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Fabry–Perot magnonic ballistic coherent transport across ultrathin ferromagnetic lamellar bcc Ni nanostructures between Fe leads

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ABSTRACT

We propose thermodynamically stable systems of ultrathin lamellar bcc Ni nanostructures between bcc Fe leads, −Fe[Ni(n)]Fe−, based on the available literature for bcc Ni overlayers on Fe(001) surfaces, and establish the necessary criteria for their structural and ferromagnetic order, for thicknesses $n \leq 6$ bcc Ni monatomic layers. The system is globally ferromagnetic. A theoretical model is presented to investigate and understand the ballistic coherent scattering of Fe spin-waves, incident from the leads, at the ferromagnetic bcc Ni nanostructure. The Ni−Ni and Ni−Fe exchange are computed using the Ising effective field theory (EFT), and the magnetic ground state of the system is constructed in the Heisenberg representation. We compute the spin-wave eigenmodes localized on the bcc Ni nanostructure, using the phase field matching theory (PFMT), illustrating the effects of symmetry breaking on the confinement of localized spin excitations. The reflection and transmission scattering properties of spin-waves incident from the Fe leads, across the embedded Ni nanostructures are investigated within the framework of the same PFMT methodology. A highly refined Fabry–Perot magnonic ballistic coherent transmission spectra is observed for these −Fe[Ni(n)]Fe− systems.

1. Introduction

Magnonics is a growing research field that proposes to use spin-waves in magnetic materials as the elementary excitation for the transport and processing of information. It deals primarily with the study of the excitation, manipulation and detection of spin-waves in magnetic materials. An advantage of magnonics over electronics is the fact that for electronic devices there are natural limits for their functioning due to the Joule heating effect. Magnetic elements and composite nanomaterials can also be insulators which is a supplementary advantage. This has stimulated the tremendous research effort in recent years to understand and manipulate the properties of magnetic materials with the objective to enhance the performance of physical devices in magnonics [1–3] and in magnon spintronics [4].

The current experimental research in magnonics is mostly concentrated on the study of spin-waves at the micrometer scale; see for example references [5,6]. Further, the research and development of logic circuits witness significant developments for the applications of spin-wave magnonics on the micrometer scale [7–9], including the use of insulating magnetic nanomaterials [9]. Though there are recent attempts to excite spin-waves at shorter wavelengths of the order of a few hundred nanometers [10], nevertheless, despite the compelling research dedicated to the emerging field of magnonics, the experimental work for the emission, manipulation and detection of spin-waves with wavelengths $\lambda \sim$ a few nm, at the lower end of the nano scale, is limited and continues to be a key challenge.

The technical development of magnetic devices for the lower end of the nano scale involves on one hand the analysis and development of novel and appropriate nanomaterials. Moreover, nanostructures of such magnetic materials, with specifically required properties, also need to be developed for the corresponding miniaturized devices of information processing and storage.

The magnetic 3d transition metals (TM), in particular Fe, Co, and Ni, which have respectively bcc, hcp, and fcc crystalline lattices, are regarded as promising magnetic nanomaterials. For example, the use of these TMs to prepare bimetallic multilayers has been a successful approach to modulate the magnetic properties of such systems [11–14]. One can expect hence that magnetic nanostructures, such as nanojunctions in magnonic circuits, of ultrathin films of TMs, or of TM alloys, can be of significant interest for the magnonics technology at the nano scale. It is reasonable hence to suppose that such technologies will require the exploitation of ultrathin films consisting of a few

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monatomic layers of these nanomaterials. The investigation of the magnonic ballistic transport across homogeneous TM nanostructures has been initiated recently to that end, in particular to identify the magnetic ground states of Fe–Co alloy ultrathin nanojunctions [15], and to compute the magnonic ballistic coherent transport across them [16]. The ballistic magnonic transport investigates, in particular, the coherent transport of spin waves across nanostructures whose typical dimensions are significantly smaller than the spinwave wavelength. This approach is outside damping effects, and is increasingly relevant in view of the objectives of the development of new nanotechnologies.

The purpose of the present work is to compute the magnonic coherent ballistic transport across an ultrathin lamellar bcc Ni nanostructure between Fe leads, −Fe[Ni(n)]Fe−, for different thicknesses of n = 2–6 Ni monatomic layers. The interest in such systems stems from the potential technological application of its proposed nanostructures. By selecting the appropriate thickness of the embedded Ni nanostructure, and if possible, by electrically and magnetically controlling its fundamental parameters, it is possible to fully control the transmission of specific magnonic frequencies, and conversely the suppression of parasitic magnonic signals in magnonic and spintronic nano-devices.

To carry out this kind of computation implies the need to fully understand the structural and magnetic properties of the bcc Ni phase of the lamellar Ni nanostructure between the Fe leads, in particular the characteristics of its magnetic order, and the nature of the exchange between the Ni atoms in the nanostructure itself, as well as the exchange between Ni and Fe atoms at the two interfaces of the system.

Fe, Co, and Ni are the three principal magnetic TMs, and have been the subject of intensive investigations in recent years to see whether their crystalline phases can be modified and under what conditions, and how their magnetic properties may be modified by these phase changes. These investigations increase our understanding of the origin of magnetism at the nano scale, and of the interplay between exchange coupling and interatomic distances, which could be in principle controlled by stabilized growth modes. They may also lead to innovative magnetic nanostructures with desired properties for physical devices in magnonics and spintronics.

In particular, the bcc phase of Ni has been investigated intensively in recent years [17–29]. Ni presents a thermodynamically stable bcc phase over a few monatomic layers, under certain conditions, in particular when in contact with Fe surfaces. We have hence a minimum reasonable understanding of this crystalline phase of ultrathin lamellar bcc Ni between Fe surfaces, and of the characteristics of its magnetic order and properties. Details will be presented and discussed, in Section 2 of the present paper.

The model computations for the spin dynamics, spin-wave scattering, and magnonic ballistic coherent transmission, at the −Fe[Ni(n)]Fe− system under study, will be developed by using the Heisenberg Hamiltonian representation for the magnetic ground state of the system, and employing the phase field matching theory (PFMT) [30–32]. This method is based on the appropriate phase matching of the magnonic states of the leads to the dynamics of the spin states at the nanojunction. The PFMT method, equivalent to the non-equilibrium Greens function method but more transparent, was developed as an imperative tool [30–37] to treat the localization and scattering problems of elementary excitations, such as magnons, phonons, and electrons, at nanostructures and molecular junctions. The PFMT yields the Landauer–Büttiker [38,39], reflection and transmission probabilities for the spin-waves incident from the bcc Fe leads onto the bcc Ni lamellar nanojunction system.

This paper is organized as follows. In Section 2 we analyze the relevant literature as regards the bcc Ni overlayers on Fe(001) surfaces, to ascertain the size and stability of potentially accessible bcc Ni nanostructures between Fe leads, in the −Fe[Ni(n)]Fe− systems; in particular, we establish the necessary and sufficient criteria for its structural and magnetic order, for different thicknesses $n \leq 6$ of bcc Ni monatomic layers. The absence of experimental and first principle calculations for the Ni–Ni and Ni–Fe exchange, motivates the use of Ising effective field theory (EFT) method to calculate this magnetic exchange, and the magnetic ground state of the system is constructed in the Heisenberg representation. In Section 3 the method used to investigate the spin dynamics is presented, and is developed, to derive the spin-waves in the Fe leads, and in particular to compute the spin-wave eigenmodes localized on the bcc Ni, using the phase field matching theory (PFMT). This illustrates the effects of symmetry breaking on the confinement of localized spin excitations at the lamellar nanostructure. In Section 4, the ballistic reflection and transmission scattering properties of the embedded Ni nanostructure are investigated within the framework of the same PFMT methodology. The magnonic ballistic reflection and transmission scattering cross sections of the system are determined and analysed. In Section 5 we present the results of our numerical applications of the theoretical model for the magnonic ballistic transport in three different −Fe[Ni(n)]Fe− systems, across the ultrathin lamellar bcc Ni nanostructures between Fe leads, and discuss them. In particular, a highly refined Fabry–Perot magnonic ballistic coherent transmission spectra is observed for these systems.

2. Magnetic order of −Fe [Ni (n)] Fe− nanostructure

In a recent work by Tian et al. [17], the body centered cubic Ni has been prepared experimentally as an ultrathin overlayer on GaAs(100) at low temperatures, and the magnetic properties of the system were measured. The interest in the Ni bcc phase goes back to the theoretical work of Moruzzi et al. [18], which shed light initially on the relationship between the magnetism of the bcc Ni phase and its lattice structure. More recently, Guo et al. [19], have computed by ab initio techniques the magnetic moment of the bcc Ni, and shown that it is ferromagnetic at a lattice constant of 0.280 nm. Parallel to the theoretical works, the experimental research of Heinrich et al. [20] and Wang et al. [21], have succeeded to prepare ultrathin layers of bcc Ni on the Fe(001) surface, by means of molecular beam epitaxy, and showed that the ferromagnetic bcc Ni phase exists only for a limited thickness of 3 to 4 monatomic layers. Further, Heinrich et al. [22], concluded that the bcc Ni monatomic layers have no effect on the magnetic properties of the Fe layers, and Bland et al. [23], indicated from their measurements of the high quality epitaxial bcc Ni overlayer, that the magnetic moment per Ni atom is of the order of $0.55\mu_B$, and that there is ferromagnetic coupling between the Fe and Ni layer magnetizations. Using a value of $0.69\mu_B$ per Ni atom, calculated by Lee et al. [24] using the total-energy full-potential linearized augmented plane-wave method, Celinski et al. [25] deduced from their proper experimental measurements values for the magnetic moments per Fe atom on adjacent Fe layers. Hashibon et al. [26], carried out ab initio calculations using density functional theory (DFT) in the local density approximation (LDA), and confirmed the stable bcc Ni phase for 3 to 4 monatomic layers on Fe(001). Brooks et al., [27], investigated the magnetic structure of the ultrathin overlayer of bcc Ni on Fe(001), grown using spin-polarized angle-resolved photoemission, and deduced a value of $0.40\mu_B$ for the magnetic moment per Ni atom, and an experimental value for the Curie temperature of the Ni overlayer greater than 300 K. In reference [17], the Curie temperature for such an ultrathin overlayer on a GaAs substrate is given as 456 K. Furthermore, despite an anomalous in-plane anisotropy, attested for the bcc Ni ultrathin overlayer on Fe(001) surface, it is shown theoretically [24], and experimentally [22,23,28] that there is strong hybridization for the magnetic coupling at the Fe–Ni interface. This is also confirmed by Mirbt et al. [29], who computed the magnetic profile in the bcc Fe(001) surface when covered by one or two monatomic layers of 3d transition metals, including Ni, and explained their calculated trends in terms of the hybridization between the 3d states of the overlayer and the Fe substrate. This implies that the experimentally obtained magnetic properties of the bcc Ni ultrathin layer, on Fe(001), are not necessarily the intrinsic properties of the bcc Ni itself.