Designing Novel Nanostructured Permanent Magnets

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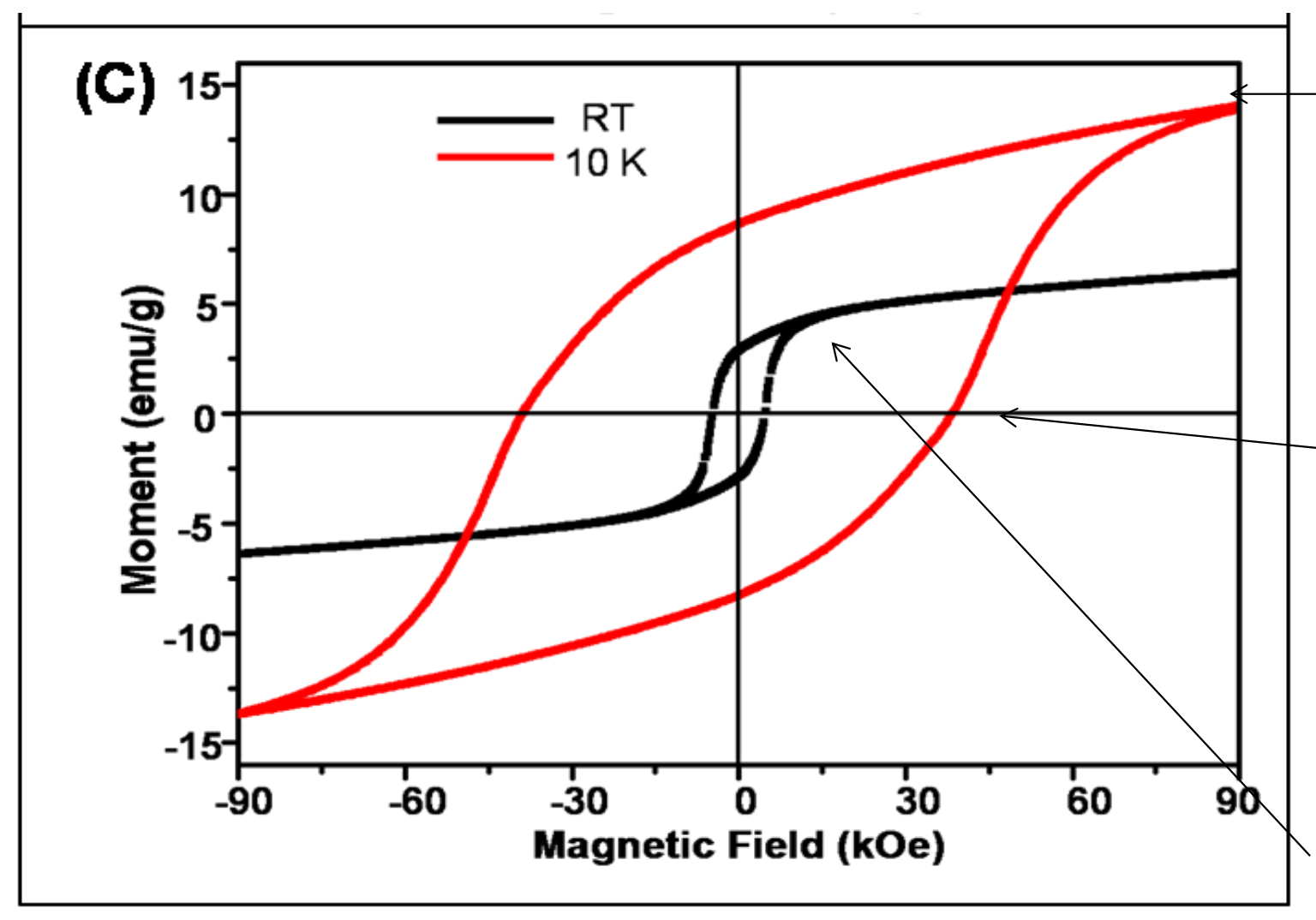
Motivation

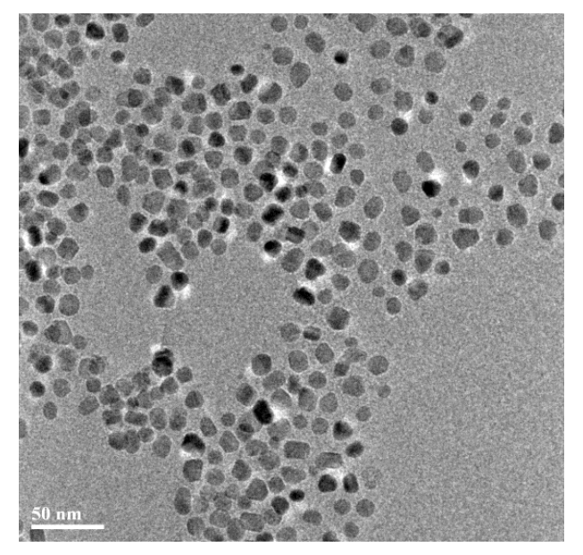
- The modeling of magnetic properties of magnetic materials is one of the key factors in producing high performance alloys, which have tremendous applications in advanced energy technologies.
- Rare earth element based alloys have been the source of high performance magnetic alloys, and have played a paramount role in the development of various technologies, including: memory devices (such as credit cards, random-access memory), sensors, and various biomedical applications.
- There is a need to replace rare earth metals with material with powerful magnetic properties.
- Our group recently found CrTe-based materials that show very promising magnetic properties in nanostructured form.
- The goal is to investigate the behavior bulk material made out of nanomagnets to predict the magnetic properties which will help screening candidate materials prior to their fabrication.
- Highly effective magnetic materials have wider hysteresis loops (or higher coercivity, refer to figure 1) and large magnetocrystalline anisotropy. Therefore, in order to predict the next novel magnetic materials, one has to simulate the magnetic properties of the material on the nanoscale and pinpoint the magnetic parameters which influence its performance and behavior.



Saturation Magnetization

Coercivity

Narrow hysteresis loop implies a small amount of dissipated energy in reversing the magnetization



Computational methods

- Object Oriented Micromagnetic Framework (OOMMF).
- Scripts written in Tcl/Tk.
- Time Evolvers which track LLG dynamics, and locate local minima in the energy surface through direct minimization techniques.
- Landau-Lifshitz-Gilbert Equation

Landau-Lifshitz Gyromagnetic ratio

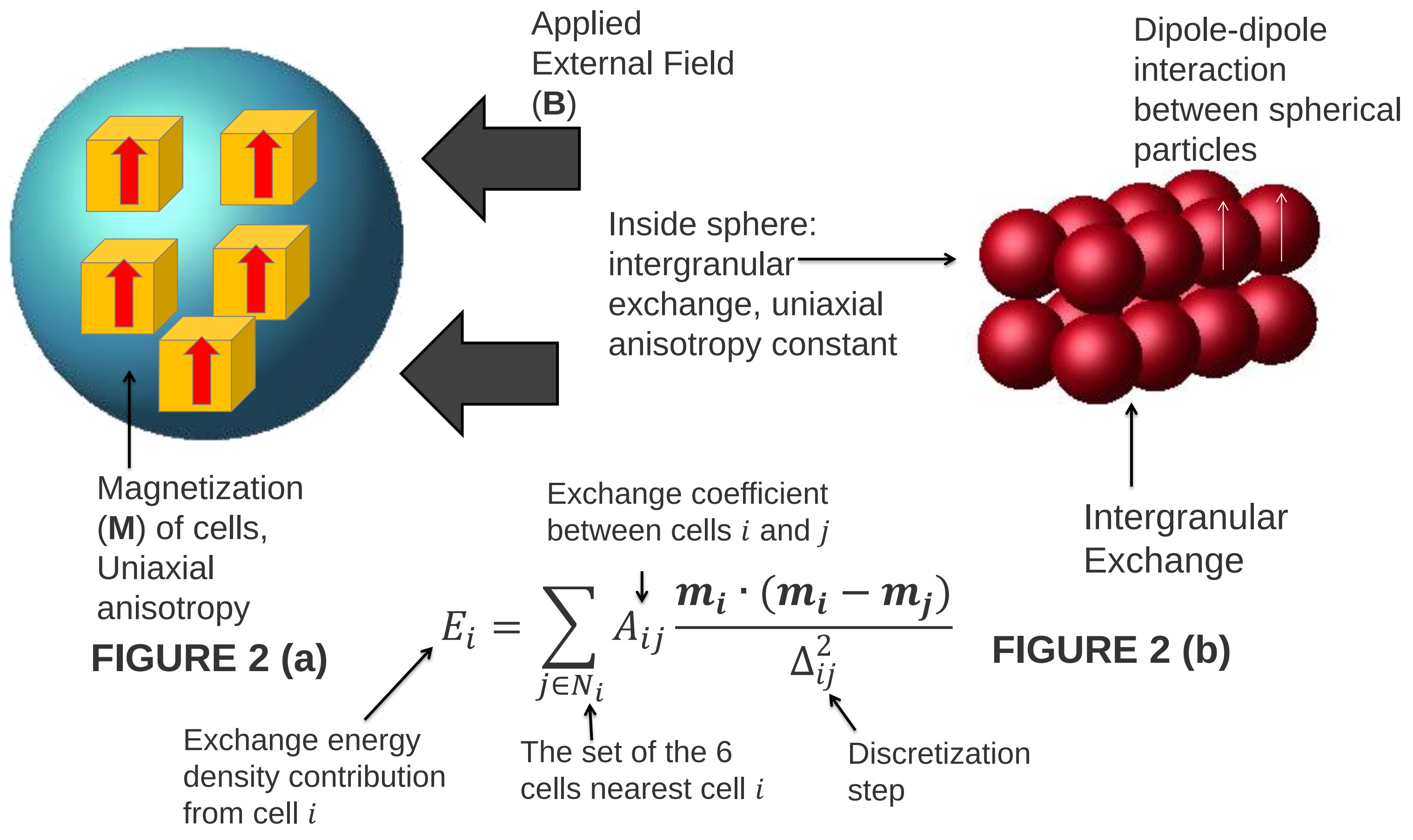
$$\frac{d\vec{\boldsymbol{M}}}{dt} = -|\gamma|\vec{\boldsymbol{M}} \times \overrightarrow{\boldsymbol{H}_{eff}} + \frac{\alpha}{\boldsymbol{M}_s}\left(\vec{\boldsymbol{M}} \times \frac{d\vec{\boldsymbol{M}}}{dt}\right)$$

Effective Field

Magnetization

- Runge-Kutta methods for integrating the LLG ODE

model



Applied External Field (**B**)

Dipole-dipole interaction between spherical particles

Inside sphere: intergranular exchange, uniaxial anisotropy constant

Magnetization (**M**) of cells, Uniaxial anisotropy

FIGURE 2 (a)

Exchange coefficient between cells i and j

$$E_i = \sum_{j \in N_i} A_{ij} \frac{\boldsymbol{m_i} \cdot (\boldsymbol{m_i} - \boldsymbol{m_j})}{\Delta_{ij}^2}$$

Intergranular Exchange

FIGURE 2 (b)

Exchange energy density contribution from cell i

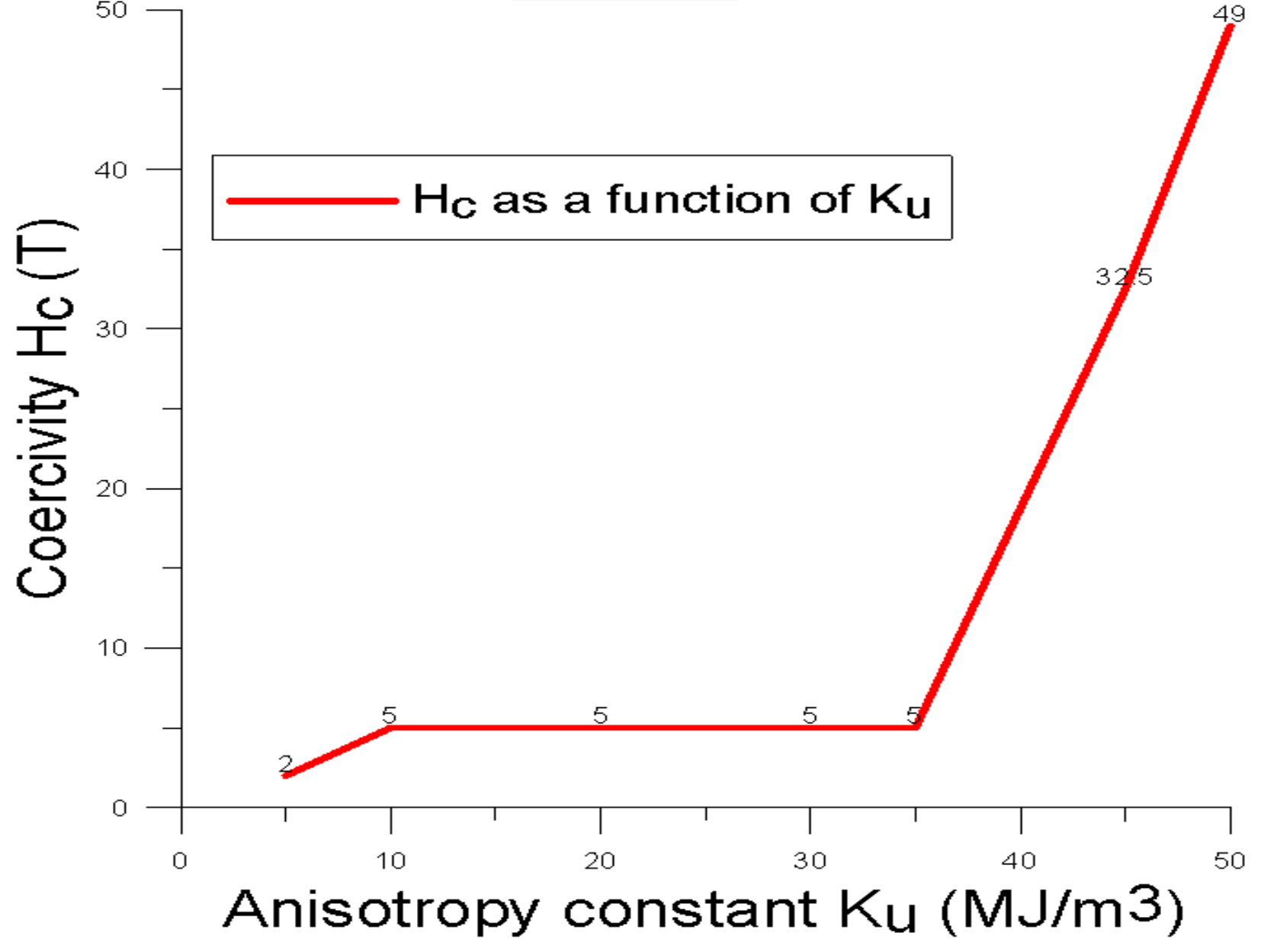
The set of the 6 cells nearest cell i

Discretization step

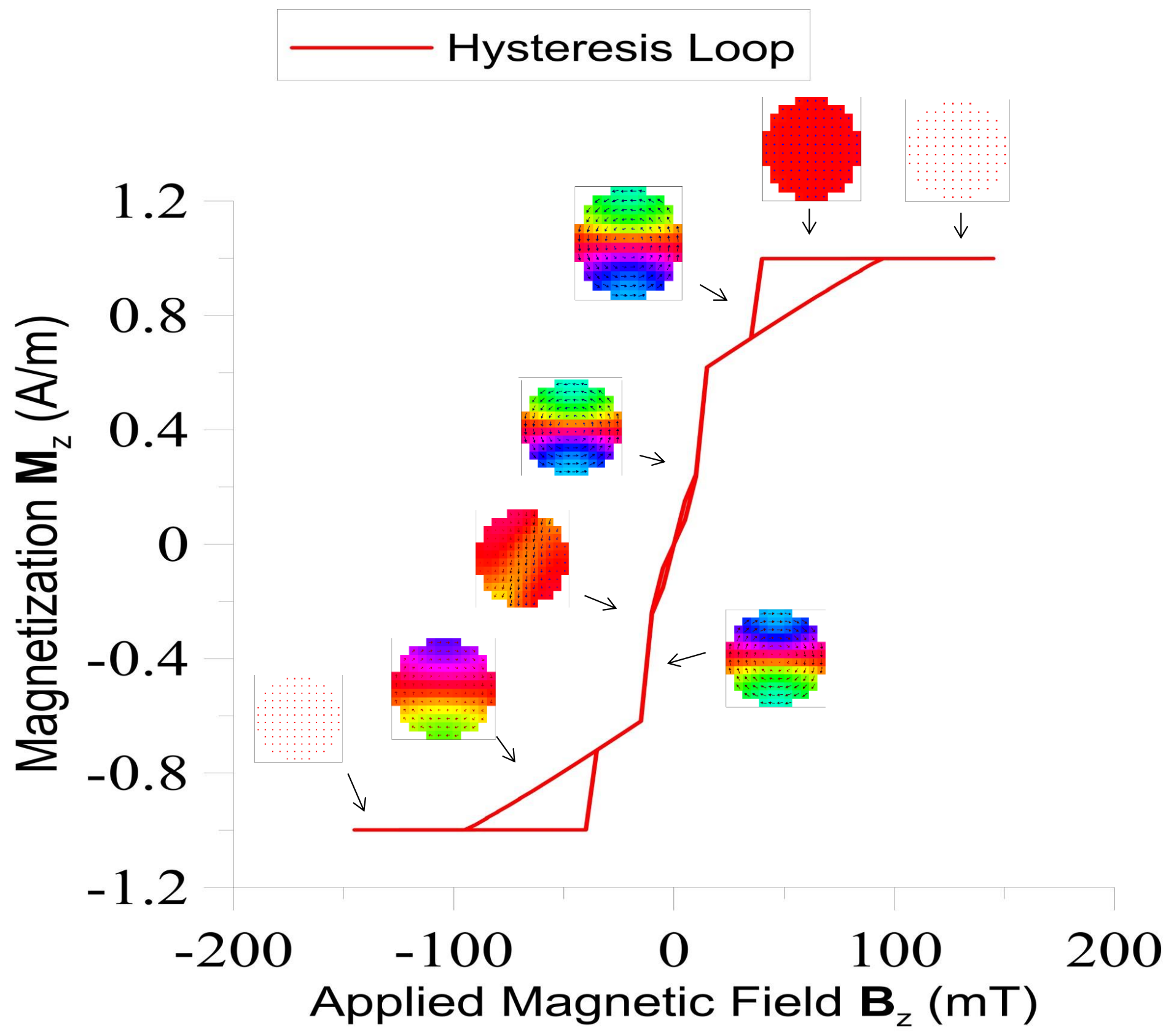
FIGURE 2 (a) represents the model of a spherical magnetic material (with radius 60 nm) that encloses individual magnetic cells of size 5nm on each side. The cells each have magnetization, and a uniform magnetic exchange constant of 13 pJ/m. The cells also have uniaxial anisotropy which will be varied and studied.

FIGURE 2 (b) represents the model of a bi-layer granular micromagnetic system. There are two layers of grains, each of which encloses magnetic cells of size 1.5 nm on each side. Each of the cells has uniaxial anisotropy which will be varied and studied, as well as 6-neighbor exchange energy which will be further examined.

Spheres



Coercivity as a function of anisotropy constant. We see the higher the uniaxial ansiotropy, the higher the coercive field. The steady coercivity at 5T corresponds to a pining field.



The hysteresis loop for a single sphere of radius 60 nm and uniaxial anisotropy constant of 30 mJ/m³ with applied magnetic field in the z direction. Inside the sphere are cells of size 5 nm on each side. We see the behavior of the sphere as it forms vortices and we see the effects of Berkhausen jumps caused by pinning fields.

Granular bi-layer

Figure 5

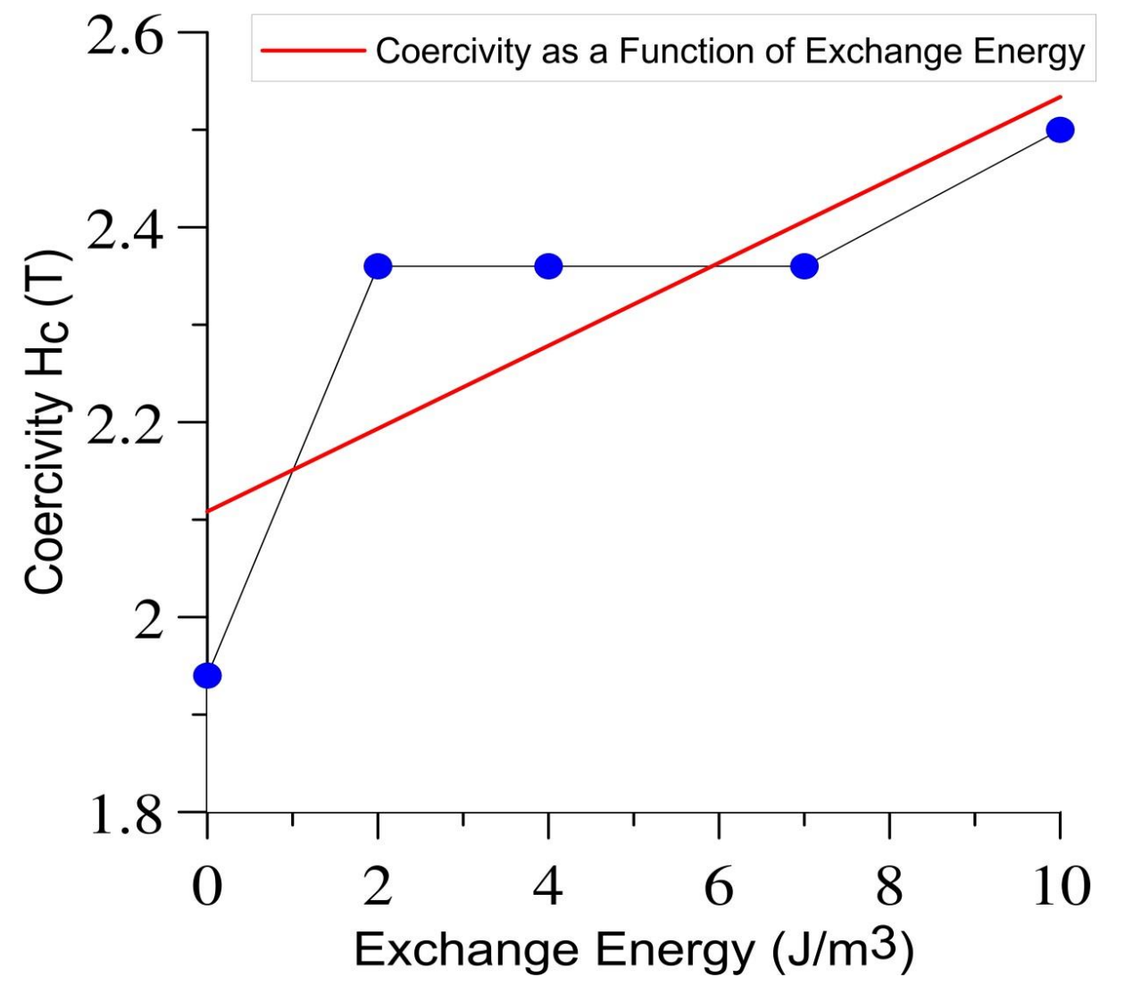


Figure 6

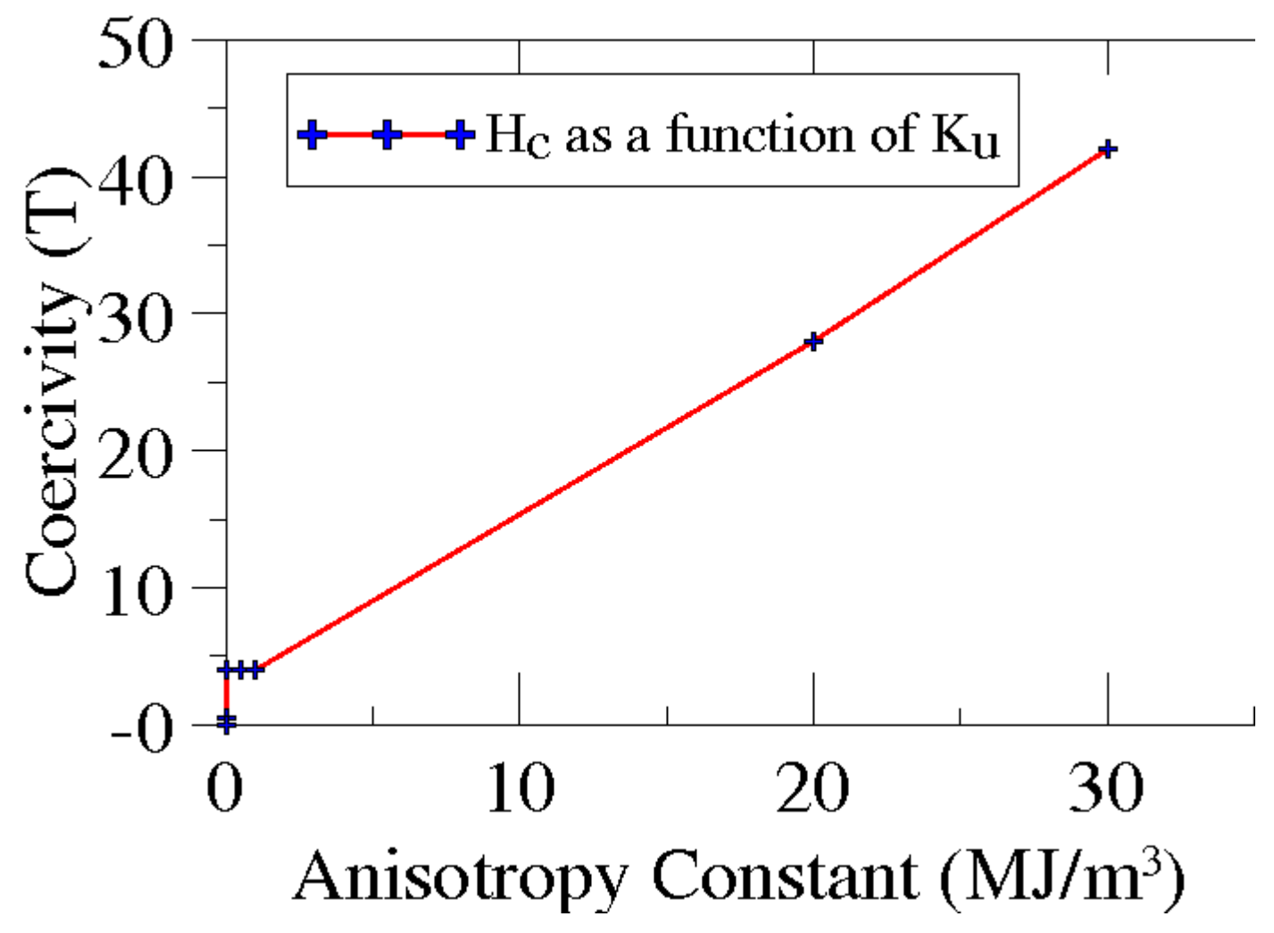


Figure 5 represents coercivity as a function of exchange energy. The system has a uniaxial anisotropy constant of 1.6 mJ/m³.

Figure 6 represents coercivity as a function of uniaxial anisotropy constant. Here, the exchange energy was kept at 5 pJ/m.

In both cases we have a region of 21 nm by 24 nm by 10.5 nm, with individual cells of size 1.5 nm on each side are enclosed.

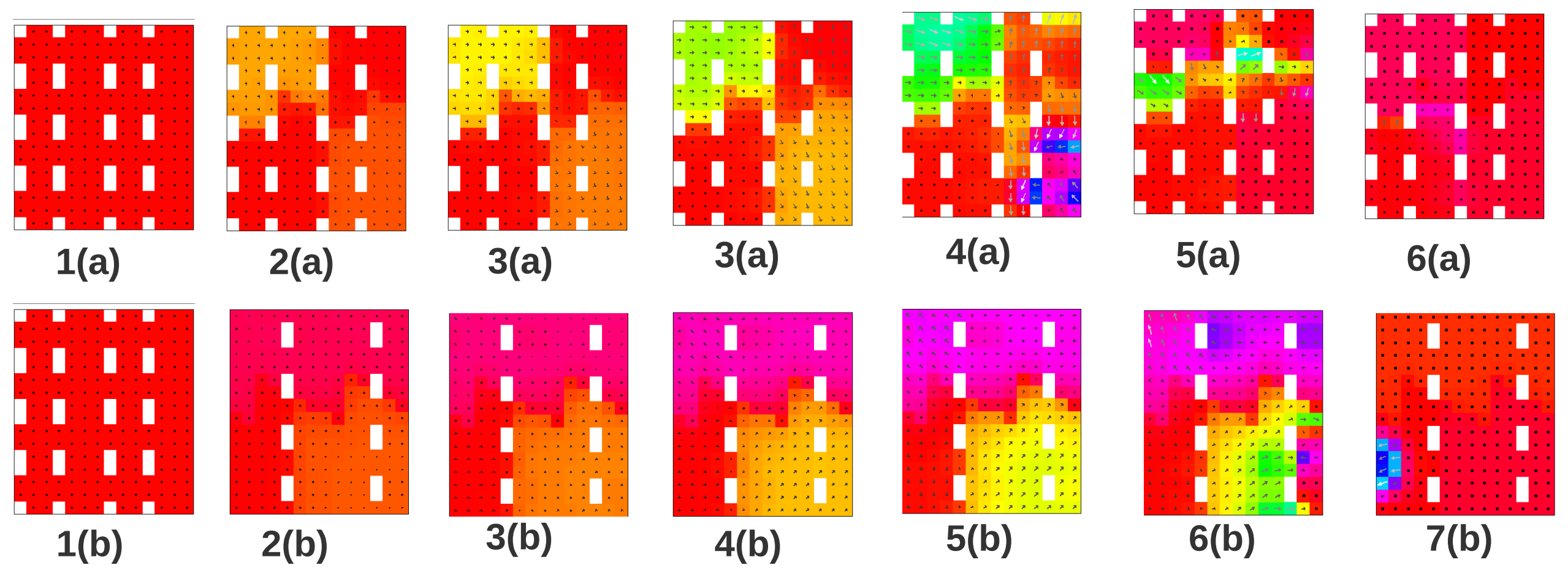


FIG. domain wall propagation of a bilayer granular structure of 1.5 nm cells with 30 MJ/m³ anisotropy and 15 pJ/m interatomic exchange. **1(a)-6(a)** is a z-slice of 2.415 nm, whereas **1(b)-7(b)** is a z-slice of 7.245 nm.

Conclusions

- We model two models of micromagnetic material: a spherical system, and a touching bi-layer system with intergranular exchange. We then obtain functions of coercivity vs anisotropy constant and coercivity vs exchange energy in the granular case.
- We show that in the case of a single sphere, small anisotropy constant corresponds to small coercivity, and small coercivity corresponds to small anisotropy and vortex switching.
- In the bi-layer granular media we see that increasing inter-granular exchange energe corresponds to increasing the coercivity, and increasing anisotropy constant corresponds to increase in coercivity.
- The results agree with the Weiss Theory of ferromagnetism.
- Some interesting results are obtained with these systems in regards to vertex switching, Berkhausen jumps, and domain wall propagations.

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