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CRADA Final Report
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NUMERICAL MODELING OF GIANT MAGNETORESISTANCE EFFECT FOR APPLICATION TO MAGNETIC DATA STORAGE

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Abstract

The giant magnetoresistance (GMR) effect is a change in the electrical resistance of a magnetically inhomogeneous material that occurs when an applied magnetic field aligns the magnetic moments in different regions of the material. GMR allows the development of very small and sensitive devices for detecting and measuring magnetic fields. Such devices have many applications including the sensing of data on magnetic disk drives and in magnetic random access memory cells. This Cooperative Research and Development Agreement between Lockheed Martin Energy Systems and IBM Almaden Research Center was a joint experimental and theoretical program to obtain a better understanding of the giant magnetoresistance effect with the goal of optimizing the effect for application to magnetic data storage devices. The CRADA was successful in developing a detailed microscopic understanding of GMR and in pointing out strategies for increasing the GMR effect.

CRADA Objectives

The objective of this CRADA was to use advanced computing techniques and architectures to model the giant magnetoresistance (GMR) effect in layered transition metal alloy systems for the purpose of understanding and optimizing this effect for application to magnetic data storage devices. The ultimate goals of the project were:

(1) to assist our industrial partner in maintaining US competitiveness in the highly competitive international market for magnetic storage devices,
(2) to develop our understanding of magnetic multilayer systems so that they may be used to build static radiation and electromagnetic pulse resistant magnetic memory devices suitable for DP applications, and
(3) to advance the art of parallel processing at DP laboratories by applying novel computer architectures to frontier problems in materials modeling.

Fulfillment of CRADA objectives

The objective and goals of the CRADA were achieved. Advanced computing techniques and architectures were used to model the giant magnetoresistance in layered transition metal alloy systems. This work has significantly increased our understanding of GMR and has suggested novel ways that the effect can be optimized for application to magnetic data storage and for other applications. This better understanding of GMR will help our industrial partner in the highly competitive international market for magnetic storage devices.

The improved model and understanding of GMR may also be helpful in the design and fabrication of non-volatile radiation and electromagnetic pulse resistant magnetic memory devices suitable for DP applications. The modeling of GMR specifically for this application will continue with follow-on support from the Defense Advanced Research Projects Agency (DARPA).

This work contributed to the advancement of the art of parallel processing at DP laboratories. The novel advances that were made in areas of portability, thread independence, and load balancing were disseminated through our project partners at Livermore and Sandia to other DP laboratories.

Benefits to Defense Programs

Defense programs need magnetic memory devices capable of withstanding ionizing radiation and electromagnetic pulses. One such device, the MRAM or magnetic random access memory, stores information in the orientation of the magnetization in tiny cells of a magnetic film. The most important factor limiting the speed and information storage density of these devices is the sensitivity of the technique for non-destructively reading the data. Currently the anisotropic magneto-resistance effect is used to sense the state of the memory cell. GMR, however, offers a much more sensitive technique for reading the data. It is estimated that an increase of a factor of two in the size of the GMR effect would provide sufficient sensitivity for MRAM to compete successfully with semiconductor dynamic random access memory in terms of speed and density. Our models of GMR have suggested strategies for achieving this goal. Pursuit of this goal continues with funding from DARPA.

Defense programs also benefited from the development of techniques for parallel processing and their dissemination to DP laboratories. This CRADA was part of a three laboratory project. In addition to the Lockheed Martin Energy Systems component, important roles were played by colleagues at Livermore and Sandia. Our Livermore colleague, in particular, learned much about parallel processing during his visits to Oak Ridge. Conversely, important contributions to this work were provided by the other laboratories.

Numerical Modeling of GMR

Giant Magnetoresistance (GMR) is a change (usually a decrease) in the electrical resistivity that occurs in a magnetically inhomogeneous material when an applied magnetic field brings the magnetic moments in different regions into alignment. It is called "giant" magnetoresistance because it can be much larger than other forms of magnetoresistance in appropriately designed structures. GMR has caused much excitement because of its potential use in devices that sense magnetic fields.

GMR has been observed in several geometries, but the geometry most interesting for applications consists of thin films made up of ultra thin ferromagnetic layers separated by ultra thin non-magnetic "spacer" layers. The resistivity in the plane of the film is lower when the magnetic moments in the different ferromagnetic layers are aligned by the application of a magnetic field.

Field sensing devices based on GMR have many important applications. One area of critical importance is in read sensors for disk drives. The continuing rapid increase in the information storage density of computer disk drives requires that the magnetic regions which store the data become smaller and smaller. Because less magnetic material is used to represent each bit of information, the magnetic field associated with this bit which is used to sense whether the bit is a zero or a one also gets smaller and much more difficult to detect. GMR will be important for next generation disk drives because it is an ideal technique for sensing the tiny fields associated with the data stored on a high density disk drive.

A second potential application of GMR which has obvious significance to DP is the use of GMR in magnetic random access memory (MRAM) devices. These devices have the advantages that they have no moving parts, they are immune to ionizing radiation and electromagnetic pulse, and that they retain their information in the absence of power. In MRAM devices information is stored in terms of the orientation of the magnetization in tiny cells in a thin magnetic film. In order to achieve high speeds and densities, it is necessary to have an extremely small and sensitive detector of magnetic fields. The GMR effect can be used to sense the direction of magnetization in the cells allowing increases in speed and density that may make GMR based MRAM competitive with semiconductor dynamic random access memory devices in commercial markets.

GMR has obvious potential for application in detection and surveillance devices. There is also expected to be a large market related to non-contact position and motion sensing. Because GMR sensors can be made extremely small and can be integrated onto integrated circuits, they may become common parts on machinery and mechanical devices.

In order to achieve the potential benefits of GMR we desired to understand the phenomenon in greater detail and, in particular, to identify the optimal structures and materials for GMR. In order to accomplish this task we developed and extended the Layer Korringa Kohn Rostoker (LKKR) technique for calculating electronic structure. The LKKR code that we used was written by Professor James M. MacLaren of Tulane University and his collaborators. The LKKR code was particularly appropriate for treating GMR because a typical GMR system consists of extremely thin alternating layers of magnetic and non-magnetic material. The first part of the project consisted of the extension of the LKKR code to treat conductivity, and the porting of the code to parallel supercomputers.

Our first calculation of the conductivity with the LKKR used a simple semi-classical approach which could be applied to periodic magnetic multilayers [1]. With this approach we were able to show qualitatively how the GMR effect can arise from the phenomenon of "potential matching". In a metal, current is carried in parallel by two spin channels, majority and minority. Potential matching can occur in magnetic systems when the exchange interaction shifts the potentials of atoms of one type and spin so that they match the potentials atoms of another type. Examples of this are Fe, Co, Ni, and Cu which match in the majority channel and Fe and Cr which match in the minority channel. The low resistivity in the matching channel leads to a "short circuit" effect and gives a higher conductivity when the moments are aligned. The matching almost always occurs in the same spin channel, although, in principle different channels on different atoms could match. This explanation of the origin of GMR together with calculations showing potential matching was described in a publication[2].

We desired more than a qualitative understanding of GMR however, and we needed the ability to understand and model GMR in non-periodic structures of the type that IBM was investigating for application to magnetic recording. For these reasons we developed a much more general and quantitative technique based on the Kubo-Greenwood approach to electron transport. We developed the formal theory and described it in a publication[3].

One of the important issues concerning GMR is the nature of the interfaces between the magnetic and non-magnetic layers. Together with our IBM colleagues we performed a joint theoretical and experimental study of the likely magnetic structure of the interface between Ni and Cu and between permalloy ($Ni_{.8}Fe_{.2}$) and Cu. We found that the Ni atoms tended to lose their moments and that the Fe atoms tended to retain their moments but these moments were likely to be easily disoriented. Our theoretical results agreed with the experimental results of our IBM colleagues who observed a loss of ferromagnetic moment for thin deposited films. These results were presented in a joint publication[4].

In order to compare our anticipated results which utilized massively parallel computers and advanced theoretical techniques to calculate the GMR for realistic models with the work of others who had applied various approaches to the free electron model, we decided to study this simple model. We found that we could solve this model exactly for magnetic multilayers. We compared this exact solution to others in the literature and found that the then most popular treatment was incorrect, however a semi-classical approach that our IBM colleagues were using worked rather well[5,6].

During this period we were working to port the LKKR code to the massively parallel computers and to extend the code to treat transport. We successfully ported the code for three quite different architectures, the shared memory architecture of the Kendall Square Research computer, the heterogeneous loosely coupled message passing architecture appropriate to workstation clusters or to the IBM-SP2 and to the planar net topology message passing architecture of the Intel Paragons.

The successful porting and development allowed us to calculate the non-local layer dependent conductivity of non-periodic systems such as the spin-valves that were being developed at IBM Almaden Research Center. The results gave a clear and quantitative picture of GMR[7,8]. One important contribution resulted from electrons that were accelerated in one ferromagnetic layer , traveled across the intervening spacer layer and contributed to the current in the second ferromagnetic layer. This effect was seen most vividly in calculations for which the scattering rate for the electrons was relatively high.

For systems in which the scattering rate for the electrons was lower, an additional effect was observed in the calculations for copper-cobalt spin valves. There can be a large contribution to the GMR that arises from a wave guide effect[9 10]. Some of the electrons in the copper spacer layer that have a relatively large momentum parallel to the interface will be totally internally reflected at the interface. Surprisingly, for reasons having to do with the electronic structure, this happens only for the majority electrons. Thus this effect adds to the effect of the preceding paragraph. This guide wave effect requires atomically smooth interfaces, so it is not yet clear if it is contributing to the GMR in samples that have been produced to date. It appears, however, to offer an excellent opportunity for increasing GMR.

Most calculations of GMR assume that the magnetic moments on adjacent ferromagnetic layers are aligned either parallel or anti-parallel. We generalized our codes so that they could be used to calculate the conductivity for an arbitrary angle between the directions of the moments in the different layers[11].

Recently, a very large ("colossal") magnetoresistance effect has been observed in certain manganate compounds. Because this effect might be a commercial rival to GMR at some future date we investigated the electronic structure of these materials. We found that their strange behavior may be related to their peculiar electronic structure which we found to be metallic for majority spin electrons and semiconducting for minority spin electrons[12].

Although commercial applications of GMR usually employ a "Current In the Plane" (CIP) geometry, there is much interest in the "Current Perpendicular to the Plane" (CPP) geometry. We spent a modest amount of effort in developing the theory for this geometry[13,14].

It is clear that understanding and controlling the physical, chemical, and magnetic structure of interfaces will be one of the keys to improving GMR. Recently we have investigated the magnetic structure of permalloy copper interfaces. We find that interdiffusion of copper and permalloy both reduces the nickel moment and lowers the strength of the exchange coupling so that the iron atoms near the interface may lose their alignment with the ferromagnetic layer [15].

We have written a popular account of GMR, its applications, and our work on it[16]. A copy of this account is attached.

Inventions

No inventions were made or reported under this CRADA.

Commercialization Possibilities

It is our assessment that the introduction of GMR read sensors into the commercial disk drive market will occur when current technology is unable to meet the sensitivity demands required by the exponential increase in drive density. This is projected to occur sometime during the next two to three years. Considering the 60% annual compounded growth rate in disk drive areal densities, significant improvements in GMR spin-valve sensitivity, possibly taking advantage of the strategies developed by this CRADA may be required within five to ten years.

GMR-based magnetic random access memory technology is much less mature. It appears that currently producible GMR spin valves may support a niche market for MRAM for non-volatile and radiation resistant applications, but significant penetration of the market now occupied by semiconductor DRAM will require a significant improvement in GMR. We are currently working with DARPA to improve the GMR for these applications.

Plans for Future Collaboration

Work has been nearly completed for a paper describing very large computer models of IBM spin valves. The results of this work indicate a surprisingly strong spin dependence of the bulk scattering rate in cobalt. We plan continue to work on this project together using funding from other sources.

Conclusions

Two basic mechanisms for GMR in the current in the plane geometry were identified. One is a non-local effect in which electrons are accelerated by the applied field in one ferromagnetic layer, travel through the spacer layer to another ferromagnetic layer where they contribute to the current. The other mechanism is a wave guide effect that can operate to significantly enhance GMR in some systems with smooth interfaces. Comparison between theory and experiments performed under this CRADA indicate that there may be a large asymmetry between the scattering rates of majority and minority electrons in elemental ferromagnets such as Co.

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