COSC-4309 Simulations
Final Project – Due July 8, 2010

Work Performed in Magnetization of Gadolinium in Vicinity of Curie Temperature

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INTRODUCTION

The system for this study is a solid cube of gadolinium which is just above its Curie temperature, indicating that, in the absence of a strong enough applied magnetic field, the material is in its paramagnetic phase. The characteristics of this phase include randomly oriented magnetic dipole moments and weak partial alignment with an external magnetic field.

As a magnetic field is applied, a torque is exerted on the individual magnetic dipole moments in an effort to align them with the easy axis of the applied field. In turn, work is performed on the system by the magnetic field to achieve alignment, while the internal energy of the system is lowered through reduction of magnetic entropy. However, since the system is near its Curie temperature, a strong enough applied field can cause the material to transition into its ferromagnetic phase, characterized by a sharp and rapid alignment relative to the applied field.

This transition is of the first order, which means that there is a latent heat exchange associated with the lowering of magnetic entropy. By the magnetocaloric effect, a material experiencing this kind of transition tends to dissipate heat as a result of the applied field. The magnetocaloric effect has strong utility value in the construction of magnetic refrigerators, since these materials can dissipate heat to their surroundings when a field is applied, then (once the dissipated heat has been removed by a thermal conduit of some sort) absorb heat once the applied field is no longer present.

Gadolinium is an excellent candidate for this for the following reasons:

- Strong magnetic moment per atom – 7.94μB compared to other elemental ferromagnets: iron (2.22μB), cobalt (1.72μB), and nickel (0.60μB).
- Reasonable Curie temperature – 293 K compared to: iron (1043 K), cobalt (1388 K), and nickel (627 K). For reference, “room temperature” is typically between 293 and 300 K.
- Can be readily bonded with other elements to tune each of the aforementioned properties.

The motivation for this study is to estimate the amount of energy that must be spent, as well as the required amount of time, in order to magnetize a sample of gadolinium. This information is very useful for the development of new electronic devices utilizing gadolinium’s unique characteristics.

BACKGROUND AND VALIDATION

Magnetization is a property which is exhibited almost exclusively due to motion of electrons orbiting a nucleus in a particular fashion. Each atom in a material exhibits some properties of magnetism, which is characterized by magnetic moments per atom and measured in terms of the Bohr magneton, which is:

\[ \mu_B = \frac{e\hbar}{2m_e} \]

where \( e \) is the elementary charge, \( \hbar \) is the reduced Planck constant \((\hbar/2\pi)\), and \( m_e \) is the mass of an electron. As mentioned previously, gadolinium has a magnetic moment of magnitude 7.94μB.

External magnetic fields tend to align these magnetic moments along the easy axis of
the applied field by exerting a torque on the dipoles:

$$\tau = m \times B$$

where $m = \mu \hat{m}$ is the magnetic moment vector in a particular orientation and $B = \mu_0 \mu_r H$ is the vector combination of the applied field $H$ and the internal magnetization per unit volume of the material $M = \frac{m}{V}$. The cross product indicates that the torque is perpendicular to both the magnetic dipole moment orientation and the B-field. Bold print indicates a vector.

From the torque, we can obtain the angular acceleration of the body about a fixed axis:

$$\tau_{net} = \frac{dL}{dt} = I \alpha$$

where $L = I \omega$ is the angular momentum vector, $I$ is the moment of inertia of the body, and $\omega$ is the angular velocity of the rotating body. Since the angular momentum is differentiated with respect to time for torque, the velocity vector becomes the angular acceleration $\alpha$. The moment of inertia for a sphere is $\frac{2mr^2}{5}$ where $m$ is mass of the body and $r$ is the radius of the spherical shape.

The angular acceleration helps determine how the magnetic dipole moments line up with each step in the simulation process:

$$\theta = \omega_0 t + \frac{1}{2} \alpha t^2$$

where $\theta$ is the angular displacement over time interval $t$.

The potential energy associated with the applied field interaction with the magnetic dipole moments is:

$$U = -m \cdot B$$

where the dot product indicates a scalar value. Therefore, as the field is aligning (by action of torque) along the easy axis of the B-field, the internal energy of the system is decreasing. Under full alignment (saturation), the only components which will be utilized in the dot product are in the same direction, thus multiplying together.

The change in potential energy of a body constitutes work performed by either the body itself or another object in the total system:

$$W = -\Delta U$$

In other words, to lower the internal energy of a system, energy must be supplied to the system. In this case, the energy is provided by the B-field.

**ASSUMPTIONS USED IN THE MODEL**

In order to actually model the system, several assumptions must be used. The limitations of calculating the statistical elements in the system lead to the conclusion that this model will only give a rough estimate of the amount of energy spent in magnetization.

First, the model assumes that the magnetic dipole moments are totally random and uniformly distributed. This assumption is not accurate due to the statistical nature of temperature as a bulk property of matter. Since the system is in the vicinity of its Curie temperature, statistically there are some regions which may have an internal energy low enough to be in their ferromagnetic phase.
The model further assumes that the temperature change by the magnetocaloric effect is adiabatic and isobaric. This means that the only energy transport in the model is through the applied magnetic field. This is not accurate, but to appropriately model the pressure and volume deformations of the system would require significantly more time and might not add anything substantial to the final result.

The model also assumes that the magnetic material under examination is gadolinium of 100% purity. This is not possible, but it is all that could be done given the time constraint of the project.

Given the size of system to be examined, the field is setup to not decay as a function of distance. Since the distance increases on the order of 1 Ångström, or $1 \times 10^{-10}$ meters, this decay would be negligible.

Due to the scarcity of information available on this subject, the critical magnetic field strength which encourages a transition in gadolinium could not be found. Therefore, the model uses the critical value obtained by Tang, et al, for Gd$_5$(Si$_{1.95}$Ge$_{2.05}$). This should serve as a rough estimate of the required magnetic field, since the main magnetic component of the aforementioned compound is gadolinium. As shown in Figure 1, the field transitions when subjected to field strength of about 19 kOe given that the system is roughly 5 K above its Curie temperature.

**Figure 1**

**SPECIFICATIONS FOR THE COMPUTER PROGRAM**

In order to simplify the calculations of the system, the model is examined for a uniform field in the $\vec{k}$ direction, with the magnetic material resting one unit away from the field source (also in the $\vec{k}$ direction). This prevents the field from being amplified beyond its desired level, since it decays quadratically as a function of distance from the field source. For distances below one unit, the quadratic decay factor $\frac{1}{d^2}$ would strengthen the applied field. We neglect this factor to simplify our process.

This has numerous benefits to the calculations. For example, in calculating torque:

$$\tau = \det \begin{vmatrix} 1 & \hat{j} & \hat{k} \\ m_i & m_j & m_k \\ 0 & 0 & B_k \end{vmatrix} = m_j B_k \hat{i} - m_i B_k \hat{j}$$

Further, the potential energy sees a similar benefit:

$$U = -m_k B_k$$

Due to time constraints, the system must be modeled based on input of a specified number of atoms as opposed to input of
physical dimensions. Each atom and its interatomic distance occupy a space on the order of 1 Ångström. Therefore, a cube with sides of 1 millimeter could contain as many as $1 \times 10^{21}$ atoms. With the number of calculations that must occur on each atom, estimations on samples of practical physical dimensions must be done as a future endeavor.

The simulation begins by allocating three-dimensional arrays to maintain the state of each magnetic dipole moment. Since each atom can be uniquely identified by (x,y,z), these coordinates will be used to retrieve each $\hat{i}$, $\hat{j}$, and $\hat{k}$ component. Further, the model must keep track of the potential energy for each dipole as well as the angular velocity from the previous step.

At initialization, the simulation establishes events at each $dt$ time segment corresponding to magnetization of the first layer in the $\hat{k}$ direction. After the first layer has been processed, it should spawn an event at the same sim_time to process the next layer.
RESULTS OF SIMULATION

in.txt:

1e6  10  1.0  10  0  3.5  0.95  1.9  2.5  91

[garretl@galaxy1 finalproj]$ ./project
End of run   1
End of run   2
End of run   3
End of run   4
End of run   5
End of run   6
End of run   7
End of run   8
End of run   9
End of run  10
*** glibc detected *** ./project: corrupted double-linked list:
0x09ca62d0 ***
.....

The simulation runs as expected, but there is an error somewhere in terminating the program. Time constraints prevented me from fixing this issue since the simulation takes about 15 minutes to run on galaxy.

As shown on the following pages, the system performs the calculations as planned. Since the system only consists of one million atoms (each face of the cube is only 1.8 nm wide!), the results are consistent with expectations. When the field strength exceeds the threshold, there is a noticeable jump in the amount of work spent in magnetizing the material. As stated previously, the assumption is that the material experiences a phase transition when it is 5 K above its Curie temperature and subjected to a field of 19 kOe (1.9 Tesla). Between 1.75 and 2.1 T, this transition occurs and the work spent in magnetization raises two orders of magnitude. This is interesting and certainly worth exploring in other possible utilities.

The convergence of simulation results is deceiving because there are actually minor variations in the calculated work. Since each line of the simulation results is the summation of the work on one million atoms, it makes sense that these variations on a scale less than $10^{-12}$ would converge to six decimal places, as in the simulation output.
With more time, the simulation could be improved by dealing with the aforementioned assumptions in a better way. Also, the result of the simulation can be made more practical given enough computing resources to model a physically tangible object, as opposed to one which is roughly 1.8 nm³.

Sources:
H. Tang, et al, “Magnetic field induced phase transitions in GdSi(Si1.95Ge2.05) single crystal and the anisotropic magnetocaloric effect” Journal of Alloys and Compounds 455, pp. 73-76, 2008.

Summary.txt:

Magnetization of Gadolinium Sample
Garret LaBove

Requested number of atoms for model: 1.000000e+06
Simulation will run with 1.000000e+06 atoms (1.000000e+02^3)
Times to run simulation: 10
Time for each run: 1.0000 seconds
Time steps in each run: 10 (dt = 0.100 seconds)

Range of field measurement: 0.000e+00 to 3.500e+00 T
Saturation threshold: 0.95
Range of sharp susceptibility: 1.900e+00 to 2.500e+00 T
Susceptibility maximum: 91.000

---- Simulation Run # 1 ----

For H = 0.00000e+00 T, 0.000000000e+00 Joules spent in 0.10 seconds
For H = 3.50000e-01 T, 2.57724486e-17 Joules spent in 0.10 seconds
For H = 7.00000e-01 T, 7.73173463e-17 Joules spent in 0.10 seconds
For H = 1.05000e+00 T, 1.54634693e-16 Joules spent in 0.10 seconds
For H = 1.40000e+00 T, 2.57724491e-16 Joules spent in 0.10 seconds
For $H = 1.75000e+00$ T, $3.86586735e-16$ Joules spent in 0.10 seconds
For $H = 2.10000e+00$ T, $1.44583437e-14$ Joules spent in 0.10 seconds
For $H = 2.45000e+00$ T, $3.08753940e-14$ Joules spent in 0.10 seconds
For $H = 2.80000e+00$ T, $3.10815736e-14$ Joules spent in 0.10 seconds
For $H = 3.15000e+00$ T, $3.13135257e-14$ Joules spent in 0.10 seconds

Total work performed: $1.086e-13$ Joules
Power consumed: $1.086e-13$ Watts

---- Simulation Run # 2 ----

For $H = 0.00000e+00$ T, $0.00000000e+00$ Joules spent in 0.10 seconds
For $H = 3.50000e-01$ T, $2.57724486e-17$ Joules spent in 0.10 seconds
For $H = 7.00000e-01$ T, $7.73173463e-17$ Joules spent in 0.10 seconds
For $H = 1.05000e+00$ T, $1.54634693e-16$ Joules spent in 0.10 seconds
For $H = 1.40000e+00$ T, $2.57724491e-16$ Joules spent in 0.10 seconds
For $H = 1.75000e+00$ T, $3.86586735e-16$ Joules spent in 0.10 seconds
For $H = 2.10000e+00$ T, $1.44583437e-14$ Joules spent in 0.10 seconds
For $H = 2.45000e+00$ T, $3.08753940e-14$ Joules spent in 0.10 seconds
For $H = 2.80000e+00$ T, $3.10815736e-14$ Joules spent in 0.10 seconds
For $H = 3.15000e+00$ T, $3.13135257e-14$ Joules spent in 0.10 seconds

Total work performed: $1.086e-13$ Joules
Power consumed: $1.086e-13$ Watts

---- Simulation Run # 3 ----

For $H = 0.00000e+00$ T, $0.00000000e+00$ Joules spent in 0.10 seconds
For $H = 3.50000e-01$ T, $2.57724486e-17$ Joules spent in 0.10 seconds
For $H = 7.00000e-01$ T, $7.73173463e-17$ Joules spent in 0.10 seconds
For $H = 1.05000e+00$ T, $1.54634693e-16$ Joules spent in 0.10 seconds
For $H = 1.40000e+00$ T, $2.57724491e-16$ Joules spent in 0.10 seconds
For $H = 1.75000e+00$ T, $3.86586735e-16$ Joules spent in 0.10 seconds
For $H = 2.10000e+00$ T, $1.44583437e-14$ Joules spent in 0.10 seconds
For \( H = 2.45000 \times 10^0 \) T, \( 3.08753940 \times 10^{-14} \) Joules spent in 0.10 seconds
For \( H = 2.80000 \times 10^0 \) T, \( 3.10815736 \times 10^{-14} \) Joules spent in 0.10 seconds
For \( H = 3.15000 \times 10^0 \) T, \( 3.13135257 \times 10^{-14} \) Joules spent in 0.10 seconds

Total work performed: \( 1.086 \times 10^{-13} \) Joules
Power consumed: \( 1.086 \times 10^{-13} \) Watts

---- Simulation Run # 4 ----

For \( H = 0.00000 \times 10^0 \) T, \( 0.00000000 \times 10^0 \) Joules spent in 0.10 seconds
For \( H = 3.50000 \times 10^{-1} \) T, \( 2.57724486 \times 10^{-17} \) Joules spent in 0.10 seconds
For \( H = 7.00000 \times 10^{-1} \) T, \( 7.73173463 \times 10^{-17} \) Joules spent in 0.10 seconds
For \( H = 1.05000 \times 10^0 \) T, \( 1.54634693 \times 10^{-16} \) Joules spent in 0.10 seconds
For \( H = 1.40000 \times 10^0 \) T, \( 2.57724491 \times 10^{-16} \) Joules spent in 0.10 seconds
For \( H = 1.75000 \times 10^0 \) T, \( 3.86586735 \times 10^{-16} \) Joules spent in 0.10 seconds
For \( H = 2.10000 \times 10^0 \) T, \( 1.44583437 \times 10^{-15} \) Joules spent in 0.10 seconds
For \( H = 2.45000 \times 10^0 \) T, \( 3.08753940 \times 10^{-14} \) Joules spent in 0.10 seconds
For \( H = 2.80000 \times 10^0 \) T, \( 3.10815736 \times 10^{-14} \) Joules spent in 0.10 seconds

Total work performed: \( 1.086 \times 10^{-13} \) Joules
Power consumed: \( 1.086 \times 10^{-13} \) Watts

---- Simulation Run # 5 ----

For \( H = 0.00000 \times 10^0 \) T, \( 0.00000000 \times 10^0 \) Joules spent in 0.10 seconds
For \( H = 3.50000 \times 10^{-1} \) T, \( 2.57724486 \times 10^{-17} \) Joules spent in 0.10 seconds
For \( H = 7.00000 \times 10^{-1} \) T, \( 7.73173463 \times 10^{-17} \) Joules spent in 0.10 seconds
For \( H = 1.05000 \times 10^0 \) T, \( 1.54634693 \times 10^{-16} \) Joules spent in 0.10 seconds
For \( H = 1.40000 \times 10^0 \) T, \( 2.57724491 \times 10^{-16} \) Joules spent in 0.10 seconds
For \( H = 1.75000 \times 10^0 \) T, \( 3.86586735 \times 10^{-16} \) Joules spent in 0.10 seconds
For \( H = 2.10000 \times 10^0 \) T, \( 1.44583437 \times 10^{-15} \) Joules spent in 0.10 seconds
For \( H = 2.45000 \times 10^0 \) T, \( 3.08753940 \times 10^{-14} \) Joules spent in 0.10 seconds
For \( H = 2.80000 \times 10^0 \) T, \( 3.10815736 \times 10^{-14} \) Joules spent in 0.10 seconds
For $H = 3.15000e+00$ T, $3.13135257e-14$ Joules spent in 0.10 seconds

Total work performed: $1.086e-13$ Joules
Power consumed: $1.086e-13$ Watts

---- Simulation Run # 6 ----

For $H = 0.00000e+00$ T, $0.00000000e+00$ Joules spent in 0.10 seconds
For $H = 3.50000e-01$ T, $2.57724486e-17$ Joules spent in 0.10 seconds
For $H = 7.00000e-01$ T, $7.73173463e-17$ Joules spent in 0.10 seconds
For $H = 1.05000e+00$ T, $1.54634693e-16$ Joules spent in 0.10 seconds
For $H = 1.40000e+00$ T, $2.57724491e-16$ Joules spent in 0.10 seconds
For $H = 1.75000e+00$ T, $3.86586735e-16$ Joules spent in 0.10 seconds
For $H = 2.10000e+00$ T, $1.44583437e-14$ Joules spent in 0.10 seconds
For $H = 2.45000e+00$ T, $3.08753940e-14$ Joules spent in 0.10 seconds
For $H = 2.80000e+00$ T, $3.10815736e-14$ Joules spent in 0.10 seconds
For $H = 3.15000e+00$ T, $3.13135257e-14$ Joules spent in 0.10 seconds

Total work performed: $1.086e-13$ Joules
Power consumed: $1.086e-13$ Watts

---- Simulation Run # 7 ----

For $H = 0.00000e+00$ T, $0.00000000e+00$ Joules spent in 0.10 seconds
For $H = 3.50000e-01$ T, $2.57724486e-17$ Joules spent in 0.10 seconds
For $H = 7.00000e-01$ T, $7.73173463e-17$ Joules spent in 0.10 seconds
For $H = 1.05000e+00$ T, $1.54634693e-16$ Joules spent in 0.10 seconds
For $H = 1.40000e+00$ T, $2.57724491e-16$ Joules spent in 0.10 seconds
For $H = 1.75000e+00$ T, $3.86586735e-16$ Joules spent in 0.10 seconds
For $H = 2.10000e+00$ T, $1.44583437e-14$ Joules spent in 0.10 seconds
For $H = 2.45000e+00$ T, $3.08753940e-14$ Joules spent in 0.10 seconds
For $H = 2.80000e+00$ T, $3.10815736e-14$ Joules spent in 0.10 seconds
For $H = 3.15000e+00$ T, $3.13135257e-14$ Joules spent in 0.10 seconds
Total work performed: 1.086e-13 Joules
Power consumed: 1.086e-13 Watts

---- Simulation Run # 8 ----

For H = 0.00000e+00 T, 0.00000000e+00 Joules spent in 0.10 seconds
For H = 3.50000e-01 T, 2.57724486e-17 Joules spent in 0.10 seconds
For H = 7.00000e-01 T, 7.73173463e-17 Joules spent in 0.10 seconds
For H = 1.05000e+00 T, 1.54634693e-16 Joules spent in 0.10 seconds
For H = 1.40000e+00 T, 2.57724491e-16 Joules spent in 0.10 seconds
For H = 1.75000e+00 T, 3.86586735e-16 Joules spent in 0.10 seconds
For H = 2.10000e+00 T, 1.44583437e-14 Joules spent in 0.10 seconds
For H = 2.45000e+00 T, 3.08753940e-14 Joules spent in 0.10 seconds
For H = 2.80000e+00 T, 3.10815736e-14 Joules spent in 0.10 seconds
For H = 3.15000e+00 T, 3.13135257e-14 Joules spent in 0.10 seconds

Total work performed: 1.086e-13 Joules
Power consumed: 1.086e-13 Watts

---- Simulation Run # 9 ----

For H = 0.00000e+00 T, 0.00000000e+00 Joules spent in 0.10 seconds
For H = 3.50000e-01 T, 2.57724486e-17 Joules spent in 0.10 seconds
For H = 7.00000e-01 T, 7.73173463e-17 Joules spent in 0.10 seconds
For H = 1.05000e+00 T, 1.54634693e-16 Joules spent in 0.10 seconds
For H = 1.40000e+00 T, 2.57724491e-16 Joules spent in 0.10 seconds
For H = 1.75000e+00 T, 3.86586735e-16 Joules spent in 0.10 seconds
For H = 2.10000e+00 T, 1.44583437e-14 Joules spent in 0.10 seconds
For H = 2.45000e+00 T, 3.08753940e-14 Joules spent in 0.10 seconds
For H = 2.80000e+00 T, 3.10815736e-14 Joules spent in 0.10 seconds
For H = 3.15000e+00 T, 3.13135257e-14 Joules spent in 0.10 seconds

Total work performed: 1.086e-13 Joules
Power consumed: 1.086e-13 Watts
---- Simulation Run #10 ----

For $H = 0.00000e+00$ T, $0.00000000e+00$ Joules spent in 0.10 seconds
For $H = 3.50000e-01$ T, $2.57724486e-17$ Joules spent in 0.10 seconds
For $H = 7.00000e-01$ T, $7.73173463e-17$ Joules spent in 0.10 seconds
For $H = 1.05000e+00$ T, $1.54634693e-16$ Joules spent in 0.10 seconds
For $H = 1.40000e+00$ T, $2.57724491e-16$ Joules spent in 0.10 seconds
For $H = 1.75000e+00$ T, $3.86586735e-16$ Joules spent in 0.10 seconds
For $H = 2.10000e+00$ T, $1.44583437e-14$ Joules spent in 0.10 seconds
For $H = 2.45000e+00$ T, $3.08753940e-14$ Joules spent in 0.10 seconds
For $H = 2.80000e+00$ T, $3.10815736e-14$ Joules spent in 0.10 seconds
For $H = 3.15000e+00$ T, $3.13135257e-14$ Joules spent in 0.10 seconds

Total work performed: $1.086e-13$ Joules
Power consumed: $1.086e-13$ Watts