Computational modeling of sublattice magnetizations of nano-magnetic layered materials

Vinod Ashokan\textsuperscript{a*}, A. Khater\textsuperscript{b,c}, M. Abou Ghantous\textsuperscript{d}

\textsuperscript{a}Department of Physics, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar (Punjab) 144 011, India
\textsuperscript{b}Physics Department, Le Mans University, 72085 Le Mans, France
\textsuperscript{c}Department of Theoretical Physics, Institute of Physics, Jan Dlugosz University, Czestochowa, Poland
\textsuperscript{d}Science Department, American University of Technology, Fidar Campus, Halat, Lebanon

Abstract

In the present work, we model the salient magnetic properties of the alloy layered ferrimagnetic nanostructures \([\text{Co}_{1-c}\text{Gd}_c]\) between magnetically ordered cobalt leads. The effective field theory (EFT) Ising spin method is used to compute reliable \(J_{\text{Co-Co}}\) and \(J_{\text{Gd-Gd}}\) exchange values for the pure cobalt and gadolinium materials in comparison with experimental data. Using the combined EFT and mean field theory (MFT) spin methods, the sublattice magnetizations of the Co and Gd sites on the individual hcp basal planes of the layered nanostructures, are calculated and analyzed. The sublattice magnetizations, effective magnetic moments per site, and compensation characteristics on the individual hcp atomic planes of the embedded nanostructures are presented as a function of temperature and the thicknesses of the layered ferrimagnetic nanostructures, for different stable eutectic concentrations \(c \leq 0.5\). In the absence of first principles calculations for these basic physical variables for the layered nanostructures between cobalt leads, the combined EFT and MFT approach, and appropriate magnetic modeling of the well-defined interfaces of these systems, yield the only available information for them at present. These magnetic variables are necessary for spin dynamic computations, and for the ballistic magnon transport across embedded nanojunctions in magnonics. The model is general, and may applied directly to other composite magnetic elements and embedded nanostructures.

Keywords: effective field theory; mean field theory; sublattice magnetization; exchange constant; cobalt-gadolinium alloy; ferrimagnetic nanojunction.

1. Introduction

Significant progress has been made in recent years in preparing and analyzing the physical properties of layered magnetic nanostructures and magnetic junctions. These systems have a panoply of technological applications in the areas of spin wave magnonics \([1-4]\), and spin-based nanoelectronics \([5-7]\). However, the study of the rare earth-transition metal (R-T) intermetallic...
nanostructure and nanojunction systems in this area is still in its infancy. A fundamental and intriguing interest associated with such R-T systems is to understand the phenomena which may arise due to the decrease of their size when quantum mechanical effects come into play, and surfaces and interfaces become critical components at the atomic scale for the physics of embedded junctions.

Magnetic materials tailored on the nanoscale offer at present the perspective of magnetic field controlled devices in which magnons are themselves used to carry and process information that is coded via their phase or amplitude. The study of the excitation, detection and manipulation of magnons in magnetic nanomaterials, such as alloy layered nanostructures and nanojunctions, and the detection of short-wavelength SW at the nanoscale remain key challenges.

There is a considerable literature on the alloy structure and ferrimagnetic properties of R-T intermetallic magnetic multilayers [8–13], thanks to the progress in thin film preparation techniques of these materials. This makes possible the preparation of novel composite R-T material nanojunctions and alloy layered nanostructures with novel physical properties and promising applications in magnonic devices. In the present work we study in particular the cobalt-gadolinium R-T system; the Co transition metal and Gd rare earth are ferromagnetic with the interesting Curie temperatures of 119.4 and 25.2 meV. Nanojunctions prepared from cobalt-gadolinium alloys in diverse multilayer formats can present hence very useful properties for device applications at room temperature. In this respect, the fundamental properties of bulk Co$_{1-c}$Gd$_c$ alloy materials at alloy concentrations $c$, have been studied intensively in the past due to their ferrimagnetic structure and anticipated potential for technological applications as magnetic storage elements, sensors and magneto optical devices [14, 15].

A greater understanding of the magnetic properties of the Co/Gd multilayers [9, 11, 12] has also been achieved. It is observed in these systems that strong asymmetric spontaneous diffusion of Co into the Gd plane occurs, forming an amorphous alloy Co$_{1-c}$Gd$_c$ interface for different alloy concentrations $c$. The interdiffusion can be controlled experimentally [11, 12] to determine the stable eutectic compositions of the Co$_{1-c}$Gd$_c$, for $c \leq 0.5$, preserving the ferrimagnetic structure of the multilayer systems. The properties of multilayers presenting alloy interfaces, at least a few atomic planes thick for thin layering, depends sensitively on the degree of material interdiffusion [9, 11]. Such interdiffusion may profoundly influence the properties of the multilayers [8], since the individual planes present exchange couplings different at their interfaces from the bulk. This has also been emphasized previously by model calculations which show that atomic scale magnetic alloyed interfaces can significantly modify the magnetic properties of multilayers [16–18]. The preparation of alloy like and composition stable nanojunctions composed of Co and Gd between cobalt leads is hence possible in principle thanks to the controlled interdiffusion process.

It should be noted that there has been attempts in the past to model the magnetic properties of bulk and layered cobalt-gadolinium systems [13, 19, 20] using the MFT method. These model calculations have been performed by adjusting in general the MFT results to fit the experimental data, using the cobalt spin $S_{Co}$ as a fitting parameter. In some of the calculations where $S_{Co}$ is assigned its fundamental value, the overall fit for the magnetization versus temperature does not give good agreement with the experimental data. Furthermore, the asymmetric choice of nearest neighbor exchange constants for cobalt $J_{Co-Co}$ and gadolinium $J_{Gd-Gd}$ is made in these references to reduce the number of adjustable parameters, but without any fundamental justification. To add
to this complex situation, there is a wide array of experimental values for the cobalt $J_{Co-Co}$ and gadolinium $J_{Gd-Gd}$ exchange available in the literature from different types of measurements \cite{21}, which does not help to clarify the situation for advanced modeling.

In a previous work \cite{22}, we compute the scattering and ballistic transport of spin waves (SW) incident from cobalt leads, on ultrathin ferrimagnetic cobalt-gadolinium $[Co_{1-c}Gd_c]_\ell$ basic nanojunction systems between the leads. The nanojunction $[Co_{1-c}Gd_c]_\ell$ itself is a randomly disordered alloy of thickness $\ell$ hcp atomic planes between matching hcp planes of the Co leads, at known stable concentrations $c \leq 0.5$ for this alloy system. To be able to carry out these computations it was necessary to compute the sublattice magnetizations and magnetic exchange constants in this system \cite{23}.

In the present work we have modeled the sublattice magnetizations and magnetic exchange constants of the alloy layered nanostructures $[Co_{1-c}Gd_c]_\ell[Co]_\ell[Co_{1-c}Gd_c]_\ell'$ between cobalt leads, at known stable concentrations $c \leq 0.5$ for the alloy. These triple-nanostructure systems are more complex than the previously studied single-nanostructure systems \cite{23}. The present work is hence motivated by the objective to compute the salient magnetic properties of the triple-nanostructures for fundamental interest, and the scattering and ballistic transport of spin waves incident from cobalt leads on complex ferrimagnetic cobalt-gadolinium nanojunction systems \cite{24}. Such complex systems have as it turns out a richer and wider range of spin wave filtering properties. The complex embedded triple-nanostructures are denoted symbolically henceforth by $[\ell'\ell] \ell'\ell$ for convenience, corresponding to the alternating alloy and pure nanostructures. The basal hcp (0001) atomic planes of the $...Co[\ell'\ell']Co...$ nanojunction systems are normal to the direction of the c-axis itself considered to be along the direction of the leads.

The alloy layered $[\ell'\ell']$ nanostructures under consideration are ultrathin $\sim 1.5$ nm composite cobalt-gadolinium alloy systems sandwiched between semi-infinite cobalt leads, and are hence different from bulk alloy and multilayer systems \cite{8,13,20}. Also, to the authors knowledge, there are no density functional theory (DFT) or first principle calculations for the cobalt-cobalt and cobalt-gadolinium exchange in the alloy layered $[\ell'\ell']$ nanostructures. There is hence effectively a need for reliable data for the exchange and sublattice magnetizations in these systems to be able to develop modeling studies for the $...Co[\ell'\ell'][Co...$ nanojunctions which are key elements for ballistic spin wave transport in magnonic devices \cite{22,25-30}. This need has motivated our EFT calculations to determine such data with no fitting parameters, using basic values $S_{Co} = 1$ and $S_{Gd} = 7/2$ as the spin references at absolute 0 K.

The outline of the paper is as follows. In section 2 we use the EFT Ising spin method to compute reliable $J_{Co-Co}$ and $J_{Gd-Gd}$ exchange for the pure crystalline cobalt and gadolinium materials in comparison with experimental data. These are then attributed to nearest neighbor $Co - Co$ and $Gd - Gd$ interactions in the $...Co[\ell'\ell'][Co...$ nanojunction systems for eutectic stable concentrations $c \leq 0.5$. The EFT and MFT methods are combined in section 3 to compute and analyze the sublattice magnetizations for the cobalt and gadolinium sites on the individual hcp basal atomic planes of the alloy layered $[\ell'\ell']$ nanostructures as a function of temperature, for the layered nanostructure thicknesses $[2'22']$ and $[3'33']$, and for variable alloy concentrations $c$. The sublattice magnetizations and corresponding ferrimagnetic compensation temperatures are shown in this section. The overall summary and conclusions are presented in section 4.
2. EFT modeling of pure Co and Gd systems

The EFT method is known to be superior to the MFT because it incorporates the contributions of the single-site spin correlations to the order parameter. We use it in the present work to model and determine the exchange for Co and Gd crystals over their ordered magnetic phase, by comparing the EFT calculated magnetization results and Curie temperatures with experimental data [31]. The exchange for Co and Gd crystals are then derived by using our EFT calculated constitutive relations \[ kT_c / zJS(S + 1) = 0.3127 \] and \[ kT_c / zJS(S + 1) = 0.3162 \], valid for cobalt and gadolinium, respectively. The EFT exchange \( J_{Co-Co} \) and \( J_{Gd-Gd} \) are in agreement with the mean values obtained from extensive experimental data given in the literature [21] for Co and Gd. The EFT magnetization and exchange results for cobalt are then used to seed the calculations of the sublattice magnetizations for the alloy layered ...

The Ising spin Hamiltonian \( H \) of a magnetically ordered system involving different contributions from exchange, anisotropy, and Zeeman effects, is the basis in the Ising EFT method to model the magnetic properties of the system [16, 33–35]. The statistical accuracy of EFT is essentially equivalent to the Zernike approximation where long range interactions are neglected. This method, however, has the advantage that it can account for short-range order correlations in complex spin systems without losing the relative simplicity of its basic approach, and permits the calculation of a wide range of magnetic variables, in analytical and numerical forms. It provides furthermore a good understanding of the phase diagrams of magnetic systems, as well as nontrivial, non-uniform convergence in the complex phase diagrams. In the EFT method, the exact spin correlation functional identity [33], and other relevant identities, are mathematically transformed by the introduction of a differential operator [16, 34, 35]. Manipulating the algebraic EFT output can become very time consuming, and to circumvent this problem we have employed powerful codes such as Mathematica [36, 37] to streamline and simplify this output.

In this paper we consider the exchange energy to be at the origin of the magnetic order, favoring the alignment of the spins. Other magnetic energy terms include the magnetic anisotropy from spin-orbit coupling, the classical magnetostatic energy including the magnetic dipole interactions, and the Zeeman term. It is known that the local spin magnetic anisotropy is smaller than the exchange. The dipolar interactions are dependant, however, on the form of the magnetic system and may be important, but are negligible in an infinite bulk, as for the crystalline Co leads. For the ultrathin Co/Gd alloy layered nanojunction, the spins are aligned in the limit of low temperatures almost uniformly along the normal to the junction. We can estimate that the dipolar energy due to the slab geometry of the nanojunction is at least two orders of magnitude smaller than the exchange energy [21, 38]. In the higher temperature limit where we expect significant Gd spin fluctuations, its spin component in the plane of the slab junction does not contribute because the corresponding dipolar coupling between two perfectly flat infinite planes vanishes in the absence of interface roughness [39]. This situation corresponds to our considered approximation for the nanojunction as presenting ideally flat interfaces. In order to derive our results in a first basic approach, we neglect hence the dipolar and anisotropy terms.

The Ising spin Hamiltonian \( H \) for the pure considered ferromagnetic Co and Gd crystals may
be expressed, in the absence of local spin anisotropy and Zeeman effects, as

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_{iz} \cdot S_{jz},$$

(1)

$i, j$ is the sum over nearest neighbors in the crystal, and $J$ corresponds to the nearest neighbors magnetic exchange that induces spin order along a selected z-axis. Co and Gd have coordination number $z = 12$, and present negligible anisotropy in the bulk crystal as compared to the exchange. A more useful form for the Hamiltonian, for computation purposes, may be written from Eq. (1) as

$$\mathcal{H} = \sum_i \sum_j (-JS_{jz})S_{iz} \equiv \sum_i \mathcal{H}_i(x) \equiv \sum_i -xS_{iz},$$

(2)

The formulation of the thermodynamic canonical averages for any required spin operator $"Op"$ may be calculated by the EFT method using the Van der Wearden’s (VdW) operator $\exp(JS_z \nabla)$ formalism for any given characteristic function $f_{Op}(x)$ of the spin system. The Mathematica code formulation $f_{Op}(x)$ may be written as

$$f_{Op}(x) = \frac{\text{Tr}(\text{Op} \cdot \exp\left[\frac{-\mathcal{H}_i(x)}{kT}\right])}{\text{Tr}(\exp\left[\frac{-\mathcal{H}_i(x)}{kT}\right]).}$$

(3)

where the VdW operator for cobalt with $S = 1$ is given, as in reference [40], by

$$\exp(JS_z \nabla) = S_z^2 \cosh(J\nabla) + S_z \sinh(J\nabla) + 1 - S_z^2.$$

(4)

$\nabla = \frac{\partial}{\partial x}$ is the differential operator, with the property

$$<\exp(a\nabla)> = f_{Op}(x)|_{x \to 0} = f_{Op}(x + a)|_{x \to 0} = f_{Op}(a).$$

(5)

The details of the EFT method are described elsewhere [36, 37, 40, 41]. Using matrix quantum mechanics, it is possible to construct algorithms to evaluate the required averages using a number of symbolic and numerical procedures which treat a large number of terms for each variable. This number increases with the spin value and the coordination number.

The canonical thermodynamic averages are given as $< Op > = <\exp(JS_z \nabla)> = f_{Op}(x)|_{x \to 0}$. In the present investigation for the pure Co and Gd crystals, the analysis is confined to computing the canonical averages of the single-site spin variables $\sigma = <S_z>$ and $q = <S_z^2>$, with reference to their basic spin values $S = 1$ for Co and $S = 7/2$ for Gd at $T = 0K$. To achieve the computations, a decoupling approximation is adopted, equivalent to neglecting the site-site correlations $< S_{iz} S_{jz} >$ but retaining the single-site correlations $< S_{iz} S_{iz} >$. This renders tractable the intricate calculations using EFT, and ensures the translation invariance of the magnetic properties over the crystal. Furthermore, this decoupling approximation makes the otherwise infinitely hierarchical EFT approach quite effective to compute the salient magnetic properties of the systems.

The comparison between the EFT calculated results for the normalized magnetizations for the Co and Gd crystals, using the EFT constitutive relations [32], $kT_c/zJS(S + 1)$, yield their respective Curie temperatures, $0.3127$ for spin $S = 1$ and $z = 12$, and $0.3162$ for spin $S = 7/2$ and $z = 12$, with their corresponding experimental measurements [31], yield their respective Curie temperatures,
namely 119.4 meV and 25.2 meV [23]. For Co with spin \( S = 1 \), the EFT calculated magnetization and Curie temperature agree with the experimental data for the exchange \( J_{Co-Co} = 15.9 \) meV. This value is in good agreement with the mean value for the hcp cobalt nearest neighbors exchange obtained from a large ensemble of experimental data [21]. For the hcp Gd with the larger spin \( S = \frac{7}{2} \), the EFT calculated magnetization and Curie temperature agree with the corresponding experimental measurements [31], for the exchange \( J_{Gd-Gd} = 0.42 \) meV. The EFT calculated \( J_{Co-Co} \) and \( \sigma_{Co} \) for sites on the cobalt leads seed from the interfaces inwards, the MFT calculations for the embedded alloy layered \([\ell' \ell''] \) nanostructure.

3. Modeling the sublattice magnetizations of the alloy layered \([\ell' \ell''] \) ferrimagnetic nanostructures between cobalt leads

Though basically amorphous, the alloy hcp atomic planes of the layered \([\ell' \ell''] \) nanostructure between cobalt leads, are modeled as crystalline atomic planes with random homogeneous distributions of Co and Gd atoms on their hcp lattice. Any site is considered to have the usual six nearest neighbors in its hcp (0001) basal plane, and another six neighbors on the two adjacent planes. The system is made of alternating hcp (0001) atomic planes, and we assume that the structural morphology of the two interfaces between the leads and the layered nanostructure are abrupt and crystalline. The advent of advanced experimental techniques for Co/Gd multilayer systems, [11, 12], permits minimizing the interface roughness, and the control of the atomic interdiffusion towards stable eutectic compositions \( c = 0.1 \) to 0.5.

To calculate the magnetic variables of interest for the individual basal atomic hcp planes of the alloy layered \([\ell' \ell''] \) nanostructures by MFT, the Brillouin’s functions are used to determine initially the spin variables \( \sigma^{(n')}_{\alpha} \) for the \( n' \)th atomic plane

\[
\sigma^{(n')}_{\alpha} = B_{\alpha}(S_{\alpha}, T, H_{\alpha}^{(n')}) = \frac{2S_{\alpha} + 1}{2} \coth \left( \frac{(2S_{\alpha} + 1)H_{\alpha}^{(n')}}{2S_{\alpha} kT} \right) - \frac{1}{2} \coth \left( \frac{H_{\alpha}^{(n')}}{2S_{\alpha} kT} \right)
\]

\( S_{\alpha} \) denotes the basic spin for the \( \alpha \) atomic element, namely Co or Gd, and \( H_{\alpha}^{(n')} \) the molecular field energy for the element \( \alpha \) in the atomic plane \( n' \) due to its interaction with its \( z = 12 \) nearest neighbors; \( kT \) is the thermal energy. The effective magnetic moment \( \tilde{M}^{(n')} \) per site in the \( n' \)th plane, whether alloy or pure, is determined hence in units of Bohr magnetons by

\[
\tilde{M}^{(n')}/\mu_B = (1 - c)g_{Co}^{(n')} \sigma_{Co}^{(n')} + cg_{Gd}^{(n')} \sigma_{Gd}^{(n')}.
\]

\( g_{\alpha}^{(n')} \) are the g factors for the corresponding alloy element on the \( n' \)th plane. The magnetization for the \( n' \)th atomic plane may be obtained by multiplying \( \tilde{M}^{(n')} \) by the number of sites per unit volume for the plane.

3.1. Alloy layered \([Co_{1-c}Gd_c]_2[Co]_2[Co_{1-c}Gd_c]_2 \) ferrimagnetic nanostructure between cobalt leads

Consider in this subsection the embedded layered \([2'22'] \) nanostructure between cobalt leads. For the ferrimagnetic alloyed atomic planes, the Co and Gd atoms are found with the respective
probabilities \((1 - c)\) and \(c\). The molecular field energy for a \(Co\) atom on the 1st hcp basal plane of the layered nanostructure at the interface with the cobalt lead, may hence be expressed as

\[
H_{Co}^{(1)} = (3\sigma_{Co}^{(b)}J_{cc}) + 6[(1 - c)\sigma_{Co}^{(1)}J_{cc} + c\sigma_{Gd}^{(1)}J_{eg}] + 3[(1 - c)\sigma_{Co}^{(2)}J_{cc} + c\sigma_{Gd}^{(2)}J_{eg}].
\] (8)

The exchange interactions are denoted by the simplified notation \(J_{CoCo} \equiv J_{cc}, J_{GdGd} \equiv J_{gg}\), and \(J_{CoGd} \equiv J_{eg}\). Equally, the molecular field energy for a \(Gd\) atom on the 1st hcp basal plane of the alloy layered nanostructure at the interface with the cobalt lead, is

\[
H_{Gd}^{(1)} = (3\sigma_{Co}^{(b)}J_{eg}) + 6[(1 - c)\sigma_{Co}^{(1)}J_{eg} + c\sigma_{Gd}^{(1)}J_{gg}] + 3[(1 - c)\sigma_{Co}^{(2)}J_{eg} + c\sigma_{Gd}^{(2)}J_{gg}].
\] (9)

In the present formulation, the seeding spin value for the lead \(Co\) atom at the interface with the alloy layered nanostructure is represented by \(\sigma_{Co}^{(b)}\), which is obtained singularly from the EFT calculations described in detail in section 2.

In contrast, the molecular field for a \(Co\) atom on the 2nd hcp basal plane of the layered nanostructure inwards from the 1st, is

\[
H_{Co}^{(2)} = 3[(1 - c)\sigma_{Co}^{(1)}J_{cc} + c\sigma_{Gd}^{(1)}J_{eg}] + 6[(1 - c)\sigma_{Co}^{(2)}J_{cc} + c\sigma_{Gd}^{(2)}J_{eg}] + 3\sigma_{Co}^{(3)}J_{cc}
\] (10)

Similarly, the corresponding molecular field for a \(Gd\) atom on the 2nd hcp basal plane of the layered nanostructure, is

\[
H_{Gd}^{(2)} = 3[(1 - c)\sigma_{Co}^{(1)}J_{eg} + c\sigma_{Gd}^{(1)}J_{gg}] + 6[(1 - c)\sigma_{Co}^{(2)}J_{eg} + c\sigma_{Gd}^{(2)}J_{gg}] + 3\sigma_{Co}^{(3)}J_{eg}
\] (11)

The hcp basal planes of the pure \([Co]_2\) layer between the alloy layers \([Co_{1-x}Gd_{x}]_2\), are designated respectively as the 3rd and 4th atomic planes. Using the symmetry properties of the layered \([2’22’]\) nanostructure, we note that \(\sigma_{Co}^{(3)} \equiv \sigma_{Co}^{(4)}\). The corresponding molecular field for a \(Co\) atom on the 3rd hcp basal plane is hence

\[
H_{Co}^{(3)} = 3[(1 - c)\sigma_{Co}^{(2)}J_{cc} + c\sigma_{Gd}^{(2)}J_{eg}] + 9\sigma_{Co}^{(3)}J_{cc}
\] (12)

The above equations can be put into matrix form

\[
\begin{pmatrix}
H_{Co}^{(1)} \\
H_{Gd}^{(1)} \\
H_{Co}^{(2)} \\
H_{Gd}^{(2)} \\
H_{Co}^{(3)}
\end{pmatrix} = 
\begin{pmatrix}
A_1 & 0 & 0 & 0 & 0 \\
0 & A_2 & 0 & 0 & 0 \\
0 & 0 & A_3 & 0 & 0 \\
0 & 0 & 0 & A_4 & 0 \\
0 & 0 & 0 & 0 & A_5
\end{pmatrix} 
\begin{pmatrix}
x_1 & x_2 & x_3 & x_4 & x_5 \\
y_1 & y_2 & y_3 & y_4 & y_5 \\
u_1 & u_2 & u_3 & u_4 & u_5 \\
v_1 & v_2 & v_3 & v_4 & v_5 \\
z_1 & z_2 & z_3 & z_4 & z_5
\end{pmatrix} 
\begin{pmatrix}
\sigma_{Co}^{(1)} \\
\sigma_{Co}^{(2)} \\
\sigma_{Gd}^{(1)} \\
\sigma_{Gd}^{(2)} \\
\sigma_{Co}^{(3)}
\end{pmatrix}
\] (13)
Figure 1: Calculated spin variables $\sigma_{\text{Co}}$ and $\sigma_{\text{Gd}}$ for Co and Gd sites on the 1st (a) and 2nd (b) hcp basal (0001) planes, of the alloy layered $[\text{Co}_{1-c}\text{Gd}_c]_2[\text{Co}]_2[\text{Co}_{1-c}\text{Gd}_c]_2$ ferrimagnetic nanostructure between cobalt leads, for different alloy concentrations $c$, as a function of $kT$ in meV. The down (up) arrows in each figure correspond to the trend of the $\sigma$ spin variations for the Co (Gd) sites with $c$ step changes.

Figure 2: Calculated magnetic moments per site, in unit of Bohr magnetons, for sites on the 1st (continuous curves) and 2nd (discontinuous curves) hcp basal (0001) planes of the alloy layered $[\text{Co}_{1-c}\text{Gd}_c]_2[\text{Co}]_2[\text{Co}_{1-c}\text{Gd}_c]_2$ ferrimagnetic nanostructure between cobalt leads. They present small differences only at the high temperature $kT$ end of the ordered phase. The down arrows follow the variation trend for the magnetic moments per site with the $c$ step changes, on the 1st (continuous arrow) and 2nd (discontinuous arrow) hcp basal (0001) planes.

and the coefficients matrix is identical to

$$
\begin{pmatrix}
  x_1 & x_2 & x_3 & x_4 & x_5 \\
  y_1 & y_2 & y_3 & y_4 & y_5 \\
  u_1 & u_2 & u_3 & u_4 & u_5 \\
  v_1 & v_2 & v_3 & v_4 & v_5 \\
  z_1 & z_2 & z_3 & z_4 & z_5
\end{pmatrix} 8
= \begin{pmatrix}
  2\beta_{cc} & 6c_j_{cg} & \beta_{cc} & 3c_j_{cg} & 0 \\
  2\beta_{cg} & 6c_j_{gg} & \beta_{cg} & 3c_j_{gg} & 0 \\
  \beta_{cc} & 3c_j_{cg} & 2\beta_{cc} & 6c_j_{cg} & 3j_{cc} \\
  \beta_{cg} & 3c_j_{gg} & 2\beta_{cg} & 6c_j_{gg} & 3j_{cg} \\
  0 & 0 & \beta_{cc} & 3c_j_{cg} & 9j_{cc}
\end{pmatrix}
$$

(14)
where $A_1 = 3\sigma_{Co}^{(B)} J_{Co}$, $A_2 = 3\sigma_{Co}^{(B)} J_{Co}$ and $\beta = 3(1 - c)$. Using Eqs. (8) to (12), and the spin variables $\sigma^{(n')}_{\alpha}$ format given by Eq. (6), it follows that Eq. (13) denotes a system of nonlinear equations to be solved for the spin variables

$$
\begin{pmatrix}
\sigma^{(1)}_{Co} \\
\sigma^{(1)}_{Gd} \\
\sigma^{(2)}_{Co} \\
\sigma^{(2)}_{Gd} \\
\sigma^{(3)}_{Co}
\end{pmatrix} =
\begin{pmatrix}
B_{Co}(S_{Co}, T, H_{Co}^{(1)}) \\
B_{Gd}(S_{Gd}, T, H_{Gd}^{(1)}) \\
B_{Co}(S_{Co}, T, H_{Co}^{(2)}) \\
B_{Gd}(S_{Gd}, T, H_{Gd}^{(2)}) \\
B_{Co}(S_{Co}, T, H_{Co}^{(3)})
\end{pmatrix}
$$

(15)

Solving the above equations numerically, we calculate the spin variables $\sigma^{(1)}_{Co}$, $\sigma^{(1)}_{Gd}$, $\sigma^{(2)}_{Co}$, $\sigma^{(2)}_{Gd}$ and $\sigma^{(3)}_{Co}$ as a function of temperature, for any given alloy concentration $c$. Note that the symmetry of the system imposes the following equalities for the spin variables

$$
\begin{pmatrix}
\sigma^{(1)}_{Co} \\
\sigma^{(2)}_{Gd}
\end{pmatrix} \equiv \begin{pmatrix}
\sigma^{(6)}_{Co} \\
\sigma^{(6)}_{Gd}
\end{pmatrix}, \quad \begin{pmatrix}
\sigma^{(2)}_{Co} \\
\sigma^{(2)}_{Gd}
\end{pmatrix} \equiv \begin{pmatrix}
\sigma^{(2)}_{Co} \\
\sigma^{(2)}_{Gd}
\end{pmatrix}, \quad \begin{pmatrix}
\sigma^{(3)}_{Co}
\end{pmatrix} \equiv \begin{pmatrix}
\sigma^{(4)}_{Co}
\end{pmatrix}
$$

(16)

The calculated spin variables $\sigma^{(n')}_{Co}$, $\sigma^{(n')}_{Gd}$ for the nominal $n' = 1$ and $n' = 2$ hcp basal planes are presented in Fig[1] as a function of temperature and for eutectic concentrations $c = [0.1, 0.5]$ in steps of 0.1.

Further, Eq. (7), and $g^{(n')}_{Co} \equiv g_{Co} = 2.2$, $g^{(n')}_{Gd} \equiv g_{Gd} = 2$ for all $n'$, yield the magnetic moments per site on the 1st and 2nd hcp basal planes as a function of temperature. These are presented for comparison in Fig[2] where a small interesting difference is observed at the high temperature $kT$ end of the ordered phase. Compensation temperatures $kT_{comp} < 21$ meV, are observed for the ferrimagnetic hcp planes for eutectic stable concentrations in the range $0.23 < c < 0.5$.

### 3.2. Alloy layered $[Co_{1-c}Gd_c]_3[Co]_3[Co_{1-c}Gd_c]$ ferrimagnetic nanostructure between cobalt leads

The layered $[3'33']$ nanostructures under consideration are symmetric about the origin here taken as the hcp plane $n = 0$. In this system the symmetry properties to be used are

$$
\begin{pmatrix}
\sigma^{(1)}_{Co} \\
\sigma^{(1)}_{Gd}
\end{pmatrix} \equiv \begin{pmatrix}
\sigma^{(9)}_{Co} \\
\sigma^{(9)}_{Gd}
\end{pmatrix}, \quad \begin{pmatrix}
\sigma^{(2)}_{Co} \\
\sigma^{(2)}_{Gd}
\end{pmatrix} \equiv \begin{pmatrix}
\sigma^{(8)}_{Co} \\
\sigma^{(8)}_{Gd}
\end{pmatrix}, \quad \begin{pmatrix}
\sigma^{(3)}_{Co} \\
\sigma^{(3)}_{Gd}
\end{pmatrix} \equiv \begin{pmatrix}
\sigma^{(4)}_{Co} \\
\sigma^{(4)}_{Gd}
\end{pmatrix}, \quad \begin{pmatrix}
\sigma^{(4)}_{Co}
\end{pmatrix} \equiv \begin{pmatrix}
\sigma^{(6)}_{Co}
\end{pmatrix}
$$

(17)

Similarly, as in the previous case $[2'22']$, another equivalent relation for the molecular field energy results can be cast here in matrix form as
The down arrows correspond to the trend of the magnetic moment variations with temperature range of the ordered phase. They distinctly on the 1st and 3rd hcp planes (discontinuous and continuous curves, respectively) are quite similar throughout the temperature range of the ordered phase. They differ significantly from the magnetic moments on the 2nd hcp plane (continuous curves). The down arrows correspond to the trend of the magnetic moment variations with $c$ step changes.

Figure 3: Calculated magnetic moments per site, in unit of Bohr magnetons, for the 1st, 2nd, and 3rd hcp basal atomic planes of the alloy layered $[Co_{1-r}Gd_{r}]_{3}[Co]_{3}[Co_{1-r}Gd_{r}]$ ferrimagnetic nanostructure. The magnetic moments per site on the 1st and 3rd hcp planes (discontinuous and continuous curves, respectively) are quite similar throughout the temperature range of the ordered phase. They differ significantly from the magnetic moments on the 2nd hcp plane (continuous curves).

Figure 4: Calculated effective magnetic moments per site in units of Bohr magnetons for the nominal: (a) 1st alloyed, $n' = 1$, and (b) 2nd alloyed, $n' = 2$, hcp basal planes, for the alloy layered $[Co_{0.53}Gd_{0.47}]_{3}[Co]_{3}[Co_{0.53}Gd_{0.47}]$ and $[Co_{0.53}Gd_{0.47}]_{3}[Co]_{3}[Co_{0.53}Gd_{0.47}]_{3}$ nanostructures between cobalt leads.

\[
\begin{pmatrix}
H^{(1)}_{Co} \\
H^{(1)}_{Gd} \\
H^{(2)}_{Co} \\
H^{(2)}_{Gd} \\
H^{(3)}_{Co} \\
H^{(3)}_{Gd}
\end{pmatrix} =
\begin{pmatrix}
A_1 \\
2 \beta_{J_{cc}} & 6 \epsilon_{J_{cc}} & \beta_{J_{cc}} & 3 \epsilon_{J_{cc}} & 0 & 0 & 0 & 0 \\
2 \beta_{J_{cc}} & 6 \epsilon_{J_{cc}} & \beta_{J_{cc}} & 3 \epsilon_{J_{cc}} & 0 & 0 & 0 & 0 \\
\beta_{J_{cc}} & 3 \epsilon_{J_{cc}} & 2 \beta_{J_{cc}} & 6 \epsilon_{J_{cc}} & \beta_{J_{cc}} & 3 \epsilon_{J_{cc}} & 0 & 0 \\
\beta_{J_{cc}} & 3 \epsilon_{J_{cc}} & 2 \beta_{J_{cc}} & 6 \epsilon_{J_{cc}} & \beta_{J_{cc}} & 3 \epsilon_{J_{cc}} & 0 & 0 \\
0 & 0 & 0 & \beta_{J_{cc}} & 3 \epsilon_{J_{cc}} & 2 \beta_{J_{cc}} & 6 \epsilon_{J_{cc}} & 3 \epsilon_{J_{cc}} \\
0 & 0 & 0 & \beta_{J_{cc}} & 3 \epsilon_{J_{cc}} & 2 \beta_{J_{cc}} & 6 \epsilon_{J_{cc}} & 3 \epsilon_{J_{cc}}
\end{pmatrix}
\begin{pmatrix}
\sigma^{(1)}_{Co} \\
\sigma^{(2)}_{Gd} \\
\sigma^{(3)}_{Co} \\
\sigma^{(3)}_{Gd} \\
\sigma^{(4)}_{Co} \\
\sigma^{(5)}_{Co}
\end{pmatrix}
\]
3.3. Alloy layered

in the core atomic planes tend to limiting solutions. With increasing concentration $c$, the variables can be generalized to larger nanostructures sandwiched between semi-infinite magnetic moments per site, on the individual hcp basal planes of the alloy layered magnetic system. Together, they differ significantly from the magnetic moments per site for the second hcp plane, throughout the temperature range of the ordered phase.

The above nonlinear equations can be solved numerically to obtain the spin variables and magnetic moments per site, on the individual hcp basal planes of the alloy layered magnetic nanostructure. Table 1 presents the calculated results for the magnetic moments on the 1st, 2nd, and 3rd hcp atomic planes for this system. The magnetic moments per site for the 1st and 3rd hcp planes (discontinuous and continuous curves, respectively) are quite similar throughout the temperature range of the ordered phase. Together, they differ significantly from the magnetic moments per site for the 2nd hcp plane, throughout the temperature range of the ordered phase.

The model approach is general and can be extended to treat individual hcp atomic planes of alloy layered [Co$_{1-c}$Gd$_c$]$_p$[Co]$_q$[Co$_{1-c}$Gd$_c$]$_r$ nanostructures, with $r, p, q \geq 1$. This procedure may be generalized to larger nanostructures sandwiched between semi-infinite Co leads, but we have found that with increasing $r, p, q$ the results for the spin variables and magnetic moments per site in the core atomic planes tend to limiting solutions.

### Table 1: Spin variable values $< S_{Gd} >$ for the Gd sites on the identified atomic planes

| $c$ | $22'$ | $33'$ |
|-----|-------|-------|
|    | $[Co_{1-c}Gd_c]_{2,L}$ | $[Co_{1-c}Gd_c]_{3,L}$ | $[Co_{1-c}Gd_c]_{3,R}$ |
| 0.1 | -1.10 | -1.10 | -1.10 |
| 0.2 | -1.03 | -1.03 | -1.03 |
| 0.3 | -0.97 | -0.97 | -0.97 |
| 0.4 | -0.91 | -0.91 | -0.91 |
| 0.5 | -0.83 | -0.83 | -0.83 |

where $A_1(kT) = 3M_{Co}(kT)J_{Co-Co}$ and $A_2(kT) = 3M_{Co}(kT)J_{Co-Gd}$. This yields the new irreducible variables

\[
\begin{pmatrix}
\sigma_{Co}^{(1)} \\
\sigma_{Co}^{(2)} \\
\sigma_{Co}^{(3)} \\
\sigma_{Co}^{(4)} \\
\sigma_{Co}^{(5)}
\end{pmatrix}
= 
\begin{pmatrix}
B_{Co}(S_{Co}, T, H_{Co}^{(1)}) \\
B_{Gd}(S_{Gd}, T, H_{Gd}^{(1)}) \\
B_{Co}(S_{Co}, T, H_{Co}^{(2)}) \\
B_{Gd}(S_{Gd}, T, H_{Gd}^{(2)}) \\
B_{Co}(S_{Co}, T, H_{Co}^{(3)}) \\
B_{Gd}(S_{Gd}, T, H_{Gd}^{(3)}) \\
B_{Co}(S_{Co}, T, H_{Co}^{(4)}) \\
B_{Gd}(S_{Gd}, T, H_{Gd}^{(4)})
\end{pmatrix}
\]

The above nonlinear equations can be solved numerically to obtain the spin variables and magnetic moments per site, on the individual hcp basal planes of the alloy layered magnetic nanostructure. Table 1 presents the calculated results for the magnetic moments on the 1st, 2nd, and 3rd hcp atomic planes for this system. The magnetic moments per site for the 1st and 3rd hcp planes (discontinuous and continuous curves, respectively) are quite similar throughout the temperature range of the ordered phase. Together, they differ significantly from the magnetic moments per site for the 2nd hcp plane, throughout the temperature range of the ordered phase.

The model approach is general and can be extended to treat individual hcp atomic planes of alloy layered [Co$_{1-c}$Gd$_c$]$_p$[Co]$_q$[Co$_{1-c}$Gd$_c$]$_r$ nanostructures, with $r, p, q \geq 1$. This procedure may be generalized to larger nanostructures sandwiched between semi-infinite Co leads, but we have found that with increasing $r, p, q$ the results for the spin variables and magnetic moments per site in the core atomic planes tend to limiting solutions.

3.3. Alloy layered $[Co_{0.53}Gd_{0.47}]_r[Co]_q[Co_{0.53}Gd_{0.47}]_r$ ferrimagnetic nanostructure between cobalt leads

This alloy layered magnetic nanostructure between cobalt leads, at the characteristic eutectic concentration $c = 0.47$, is particularly interesting since Co/Gd magnetic multilayers at the same
Figure 5: Calculated spin variables $\sigma_{\text{Co}}^{(n)}$ and their detailed variations as a function of temperature on the nominal $n'$ cobalt hcp basal planes inside the alloy layered ferrimagnetic nanostructures $[\text{Co}_{0.53}\text{Gd}_{0.47}]_2[\text{Co}]_2[\text{Co}_{0.53}\text{Gd}_{0.47}]_2$ and $[\text{Co}_{0.53}\text{Gd}_{0.47}]_3[\text{Co}]_3[\text{Co}_{0.53}\text{Gd}_{0.47}]_3$ in comparison with the temperature variation of the spin variable $\sigma_{\text{Co}}^{(B)}$ on the cobalt leads; see details in the text.

composition have been reported to be very stable. We have applied hence the EFT-MFT model analysis to calculate the spin variables $\sigma_{\text{Co}}^{(n)}$ and $\sigma_{\text{Gd}}^{(n)}$, and the effective magnetic moments per site, for the individual hcp basal planes of the corresponding layered ferrimagnetic nanostructures between cobalt leads, as a function of temperature, eutectic concentration, and thicknesses $\ell = 2$ and 3. The integer $n'$ numbers the hcp planes from 1 to 6 for $\ell = 2$, and from 1 to 9 for $\ell = 3$.

The calculated effective magnetic moments per site in units of Bohr magnetons for the alloyed nominal 1st, $n' = 1$, and 2nd, $n' = 2$, hcp basal planes for the alloy layered ferrimagnetic nanostructures $[\text{Co}_{0.53}\text{Gd}_{0.47}]_2[\text{Co}]_2[\text{Co}_{0.53}\text{Gd}_{0.47}]_2$ and $[\text{Co}_{0.53}\text{Gd}_{0.47}]_3[\text{Co}]_3[\text{Co}_{0.53}\text{Gd}_{0.47}]_3$ are presented in Fig.4. It is observed that the computed effective magnetic moments per site as a function of temperature on the nominal $n' = 1$ hcp basal planes do not vary significantly with increasing nanostructure thickness, see Fig.4(a). This can be understood clearly since the corresponding matrix elements in Eq.18 do not change significantly with increasing thickness. In contrast, it is observed that the effective magnetic moments per site on the nominal $n' = 2$ hcp basal planes do vary significantly with increasing thickness, see Fig.4(b). This is expected physically owing to the changes of the corresponding effective molecular fields for Co and Gd sites. The observed variations start at $\approx 15$ meV and persist for higher temperatures, including room temperature $\approx 26$ meV.

It is also interesting to compute spin variables $\sigma_{\text{Co}}^{(n)}$, and their detailed variations as a function of temperature on the nominal $n'$ cobalt hcp basal planes inside the alloy layered ferrimagnetic nanostructures, in comparison with the temperature variation of the spin variable $\sigma_{\text{Co}}^{(B)}$ on the cobalt leads. This is done for the $[\text{Co}_{0.53}\text{Gd}_{0.47}]_2[\text{Co}]_2[\text{Co}_{0.53}\text{Gd}_{0.47}]_2$ layered nanostructure between cobalt leads, for thicknesses $\ell = 2$ and 3. The calculated results are presented in Fig.5. As is
physically expected, the $\sigma^{(B)}_{Co}$ is $\geq \sigma^{(n')}_{Co}$ for all pure Co hcp planes $n'$ inside the layered thicknesses $\ell$, at all temperatures of the ordered ferrimagnetic phase. Also as expected, $\sigma^{(5)}_{Co}$ is $\geq \sigma^{(4)}_{Co}$ for the alloy layered $[Co_{0.53}Gd_{0.47}]_3[Co]_3[Co_{0.53}Gd_{0.47}]_3$ ferrimagnetic nanostructure between cobalt leads, and both are greater or equal to the $\sigma^{(3)}_{Co}$ of the $[Co_{0.53}Gd_{0.47}]_2[Co]_2[Co_{0.53}Gd_{0.47}]_2$ layered nanostructure. Note that the $n' = 3$ pure cobalt plane for the [2'22'] layered nanostructure is equivalent nominally to the $n' = 4$ pure cobalt plane for the [3'33'] layered nanostructure. The results confirm a physical trend which is expected, and which would lead to limiting values with increasing thickness of the layered ferrimagnetic structure between cobalt leads.

We emphasize that the basic physical variables, such as the exchange and sublattice magnetizations for Co and Gd sites for the embedded layered nanostructures between cobalt leads, are necessary elements for the computations of the spin dynamics of magnetic nanojunctions in the field of magnonics, as for the ballistic magnon transport [24]. In Table 1 we present an example for the calculated spin variables $<S_{Co}> \approx 1$ throughout the system, and $<S_{Gd}>$ on the identified atomic planes 1, 2, ..., $\ell$, of the layered ...Co)[2'22'][Co... and ...Co][3'33'][Co... nanostructures between cobalt leads, at room temperature $T=300K$ and stable eutectic compositions $c \leq 0.5$, using the EFT-MFT combined method.

4. Summary and conclusions

In the present work, we model the salient magnetic properties of the alloy layered ferrimagnetic $[Co_{1-c}Gd_c]_\ell[Co]_\ell[Co_{1-c}Gd_c]_\ell$ nanostructures between magnetically ordered cobalt leads. In particular we have calculated and analyzed the sublattice magnetizations of the Co and Gd sites on the individual hcp basal planes of the alloy layered nanostructures, using the combined EFT and MFT methods. The sublattice magnetizations and effective magnetic moments per site, are presented as a function of temperature and thicknesses of the layered nanostructure, for different stable alloy eutectic concentrations $c \leq 0.5$ on the alloyed nanostructure. The model is general, and may applied directly to other composite magnetic elements and embedded nanostructures.

In the absence of first principles calculations for these basic physical variables for the alloy layered nanostructures between cobalt leads, the combined EFT and MFT approach yields the only available information for them at present.

The calculated exchange, and spin variables $<S_{Gd}>$ and $<S_{Co}>$, for the cobalt and gadolinium sites on the identified hcp basal planes of the alloy layered $[Co_{1-c}Gd_c]_\ell[Co]_\ell[Co_{1-c}Gd_c]_\ell$ ferrimagnetic nanostructures between cobalt leads, are essential for the self-consistent analysis of the system spin dynamics and the coherent ballistic magnon transport across such nanostructures. This illustrates the importance of the calculated results for applications in the fields of magnonics.

The Ising EFT method serves to determine the exchange constants for Co and Gd sites of pure crystals, characterized by their fundamental quantum spins, by comparing the calculated EFT results with the corresponding experimental data. The sublattice magnetizations for the Co and Gd sites in the nanostructure are computed by seeding the MFT computations on the alloy layered ferrimagnetic nanostructure by the EFT results of the cobalt leads from the interface inwards.
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