Journal of Science: Advanced Materials and Devices 1 (2016) 31–44

Contents lists available at ScienceDirect

Journal of Science: Advanced Materials and Devices

journal homepage: www.elsevier.com/locate/jsamd

Review article

Theoretical methods for understanding advanced magnetic materials: The case of frustrated thin films

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ARTICLE INFO

Article history:
Received 3 April 2016
Accepted 16 April 2016
Available online 22 April 2016

Keywords:
Theory of magnetism
Magnetic thin films
Surface spin waves
Frustrated spin systems
Magnetic materials
Phase transition
Monte Carlo simulation
Statistical physics

ABSTRACT

Materials science has been intensively developed during the last 30 years. This is due, on the one hand, to an increasing demand of new materials for new applications and, on the other hand, to technological progress which allows for the synthesis of materials of desired characteristics and to investigate their properties with sophisticated experimental apparatus. Among these advanced materials, magnetic materials at nanometric scale such as ultra thin films or ultra fine aggregates are no doubt among the most important for electronic devices.

In this review, we show advanced theoretical methods and solved examples that help understand microscopic mechanisms leading to experimental observations in magnetic thin films. Attention is paid to the case of magnetically frustrated systems in which two or more magnetic interactions are present and competing. The interplay between spin frustration and surface effects is the origin of spectacular phenomena which often occur at boundaries of phases with different symmetries: reentrance, disorder lines, coexistence of order and disorder at equilibrium. These phenomena are shown and explained using of some exact methods, the Green's function and Monte Carlo simulation. We show in particular how to calculate surface spin-wave modes, surface magnetization, surface reorientation transition and spin transport.

1. Introduction

Material science has made a rapid and spectacular progress during the last 30 years, thanks to the advance of experimental investigation methods and a strong desire of scientific community to search for new and high-performance materials for new applications. In parallel to this intensive development, many efforts have been devoted to understanding theoretically microscopic mechanisms at the origin of the properties of new materials. Each kind of material needs specific theoretical methods in spite of the fact that there is a large number of common basic principles that govern main properties of each material family.

In this paper, we confine our attention to the case of magnetic thin films. We would like to show basic physical principles that help us understand their general properties. The main purpose of the paper is not to present technical details of each of them, but rather to show what can be understood using each of them. For technical details of a particular method, the reader is referred to numerous references given in the paper. For demonstration purpose, we shall use magnetically frustrated thin films throughout the paper. These systems combine two difficult subjects: frustrated spin systems and surface physics. Frustrated spin systems have been subject of intensive studies during the last 30 years [1]. Thanks to these efforts many points have been well understood in spite of the fact that there remains a large number of issues which are in debate. As seen below, frustrated spin systems contain many exotic properties such as high ground-state degeneracy, new symmetries, successive phase transitions, reentrant phase and disorder lines. Frustrated spin systems serve as ideal testing grounds for theories and approximations. On the other hand, during the same period surface physics has also been widely investigated both experimentally and theoretically. Thanks to technological progress, films and surfaces with desired properties could be fabricated and characterized with precision. As a consequence, one has seen over the years numerous technological applications of thin films, coupled thin films and super-lattices, in various domains such as magnetic sensors, magnetic recording and data storage. One of the spectacular effects is

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Peer review under responsibility of Vietnam National University, Hanoi.

http://dx.doi.org/10.1016/j.jsamd.2016.04.009

the colossal magnetoresistance [2,3] which yields very interesting transport properties. The search for new effects with new mechanisms in other kinds of materials continues intensively nowadays as never before.

Section 2 is devoted to the presentation of the main theoretical background and concepts to understand frustrated spin systems and surface effects in magnetic materials. Needless to say, one cannot cover all recent developments in magnetic materials but an effort is made to outline the most important ones in our point of view. Section 3 is devoted to a few examples to illustrate striking effects due to the frustration and to the presence of a surface. Concluding remarks are given in Section 4.

2. Background

2.1. Theory of phase transition

Many materials exhibit a phase transition. There are several kinds of transition, each transition is driven by the change of a physical parameter such as pressure, applied field, temperature (T), … The most popular and most studied transition is no doubt the one corresponding to the passage from a disordered phase to an ordered phase at the so-called magnetic ordering temperature or Curie temperature T_c. The transition is accompanied by a symmetry breaking. In general when the symmetry of one phase is a subgroup of the other phase the transition is continuous, namely the first derivatives of the free energy such as internal energy and magnetization are continuous functions of T. The second derivatives such as specific heat and susceptibility, on the other hand, diverge at T_c. The correlation length is infinite at T_c. When the symmetry of one phase is not a symmetry subgroup of the other, the transition is in general of first order: the first derivatives of the free energy are discontinuous at T_c. At the transition, the correlation length is finite and often there is a coexistence of the two phases. For continuous transitions, also called second-order transition, the nature of the transition is characterized by a set of critical exponents which defines its “universality class”. Transitions in different systems may belong to the same universality class.

Why is the study of a phase transition interesting? As the theory shows it, the characteristics of a transition are intimately connected to microscopic interactions between particles in the system.

The theory of phase transitions and critical phenomena has been intensively developed by Landau and co-workers since the 50's in the framework of the mean-field theory. Microscopic concepts have been introduced only in the early 70's with the renormalization group [4–6]. We have since then a clear picture of the transition mechanism and a clear identification of principal ingredients which determine the nature of the phase transition. In fact, there is a small number of them such as the space dimension, the nature of interaction and the symmetry of the order parameter.

2.2. Frustrated spin systems

A spin is said ”frustrated” when it cannot fully satisfy all the interactions with its neighbors. Let us take a triangle with an antiferromagnetic interaction $J(<0)$ between two sites: we see that we cannot arrange three Ising spins (± 1) to satisfy all three bonds. Among them, one spin satisfies one neighbor but not the other. It is frustrated. Note that any of the three spins can be in this situation. There are thus three equivalent configurations and three reverse configurations, making 6 the number of “degenerate states”. If we put XY spins on such a triangle, the configuration with a minimum energy is the so-called “120-degree structure” where the two neighboring spins make a 120° angle. In this case, each interaction bond has an energy equal to $|J|\cos(2\pi/3) = -|J|/2$, namely half of the full interaction: the frustration is equally shared by three spins, unlike the Ising case. Note that if we go from one spin to the neighboring spin in the trigonometric sense we can choose $\cos(2\pi/3)$ or $-\cos(2\pi/3)$ for the turn angle: there is thus a two-fold degeneracy in the XY spin case. The left and right turn angles are called left and right chiralities. In an antiferromagnetic triangular lattice, one can construct the spin configuration from triangle to triangle. The frustration in lattices with triangular plaquettes as unit such as in face-centered cubic and hexagonal-close-packed lattices is called “geometry frustration”. Another category of frustration is when there is a competition between different kinds of incompatible interactions which results in a situation where no interaction is fully satisfied. We take for example a square with three ferromagnetic bonds $J(>0)$ and one antiferromagnetic bond $-J$, we see that we cannot ”fully” satisfy all bonds with Ising or XY spins put on the corners.

Frustrated spin systems are therefore very unstable systems with often very high ground-state degeneracy. In addition, novel symmetries can be induced such as the two-fold chirality seen above. Breaking this symmetry results in an Ising-like transition in a system of XY spins [7,8]. As will be seen in some examples below, the frustration is the origin of many spectacular effects such as non collinear ground-state configurations, coexistence of order and disorder, reentrance, disorder lines, multiple phase transitions, etc.

2.3. Surface magnetism

In thin films the lateral sizes are supposed to be infinite while the thickness is composed of a few dozens of atomic layers. Spins at the two surfaces of a film lack a number of neighbors and as a consequence surfaces have physical properties different from the bulk. Of course, the difference is more pronounced if, in addition to the lack of neighbors, there are deviations of bulk parameters such as exchange interaction, spin-orbit coupling and magnetic anisotropy, and the presence of surface defects and impurities. Such changes at the surface can lead to surface phase transition separated from the bulk transition, and surface reconstruction, namely change in lattice structure, lattice constant [9], magnetic ordering, … at the surface [10–12].

Thin films of different materials, different geometries, different lattice structures, different thicknesses … when coupled give surprising results such as colossal magnetoresistance [2,3]. Microscopic mechanisms leading to these striking effects are multiple. Investigations on new artificial architectures for new applications are more and more intensive today. In the following section, we will give some basic microscopic mechanisms based on elementary excitations due to the film surface which allows for understanding macroscopic behaviors of physical quantities such as surface magnetization, surface phase transition and transition temperature.

2.4. Methods

To study properties of materials one uses various theories in condensed matter physics constructed from quantum mechanics and statistical physics [13,14]. Depending on the purpose of the investigation, we can choose many standard methods at hand (see details in Refs. [15,16]):

(i) For a quick obtention of a phase diagram in the space of physical parameters such as temperature, interaction strengths, … one can use a mean-field theory if the system is simple with no frustration, no disorder, … Results are reasonable in three dimensions, though critical properties cannot be correctly obtained