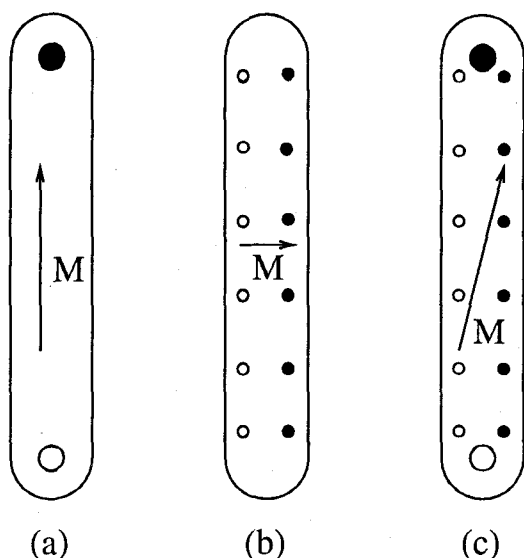


Fig. 1. (a) A particle with longitudinal magnetization, showing the north (filled circle) and south (open circle) point poles that are used to approximate it. (b) A particle with transverse magnetization in the plane of the figure, showing the strings of poles that approximate it. (c) The general case:  $M$  has both a longitudinal and a transverse component.

to +400 Oe in steps of 80 Oe, then decreased in steps to -400 Oe, and then returned to +400 Oe.

The resulting magnetization is shown in Fig. 2. Four curves are shown, corresponding to high and low (6% and 3%) volume fraction and fast and slow magnetic field sweep (2000 $\Delta t$  and 3000 $\Delta t$  per point, corresponding to 75 and 50 complete cycles per second, respectively). As expected, the loop is narrower for the slower sweep rates. The volume fraction has a surprisingly small effect on the hysteresis curve.

Several points on the loop are labeled, and Fig. 3 shows the particle configurations at these points. Note that the alignment starts very slowly as the field is increased, and the system aligns very rapidly as it approaches point (b) of Fig. 2. Although the magnetization is over 80% of its saturation value when  $H = 320$  Oe (Fig. 3(b)), many particles still do not appear aligned. We reach the coercive field at approximately point (d), where the particles are still aligned and in fact can be seen to be beginning to form a layered structure reminiscent of a smectic liquid crystal (this has been seen previously when the field is turned on during the aggregation process [6].) This structure is then destroyed in the reversal that takes place near (e).

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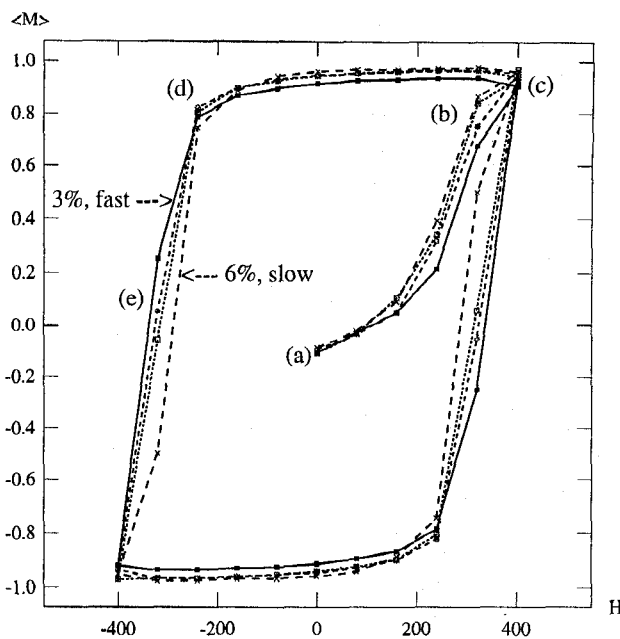
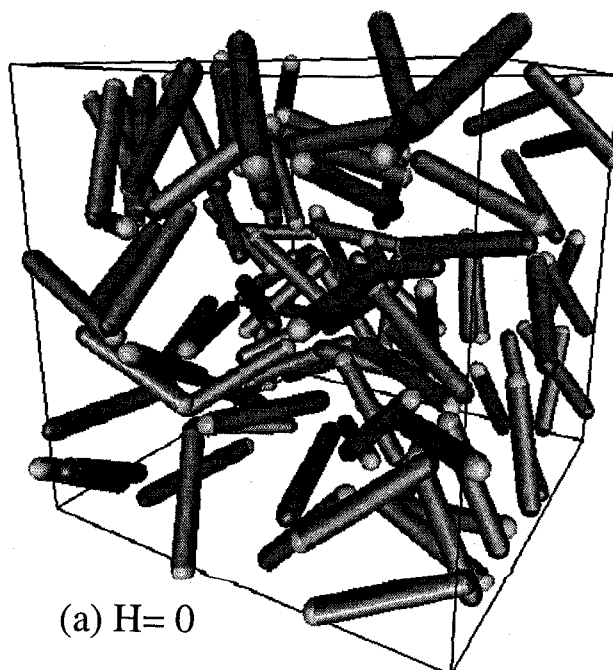


Fig. 2. Hysteresis loop, showing magnetization as a function of magnetic field. Innermost curve (long dashes): 6% volume fraction, slow field sweep (80,000 Oe/sec or 50 Hz); dots: 3%, 50 Hz; short dashes: 6%, 75 Hz; solid line: 3%, 75 Hz. Labels (a), (b), ... indicate points on the solid line for which snapshots are shown in Fig. 3.

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(a)  $H=0$

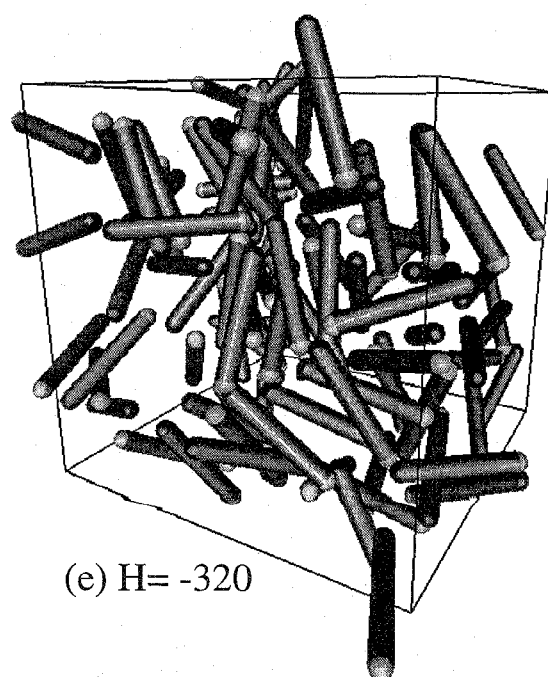
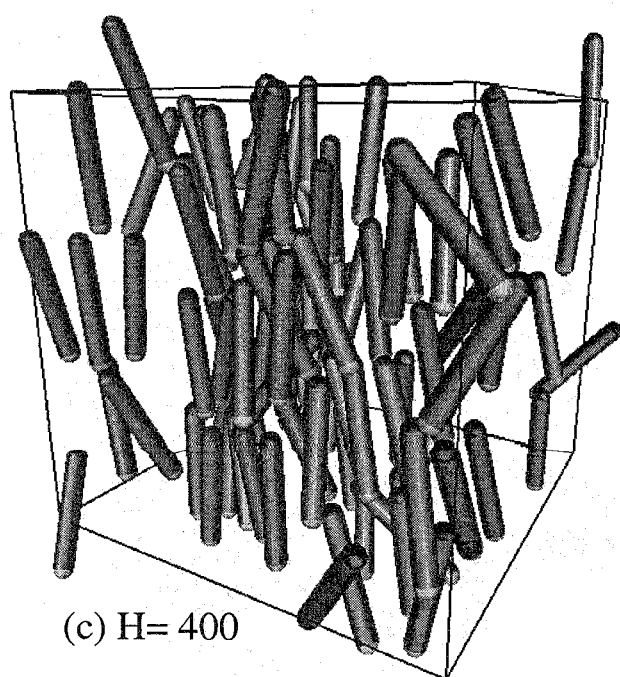
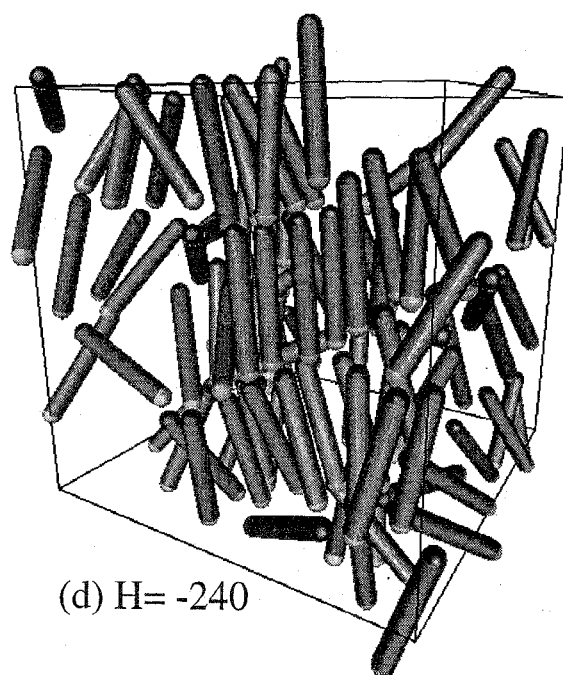
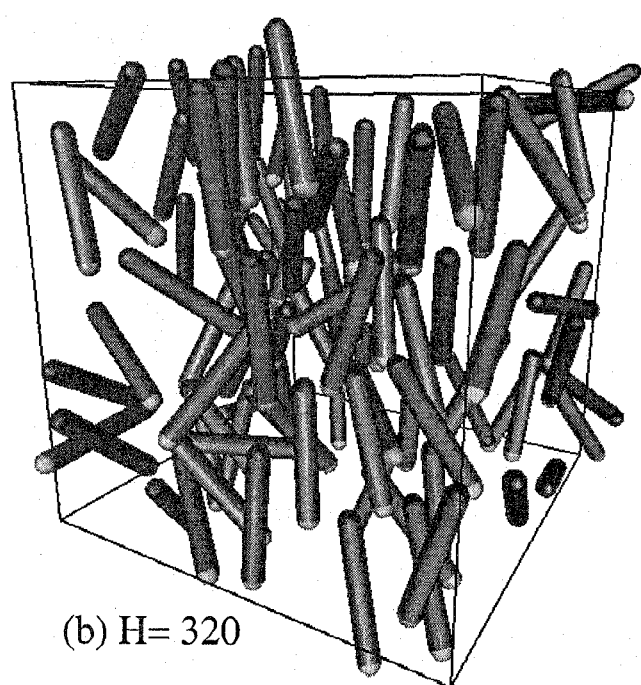


Fig. 3. Snapshots of the magnetic ink at the points marked (a), (b), (c), (d), and (e) in Fig. 2.