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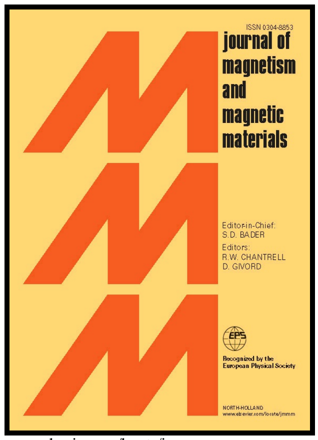

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Self-Consistent Model of a Solid for the Description of Lattice and Magnetic Properties

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Abstract

In the paper a self-consistent theoretical description of the lattice and magnetic properties of a model system with magnetoelastic interaction is presented. The dependence of magnetic exchange integrals on the distance between interacting spins is assumed, which couples the magnetic and the lattice subsystem. The framework is based on summation of the Gibbs free energies for the lattice subsystem and magnetic subsystem. On the basis of minimization principle for the Gibbs energy, a set of equations of state for the system is derived. These equations of state combine the parameters describing the elastic properties (relative volume deformation) and the magnetic properties (magnetization changes).

The formalism is extensively illustrated with the numerical calculations performed for a system of ferromagnetically coupled spins $S=1/2$ localized at the sites of simple cubic lattice. In particular, the significant influence of the magnetic subsystem on the elastic properties is demonstrated. It manifests itself in significant modification of such quantities as the relative volume deformation, thermal expansion coefficient or isothermal compressibility, in particular, in the vicinity of the magnetic phase transition. On the other hand, the influence of lattice subsystem on the magnetic one is also evident. It takes, for example, the form of dependence of the critical (Curie) temperature and magnetization itself on the external pressure, which is thoroughly investigated.

Keywords: magnetoelastic coupling, ferromagnetism, thermodynamics of magnets, Curie temperature, magnetization, thermal expansion, isothermal compressibility

1. Introduction

Thermodynamics of magnetic solids is a subject of interest of solid state physicists since many years [1]. From the point of view of methodology, some analogy to systems described by the volume and pressure is exploited, namely the thermodynamic magnetic variables: magnetic field h and magnetization m correspond to the respective mechanical variables - pressure p and volume V, considered at some temperature T (see for example Ref. [2]). Therefore, the magnetic equation of state involves three variables: h, m and T.

In majority of cases both the subsystems of solid state (magnetic and lattice one) are described separately, with no coupling between them. In such situation, the lattice-related properties of the magnetic solid are considered as fully independent on magnetic properties, leading to another equation of state interrelating p, V and T. However, such approach neglects the magnetoelastic interactions which occur between these subsystems. The simplest source of such coupling is the fact that the magnetic exchange integral between magnetic moments depends on their mutual distance, thus is a volume-dependent quantity. The magnetoelastic interactions are basis for such effects as the magnetostriction and piezomagnetism, which are important from the point of view of possible applications. They are also responsible for sensitivity of any magnetic properties (for example, the critical temperature) to external pressure.

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