



Spin dynamics and magnonic characteristics of a magnetically ordered fcc Fe-Ni alloy monolayer on an fcc Ni slab substrate

Lamia Saim^a, Elie A. Moujaes^{b,*}, Antoine Khater^{c,d}, Rachid Tigrine^a

^a Laboratoire de Physique et Chimie Quantique, University Mouloud Mammeri de Tizi-Ouzou, B.P. No. 17 RP, 15000 Tizi-Ouzou, Algeria

^b Departamento de Física, Universidade Federal de Rondônia, 76900-900 Porto Velho, Brazil

^c Department of Physics, Le Mans University, 72085 Le Mans, France

^d Institute of Physics, Jan Dlugosz University, Am. Armii Krajowej 13/15, Czestochowa, Poland

ARTICLE INFO

Keywords:

Magnonics
Nickel slab substrate
Spin dynamics
Ordered alloy
Density functional theory
Localized states

ABSTRACT

We investigate the surface spin dynamics and magnonic characteristics of a magnetically ordered fcc Fe-Ni alloy monolayer on a Ni magnetic slab substrate. The calculations are performed using the Heisenberg Hamiltonian representation for the magnetic ground state of the system. Using the Spin Polarized Relativistic Korringa-Kohn-Rostoker (SPRKKR) method, the relevant magnetic exchange parameters are computed, taking into account the nearest and next nearest Fe-Fe interactions. This establishes the appropriate Heisenberg Hamiltonian. The Phase Field Matching Theory (PFMT) is applied to compute the spin dynamics and surface magnonics of the system, and thus determine the spin wave eigenmodes localized at the surface but propagating in its plane with surface group velocities; these intrinsic eigenmodes constitute basic elements for the magnonic characteristics of the system. The inclusion of the Fe-Fe interactions alters the highest magnonic mode compared to the case when such interactions are absent. The localized densities of states (LDOS) for the irreducible representative magnetic sites at the surface nanostructure are extracted from our computed PFMT Green's functions. The model is general, and can be applied to different ultrathin layered magnetic alloys on magnetically ordered substrates.

1. Introduction

Motivated by the endeavor to produce magnetic field controlled devices by using spin waves (instead of electrons) to carry and process information, the field of magnonics is born [1]. This new field aims at studying, detecting and manipulating spin waves in magnetic materials. It is superior to the field of *electronics* in the sense that it does not use electric currents, thus avoiding significant Joule heating effects which limit the efficiency, capacity and lifetime of electronic devices. Additionally, it is different from the field of *spintronics* [2], which although makes use of just the spin moment of the electric charge, is still destined to depend on itinerant electrons. Techniques in this field can be applied to boost the performance of physical devices [3,4]. The study of spin dynamics constitutes the basic first step for the production of magnonic devices. This is achieved through the investigation of the propagation of spin waves inside magnetic materials which allows the observation of new magnetic phenomena in the systems under study [5–8].

Experimentally, early investigations in magnonics started with ferromagnetic [9] on the millimetre to micrometre [10,11] time scales. Wave-based data processing by spin waves proved to be an optimistic

approach to conquer the challenges which CMOS based logic networks are facing; in fact it is now possible to combine and separate spin waves of various frequencies to process simultaneous data in single magnonic devices [12]. On the nano scale level, engineered spin-textures were used as building blocks of spin-wave based computing devices [13]; however the experimental attempts to emit, manipulate and detect spin waves are accessible at only a few hundreds of nanometres [14] where the detection of those occurring at the lower end of the nano scale is still limited and remains a main challenge.

Magnetic nanomaterials belong to the general class of materials that are vital in various areas such as medicine [15,16], and catalysis [17]. In magnetic tunnel junction (MTJ) technology, magnetic nanomaterials made from transition metals (TM), such as Fe, Ni and Co, can be constructed to modulate the spintronics properties of ultrathin junctions containing bimetallic nanolayers [18]. Also, magnetic ultrathin nanojunctions consisting of a few TM atomic monolayers, are significantly interesting for modulating magnonics phase fields. Recently, the study of homogeneous magnetically ordered TM alloy nanostructures was initiated by constructing the ground states of Fe-Co alloy nanojunctions, $[\text{Gd}_{1-x}\text{Co}_x]_n$ nanojunctions with Co leads, as well as the computation of

* Corresponding author.

E-mail address: eamoujaes@unir.br (E.A. Moujaes).

<https://doi.org/10.1016/j.jmmm.2020.166958>

Received 6 December 2019; Received in revised form 2 March 2020; Accepted 28 April 2020

Available online 01 May 2020

0304-8853/ © 2020 Elsevier B.V. All rights reserved.

the site magnetizations in the n -layered alloy for diverse concentrations c [19–21].

By evaluating the reflectance and transmittance fields of the incident lead spinwaves, the corresponding coherent ballistic transport across TM nanojunctions, whose dimensions are relatively smaller than the spinwave wavelength, can also be examined. This has been successfully explored for the Fe-Co alloy nanojunctions with Fe leads [21], Gd-Co alloy nanojunctions with Co leads [22], Fe-Ni alloy nanojunctions with Fe and Co leads [23], and ultrathin lamellar bcc Ni monolayers of different thicknesses between Fe leads [24]. The exchange constants for the above calculations were obtained for nearest neighbours using the Effective Field Theory (EFT) [25] and the virtual crystal approximation (VCA) [26–29]. The computations of the spin dynamics in these systems, based on a Heisenberg Hamiltonian, are acquired by employing the Phase Field Matching Theory (PFMT) [21–24] based on the appropriate phase matching of the spinwave Bloch states of the leads to the localized spin dynamic states in the nanojunction scattering region.

For advanced magnonic technologies, an important type of magnetic nanomaterial consists of ultrathin magnetic films (of a few alloy monolayers). In complex magnonic circuitry, it is often used as magnetic modulable and controllable surface systems on slab substrates or nanojunction systems between magnetic leads, especially those using Fe, Ni and Co.

An earlier interest in spin-injection into a semiconductor-based device has motivated the study of the structural and magnetic properties of a few atomic monolayers Ni/Fe and Fe/Ni epitaxially grown on GaAs [30]. It was shown that a proper choice of Fe and Ni sequences (Fe/Ni/GaAs) and their thickness of up to three atomic monolayers, induced the rotation of magnetization from the in-plane to the out-of-plane direction, thanks to the change of the effective anisotropy of the monolayers. This change was found for a series of ultrathin Fe films of a few monolayers grown on Ni films with constant thickness on top of Si substrates [31]. Currently, the study of ultrathin alloy Fe-Ni monolayers on different substrates, [32–34], is of interest.

Furthermore, some theoretical research work has also been done on the magnetic properties of ultrathin fcc Fe nanostructures on Cu(111) surfaces using ab initio techniques [35], and of an $\text{Fe}_{1-x}\text{Ni}_x$ monolayer on Cu(001) substrate using the spin-polarized linear muffin-tin orbitals Green's-function technique and the Korringa-Kohn-Rostoker Green's function method [36]. The magnetic properties of ultrathin TM films on 4d substrates have also been extensively considered in [37].

In this paper, we investigate in depth the magnetic ground state and the spin dynamics of the system of a monolayer of fcc $\text{Fe}_{0.5}\text{Ni}_{0.5}$ alloy as the topmost surface monolayer on an fcc Ni slab substrate of sub-microscopic width much greater than the width of an atomic monolayer. Our choice comes from the fact that the system is important in magnonics from a technological point of view; furthermore it is a stable system since the ordered $\text{Fe}_{0.5}\text{Ni}_{0.5}$ fcc structure has, according to DFT calculations, the lowest energy of all the alloy configurations with the same stoichiometry [38–40]. Nonetheless, its spin dynamics have not been addressed before. Here, we use DFT techniques to determine the various exchange parameters, and the Phase Field Matching Theory (PFMT) to compute the spin dynamics and the localized magnonic modes at the surface. Our theoretical model which applies to the present system, can be extended directly to an ultrathin nanometric film of a few alloy monolayers at the surface. Varying the surface film thickness can modulate and control the number and behavior of surface localized eigenmodes which are basic elements for the magnonic properties of such nanostructures.

The paper is organized as follows: In Section 2, The magnetic ground state of the system is constructed adopting the Heisenberg representation, and ab initio computations are developed to compute the nearest and next nearest neighbor magnetic exchange between the different Ni and Fe sites of the system, using the Spin Polarized Relativistic Korringa-Kohn-Rostoker (SPKKR) technique. In Section 3, the

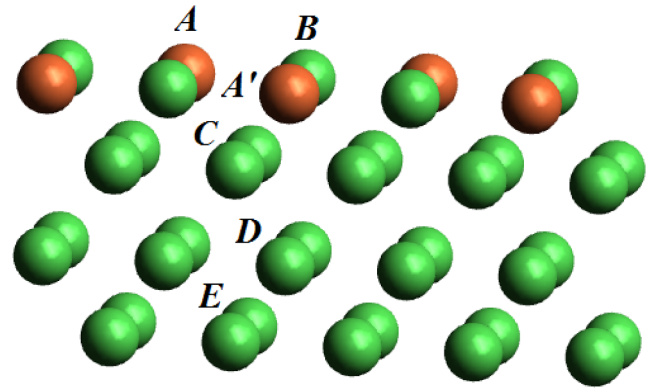


Fig. 1. Schematic representation of the magnetically ordered fcc monolayer $\text{Fe}_{0.5}\text{Ni}_{0.5}$ alloy on an fcc Ni substrate. The brown balls represent Fe sites in the alloy denoted by A and A'. The green balls identify Ni sites, labeled B in the alloy monolayer. As one goes deeper into the substrate, Ni sites C, D and E are encountered.

theoretical model is established in detail using the Phase Field Matching Theory (PFMT) to obtain the spin dynamics of the system, and compute the spin waves, notably the localized eigenmodes at the surface alloy monolayer which are basic to characterize the system magnonic properties. Theoretical and numerical results, followed by a discussion, are presented in Section 4 and the conclusions are given in Section 5.

2. DFT computations of the system's magnetic order and exchange parameters

The structure of the magnetically ordered monolayer alloy on the Ni substrate (which is the configuration shown in Fig. 1) is constructed as a 2D fcc slab of 40 atoms cut along the [001] direction using the X BAND graphical interface implemented in the Spin Polarized Relativistic Korringa-Kohn-Rostoker (SPKKR) code [41,42]. The first three layers are of Ni whilst the fourth layer represents the $\text{Fe}_{0.5}\text{Ni}_{0.5}$ alloy. The slab has an orthorhombic primitive structure and thus belongs to the $Pmmm$ space group. The lattice parameter is chosen to be that of fcc Ni ($a_{\text{Ni}} = 3.49 \text{ \AA}$).

The first step towards obtaining the magnetic exchange constants (J) is a self consistent potential calculation (SCF). Since TM elements are involved, the angular momenta expansion for the major component of the wave function l_{max} was set to 3. During the SCF cycles, a Brillouin zone (BZ) integration with a special point method was used with a grid of 400 k-points. To achieve convergence, we have used a BROYDEN2 scheme [43] with a scalar relativistic Vosko-Wilk-Nusair (VWN) exchange correlation potential [44]. The Ewald parameter which determines the relative weight of the real and reciprocal space lattice sums is set to 0.3, and both the cutoff radii in real and reciprocal spaces are restricted to a value of 3.3. The weakly bound states are treated as core states, and the upper end of the energy path E_{max} is set to the Fermi energy E_F . Regarding the real part of the lowest energy value we have used $E_{\text{min}} = 0.2 \text{ Ry}$, and the number of E mesh points was set to 30. Since slab calculations are usually slow, the SCF mixing parameter was set to 0.07 to accelerate the convergence with a maximum number of SCF iterations of 300. If desired, the new converged self consistent potential can then be used to compute the total (TDOS) and partial (PDOS) density of states of each Ni/Fe site using a denser grid of 850k-points and a higher E mesh points of 50.

The SPKKR package calculates the magnetic exchange constants J for the Heisenberg Hamiltonian of the system:

$$\mathcal{H} = - \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j,$$

where $\vec{S}_i$ and $\vec{S}_j$ represent the spins at sites i and j and J_{ij} are the

exchange constants between the different sites. The calculations are based on the KKR Green's functions following the formulation of Liechtenstein et al. [45]. The exchange constants are calculated with respect to a referential central site i of a cluster of atoms with the radius $R_{clus} = \max|\vec{R}_i - \vec{R}_j|$, $\vec{R}_i$ and $\vec{R}_j$ being the positions of sites i and j respectively. We have taken between 0 and 1.0 to include nearest and next nearest neighbours. For completeness, the computations are undertaken using different referential sites.

The nearest neighbour exchange interactions between Fe and Ni atoms in the two topmost monolayers at the surface, between Ni atoms in the alloy monolayer and Ni atoms in the slab substrate, and between Ni atoms within the substrate are computed within a DFT framework. Given their importance, the Fe-Fe next nearest neighbour interactions in the surface alloy monolayer will be also determined. On the other hand, the Ni-Ni next nearest neighbour interactions within the alloy plane are small and will therefore be neglected. With the exchange constants at hand, the overall Heisenberg Hamiltonian is then established to predict the system's spin dynamics.

3. Theoretical model for the system's magnonic characteristics

3.1. Computation of the substrate and surface magnon modes

The ordered alloy monolayer is built up by substituting an Fe atom for every other Ni atom in the topmost original surface Ni monolayer. Note that the surface breaks the symmetry along the z-direction which, in our case, is perpendicular to the whole system.

It is instructive at first to analyze the magnonic properties of the bulk fcc Ni as a reference. This is well known, and leads to a single propagating spin wave (SW) mode over the fcc crystallographic structure; the bulk magnon dispersion can be written as

$$\Omega(\phi_x, \phi_y, \phi_z) = 12 - 4(\cos(\phi_y)\cos(\phi_z) + \cos(\phi_x)\cos(\phi_y) + \cos(\phi_x)\cos(\phi_z)),$$

where ϕ_x , ϕ_y and ϕ_z are normalized dimensionless phases that run over the fcc first Brillouin zone (BZ). $\Omega(\phi_x, \phi_y, \phi_z)$ is a dimensionless normalized energy parameter given by $\hbar\omega/(J_V S_{Ni})$, where J_V represents the magnetic exchange constant between two nearest neighbour Ni sites in the bulk region, and S_{Ni} is the spin per Ni site. Fig. 2(a) shows the magnonic dispersion curves for bulk fcc Ni corresponding to $\phi_y = \phi_x = 0$ and to $\phi_y = \pi/2$, $\phi_x = 0$ for $-\pi \leq \phi_z \leq \pi$. In the first case, the propagating SWs occur for $0 \leq \Omega \leq 16$, while for the second case they occur for $8 \leq \Omega \leq 16$. The group velocities of the SW mode along the two different BZ paths are shown in Fig. 2(b).

Generally, the equation of the precessional motion of a spin vector U on an fcc site with coordinates n , s and m can be written as

$$\begin{aligned} \Omega U_{Ni}(n, s, m) = & 12U_{Ni}(n, s, m) - U_{Ni}(n-1, s-1, m) \\ & - U_{Ni}(n+1, s+1, m) - U_{Ni}(n+1, s-1, m) \\ & - U_{Ni}(n+1, s, m+1) - U_{Ni}(n, s-1, m+1) \\ & - U_{Ni}(n-1, s, m+1) - U_{Ni}(n, s+1, m+1) \\ & - U_{Ni}(n, s-1, m-1) - U_{Ni}(n+1, s, m-1) \\ & - U_{Ni}(n-1, s, m-1) - U_{Ni}(n, s+1, m-1) \\ & - U_{Ni}(n-1, s+1, m), \end{aligned} \quad (1)$$

with $U_{Ni}(n \pm 1, s, m) = U_{Ni}(n, s, m)e^{\pm i\phi_x}$, $U_{Ni}(n, s \pm 1, m) = U_{Ni}(n, s, m)e^{\pm i\phi_y}$ and $U_{Ni}(n, s, m \pm 1) = U_{Ni}(n, s, m)e^{\pm i\phi_z}$, $\{e^{\pm i\phi_x}$, $e^{\pm i\phi_y}$ and $e^{\pm i\phi_z}\}$ being the corresponding phase factors.

As can be inferred from Fig. 1, A and B belong to the ordered alloy monolayer, C to the first Ni atomic plane in contact with the alloy, D to the so called matching region and E to the bulk region.

The spin dynamics of our system is obtained by resolving the spin precession equations of motion of the spin vectors situated on the representative sites A, B, C, D and E. Using Eq. (1), the nearest and next nearest neighbour interactions for site A yield:

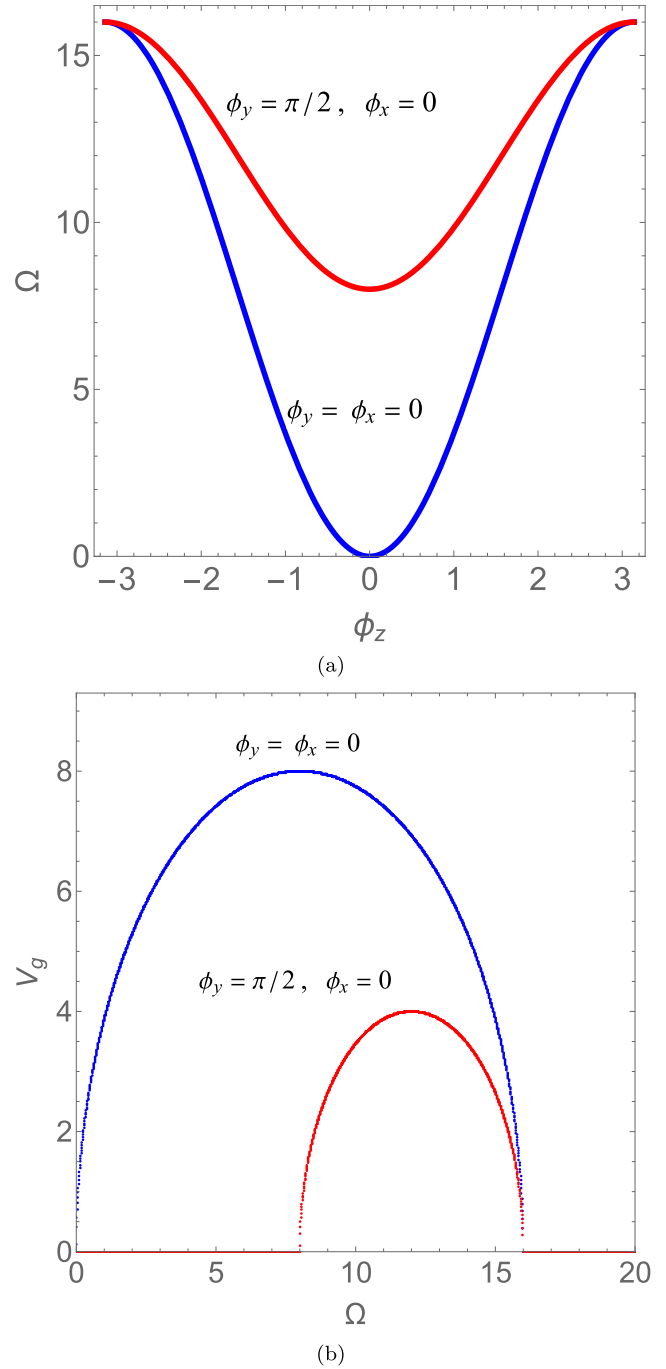


Fig. 2. (a) Dispersion curves representing spin wave (SW) bands generated by the single mode of bulk Ni along two arbitrary directions in the Brillouin zone, ($\phi_y = \phi_x = 0$, $\phi_y = \pi/2$, $\phi_x = 0$) with $-\pi \leq \phi_z \leq \pi$. $\Omega = \hbar\omega/(J_V S_{Ni})$ is a dimensionless frequency normalized with respect to the exchange and spin values. (b) Group velocity of the single propagating mode of fcc bulk Ni along the two paths depicted in (a).

$$\begin{aligned} & [\Omega - 8J_1J_2 + J_2J_4(-4 + 2\cos(2\phi_x) + 2\cos(2\phi_y))]U_A \\ & + J_1J_2(1 + e^{-2i\phi_x} + e^{2i\phi_y} + e^{-2i\phi_x}e^{2i\phi_y})U_B \\ & + J_1J_2(1 + e^{-2i\phi_x} + 2e^{-i\phi_x}\cos(\phi_y))U_C = 0. \end{aligned}$$

For site B, only the eight nearest neighbors are considered, giving:

$$\begin{aligned} & [\Omega - 4(J_1 + J_3)]U_B \\ & + J_1(1 + e^{2i\phi_x}e^{-2i\phi_y} + e^{2i\phi_x} + e^{-2i\phi_y})U_A \\ & + J_3(1 + e^{-2i\phi_y} + 2e^{-i\phi_y}\cos(\phi_x))U_C = 0. \end{aligned}$$

The 12 nearest neighbours for site C yield:

$$[\Omega - 2J_1 - J_3(10 - 4\cos(\phi_x)\cos(\phi_y))]U_C + J_1(1 + e^{2i\phi_x})U_A + J_3(1 + e^{2i\phi_y})U_B + J_3(1 + e^{2i\phi_y} + 2e^{i\phi_y}\cos(\phi_x))U_D = 0.$$

For site D, the equation for the 12 nearest neighbours reads:

$$[\Omega - J_3(12 - 4\cos(\phi_x)\cos(\phi_y))]U_D + J_3(1 + e^{-2i\phi_y} + 2e^{-i\phi_y}\cos(\phi_x))U_C + J_3(1 + e^{-2i\phi_y} + 2e^{-i\phi_y}\cos(\phi_x))U_E = 0.$$

Finally, for the Ni site E, 12 nearest neighbours are also involved and the equation takes the form:

$$[\Omega - 8J_3 - 4 + 4J_3\cos(\phi_x)\cos(\phi_y)]U_E + J_3(1 + e^{2i\phi_y} + 2e^{i\phi_y}\cos(\phi_x))U_D + (1 + e^{2i\phi_y} + 2e^{i\phi_y}\cos(\phi_x))U_F = 0.$$

U_A , U_B , U_C , U_D and U_E are spin precession amplitudes at sites A, B, C, D and E respectively. Theoretically, since the Ni substrate bulk can be assumed semi-infinite, one of the nearest neighbors of the Ni atom on site E, will be on a layer beneath (not shown in the figure), and will be called site F; its spin precession amplitude will be denoted by U_F .

For algebraic convenience, we define $\Omega = \hbar\omega/(J_V S_{Ni})$, $J_1 = J_{FeNi}/J_V$, $J_2 = S_{Fe}/S_{Ni}$, $J_3 = J_{NiNi}/J_V$ and $J_4 = J_{FeFe}/J_V$, where S_{Fe} and S_{Ni} are the spins at Fe and Ni sites respectively.

The above system of equations forms a rectangular 5×6 dynamical matrix (M_D) which is not possible to diagonalize. Therefore it is instructive to define a 6×5 matching matrix. The role of this matrix is to establish the relationships that make it possible to connect the spin displacements belonging to the surface area (layers containing A, A' and B) and those of the evanescent modes of the perfect waveguide (layers containing Ni atoms at sites E and F).

To determine M_R , we have to define a Hilbert space with a basis $\{|R\rangle\}$, used to study the precessional motion of the spins in the matching region (layers containing atoms C and D). For a site belonging to the matching region in our $Fe_{0.5}Ni_{0.5}/Ni(100)$ system, the precession amplitudes can be written as

$$U_{\alpha\beta}(n, s, m) = \sum_{\nu} Z_{\nu}^m w_{\beta}(\alpha, \nu) R_{\nu}, \quad (2)$$

where R_{ν} is a unitary vector characterizing the evanescent waves, ν in basis $\{|R\rangle\}$; α represents one of the three directions x, y or z , and β the atomic sites in the matching region. $w_{\beta}(\alpha, \nu)$ are weighted coefficients associated with different evanescent modes and Z are phase factors for the Ni (100) surfaces satisfying the evanescence condition along the z direction into the slab substrate, normal to the alloy surface.

If we denote by $|U\rangle$ the spin precession vector of sites in the surface region, then it can be written as a block matrix comprising two parts: the irreducible part ($|Irr\rangle$) and the matching part ($|Mat\rangle$) which are matrices of dimensions 4×1 and 2×1 respectively where the former consists of displacements of sites forming the surface region (sites A, B, C and D). In a matrix form, M_R can be defined through

$$|U\rangle = \begin{pmatrix} |Irr\rangle \\ |Mat\rangle \end{pmatrix} = \begin{pmatrix} Id & 0 \\ 0 & R_1 \\ 0 & R_2 \end{pmatrix} \cdot \begin{pmatrix} |Irr\rangle \\ |R\rangle \end{pmatrix} = M_R \cdot \begin{pmatrix} |Irr\rangle \\ |R\rangle \end{pmatrix}.$$

I_d is a 4×4 identity matrix, and R_1 and R_2 define 1×1 square matrices (coefficients) which depend on the number of propagating modes of the perfect slab substrate regions. As a result, M_R is identified as:

$$M_R = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & R_1 \\ 0 & 0 & 0 & 0 & R_2 \end{pmatrix}.$$

The product of the M_D and M_R matrices form a square 5×5 matrix M_S . The localized states Ω induced by the ordered FeNi alloy monolayer can be accessed by setting $\det[M_S(5 \times 5)] = 0$. More details on how to form the matrix M_S can be found in various previous publications [29,22,46–49].

3.2. Computation of the surface magnonic local densities of states (LDOS)

In the Ni substrate the density of states (DOS) per site is strictly the same over all sites. In contrast, the magnetic sites at the surface of the present system have different atomic environments, and they hence present different local densities of states (LDOS) as a function of the sites. In this work, the most direct way to calculate the magnonic (LDOS) in the vicinity of the $Fe_{50}Ni_{50}/Ni(100)$ alloy surface, is through a formalism based essentially on the Green's functions and the PFMT matching technique. The Green operator G , obtained from the square matrix (M_S) of the system, can be expressed in the following form [47–50]

$$G(\phi_x, \phi_y, \Omega + i\epsilon) = [(\Omega + i\epsilon)I - M_S(\phi_x, \phi_y, Z, J_i)]^{-1}, \quad (3)$$

where Ω is the normalized frequency, ϵ is a tiny imaginary part added to avoid divergences in the calculations, and $(\phi_x$ and $\phi_y)$ are the phase factors along the x and y directions within the Brillouin zone in the range $[-\pi, \pi]$. Z is the previously defined phase factor and J_i are the system's exchange constants.

The spectral density matrix for a wave vector on the alloy surface, is given by the following relation

$$\rho_{(\alpha,\gamma)}^{(l,l')}(\phi_x, \phi_y, \Omega, Z, J_i) = \sum_m C_{\alpha,m}^l C_{\gamma,m'}^{l'} \delta(\Omega - \Omega_m) = \lim_{\epsilon \rightarrow 0^+} [Im G_{\alpha\gamma}^{ll'}(\phi_x, \phi_y, J_i, \Omega + i\epsilon)]. \quad (4)$$

In Eq. (4), l and l' represent two different spins on the atomic layers in the vicinity of the alloy surface, where α and $\gamma = x, y, z$ directions. $C_{\alpha,m}^l$ is the component of the spin precession vector l for the magnonic energy branch Ω_m , $Im G_{\alpha\gamma}^{ll'}$ is the imaginary part of the corresponding Green's function obtained from Eq. (3) and δ is the well known Dirac delta function.

The bulk density of states (DOS) is evaluated as the sum over all wave vector values corresponding to phase factors ϕ_x and ϕ_y at an energy $E = \hbar\Omega$ and is given by

$$D(\Omega) = \sum_{l\alpha} \sum_{\phi_x, \phi_y} \rho_{(\alpha,\gamma)}^{(l,l)}(\phi_x, \phi_y, \Omega, Z, J_i) = -\frac{1}{\pi} \sum_{l\alpha} \sum_{\phi_x, \phi_y} \lim_{\epsilon \rightarrow 0^+} [Im G_{\alpha\alpha}^{ll}(\phi_x, \phi_y, J_i, \Omega + i\epsilon)]. \quad (5)$$

On the other hand, the local density of states (LDOS) on a given site l belonging to an atomic layer near the alloy surface can then be computed as

$$D_l(\Omega) = \sum_{\alpha} \sum_{\phi_x, \phi_y} \rho_{(\alpha,\gamma)}^{(l,l)}(\phi_x, \phi_y, \Omega, Z, J_i) = -\frac{1}{\pi} \sum_{\alpha} \sum_{\phi_x, \phi_y} \lim_{\epsilon \rightarrow 0^+} [Im G_{\alpha\alpha}^{ll}(\phi_x, \phi_y, J_i, \Omega + i\epsilon)]. \quad (6)$$

4. Results and discussions

The exchange constants of the spin dynamic equations, DFT computed in Section 2, have the values: $J_{FeNi} = 8.73$ meV, $J_{NiNi} = 1.74$ meV for the nearest neighbours at the surface monolayer, $J_V = 7.21$ meV for Ni-Ni interactions in the bulk, and $J_{FeFe} = 6.82$ meV for next nearest Fe-Fe neighbours. This implies that the ratios $J_1 = 1.21$, $J_2 = 1$, $J_3 = 0.24$, $J_4 = 0.95$ and the spins are $S_{Fe} = S_{Ni} = 1$. Substituting these values in the above set of five equations to form the corresponding square matrix M_S and solving for the modes, we obtain the magnon dispersion curves

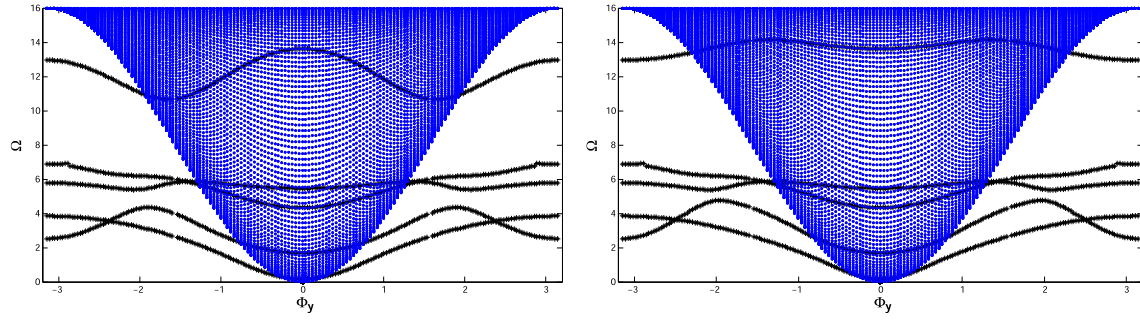


Fig. 3. (Left) No next nearest neighbour Fe-Fe magnetic exchange interactions in the surface alloy monolayer and (Right) With next nearest neighbour Fe-Fe magnetic exchange interactions. The black curves indicate dispersion branches, in the Brillouin zone, of the localized magnons at the surface of the system of an $\text{Fe}_{0.5}\text{Ni}_{0.5}$ alloy monolayer on Ni(100) substrates. These spin wave (magnon) eigenmodes propagate along the x- and y-directions, but are evanescent into the slab. The shaded regions represent the projected magnon bands of bulk Ni.

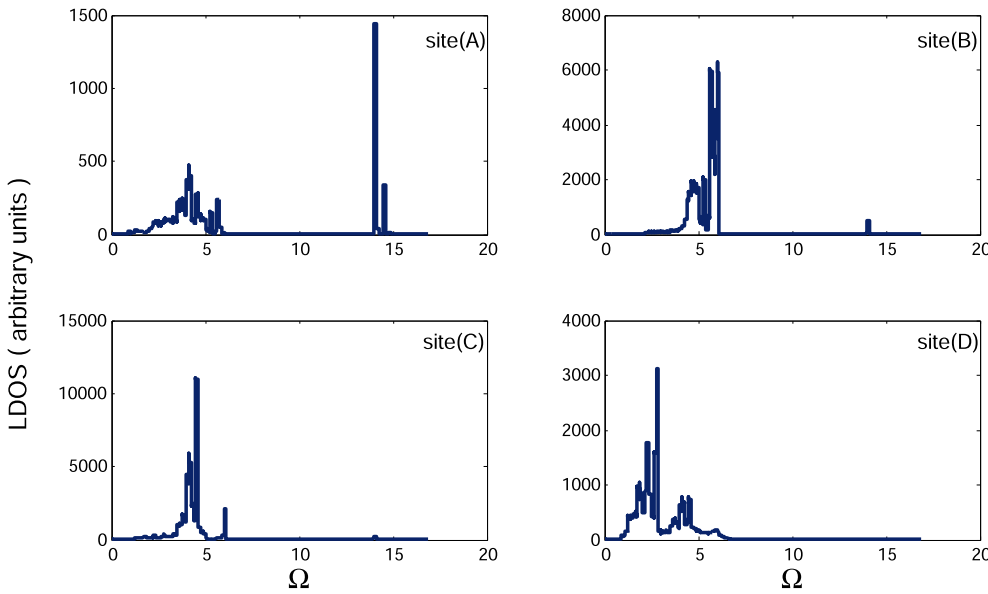


Fig. 4. Local density of states (LDOS), in arbitrary units, as a function of the normalized frequency Ω for Fe and Ni on the alloy (sites A and B) as well as for Ni sites belonging to the substrate layers (sites C and D). The Fe-Fe interactions are taken into consideration.

of Fig. 3.

To emphasize the importance of the DFT computations regarding the magnetic ground state of the system of a monolayer of fcc $\text{Fe}_{0.5}\text{Ni}_{0.5}$ alloy at the surface of an fcc Ni substrate, we present for comparison in Fig. 3(a) and Fig. 3(b) the structures of the dispersion of the surface localized magnon modes when next nearest neighbour Fe-Fe interactions are absent and present, respectively. The shaded area in the graphs represents the projection of the bulk fcc Ni magnon bands propagating along the y-direction.

In the absence of the Fe-Fe interactions, there are two branches of localized spin wave modes within $[0 - 3.69]$ and $[1.53 - 4.35]$ intervals of Ω . The third and fourth localized dispersion modes belong to the intermediate ranges $[4.74 - 5.82]$ and $[5.32 - 6.90]$ whilst the highest energy dispersion mode lies within $[10.29 - 12.96]$. Taking the Fe-Fe interactions into account, the only significant change occurs for the highest energy mode, which now propagates within a larger range within $[12.93 - 14.18]$. A smaller change occurs for one of the lowest magnonic modes namely $[1.53 - 4.35]$, which now has a slightly larger window of propagation in the range $[1.53 - 4.85]$.

The local density of states (LDOS), which in principle is a measurable quantity, incorporates the specific contributions from the localized spin-wave modes and the resonances, on sites A, B, C and D of the system as shown in Fig. 4. These are in arbitrary units and are demonstrated as a function of the normalized frequency Ω taking into account the realistic Fe-Fe interactions. These results reveal that for sites of type A, most of the contributions come from the $0 \leq \Omega \leq 6$

range with a unique high frequency contribution with the largest LDOS peak occurring at $\Omega \sim 14.01$. Restrictively, only the low frequency range ($0 \leq \Omega \leq 6$) contribute to the sites referred to as B, C and D with largest peaks taking place at ~ 6.00 , ~ 4.53 and 2.76 respectively. Due to symmetry, we expect that the resonant maximum frequency for site E would be the same as that for site D.

5. Conclusions

In this work, we have developed a robust theoretical model to investigate and establish the magnonic characteristics of the system of an ordered magnetic alloy monolayer $\text{Fe}_{0.5}\text{Ni}_{0.5}$ on Ni(100) slab substrates. Our results can be useful for ongoing research in magnonics and spintronics. The model consists of two complementary parts; the first is the DFT computations of the magnetic order and the exchange network between Ni and Fe irreducible representative sites at the surface nanostructure and in the bulk substrate; the second applies the PFMT method, both analytically and numerically, to compute the spin dynamics and establish the magnonic characteristics of the system.

The Fe-Fe next nearest neighbour exchange interactions within the surface alloy monolayer are essential for a realistic understanding of the magnonic characteristics of the system. When such interactions are considered, the highest mode propagates within a higher energy range and the propagation range of atoms within the matching region undergoes a marginal increase of around 0.5. The local densities of states (LDOS) have also been analyzed showing the resonant magnonic

energies for the different representative sites constituting the system. Exploring the effects of piling two or more magnetically ordered alloy monolayers, whether $\text{Fe}_{0.5}\text{Ni}_{0.5}$ or other alloys onto the Ni slab substrate, might cause more interesting changes to the magnonic dispersion branches; this will be the goal of a future work under preparation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

The DFT computations of the exchange parameters were performed on supercomputers at King AbdulAziz University's High Performance Computing Center (Aziz HPCC) (<http://hpc.kau.edu.sa>).

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at <https://doi.org/10.1016/j.jmmm.2020.166958>.

References

- [1] V.V. Kruglyak, S.O. Demokritov, D. Grundler, *J. Phys. D* 43 (2010) 264001.
- [2] S.A. Wolf, A.Y. Chitchekanova, D.M. Treger, *IBM J. Res. Dev.* 50 (2006) 101–110.
- [3] B. Lenk, H. Ulrichs, F. Garbs, M. Münzenberg, *Phys. Rep.* 507 (2011) 107–136.
- [4] S. Nikitov, T. Tailhades, *J. Magn. Magn. Mater.* 236 (2001) 320.
- [5] M. Binder, A. Weber, O. Mosendz, G. Woltersdorf, M. Izquierdo, I. Neudecker, J.R. Dahn, T.D. Hatchard, J. Thiele, C. Back, M. Scheinfein, *Phys. Rev. B* 74 (2006) 134404.
- [6] I. Radu, K. Vahaplar, C. Stamm, T. Kachel, N. Pontius, H.A. Dürr, T.A. Ostler, J. Barker, R.F.L. Evans, R.W. Chantrell, A. Tsukamoto, A. Itoh, A. Kirilyuk, Th. Rasing, A.V. Kimel, *Nature* 472 (2011) 205.
- [7] A. Mekonnen, A.R. Khorsand, M. Cormier, A.V. Kimel, A. Kirilyuk, A. Hrabec, L. Ranno, A. Tsukamoto, A. Itoh, Th. Rasing, *Phys. Rev. B* 87 (2013) 180406.
- [8] Kh. Zakeri, *Phys. Reports* 545 (2014) 47.
- [9] A.V. Chumak, A.A. Serga, S. Wolff, B. Hillebrands, M.P. Kostylev, *J. Appl. Phys.* 105 (2009) 083906.
- [10] M. Tsoi, A.G.M. Jansen, J. Bass, W.C. Chiang, V. Tsoi, P. Wyder, *Nature* 406 (2000) 462.
- [11] M. Krawczyk, D. Grundler, *J. Condensed Matter* 26 (2014) 123202.
- [12] F. Heussner, M. Nabinger, T. Fischer, T. Brächer, A.A. Serga, B. Hillebrands, P. Pirro, *Phys. Status Solidi RRL* 1800409–1800415 (2018).
- [13] E. Albisetti, D. Petti, G. Sala, R. Silvani, S. Tacchi, S. Finizio, S. Wintz, A. Calò, X. Zheng, J. Raabe, E. Riedo, R. Bertacco, *Comms. Phys.* 1 (2018) 56.
- [14] S. Wintz, V. Tiberkevich, M. Weigand, J. Raabe, J. Lindner, A. Erbe, A. Slavin, J. Fassbender, *Nat. Nanotechnol.* 11 (2016) 948.
- [15] T. Guo, M. Lin, J. Huang, C. Zhou, W. Tian, H. Yu, X. Jiang, J. Ye, Y. Shi, Y. Xiao, X. Bian, X. Feng, *J. Nanomater.* 8 (2018) 1–8.
- [16] A. Akbarzadeh, M. Samiei, S. Davaran, *Nanoscale Res. Lett.* 7 (2012) 144.
- [17] L.M. Rossi, N.J.S. Costa, F.P. Silva, R. Wojcieszak, *Green Chem.* 16 (2014) 2906–2933.
- [18] P.K. Amiri, *Electron Device Lett., IEEE* 32 (2011) 57–59.
- [19] V. Ashokan, M. Abou Ghantous, A. Khater, *J. Mag. Mag. Mat.* 396 (2015) 16.
- [20] M. Abou Ghantous, A. Khater, D. Ghader, V. Ashokan, *J. Appl. Phys.* 113 (2013) 094303.
- [21] V. Ashokan, M. Abou Ghantous, D. Ghader, A. Khater, *Thin Solid Films* 616 (2016) 6.
- [22] V. Ashokan, M. Abou Ghantous, D. Ghader, A. Khater, *J. Mag. Mag. Mat.* 363 (2014) 66.
- [23] E.A. Moujaes, A. Khater, M. Abou Ghantous, V. Ashokan, *Materialia* 4 (2018) 373–387.
- [24] A. Khater, L. Saim, R. Tigrine, D. Ghader, *Surf. Sci.* 672–673 (2018) 47–55.
- [25] E.A. Moujaes, A. Khater, M. Abou Ghantous, *J. Magn. Magn. Mater.* 391 (2015) 49.
- [26] T.G. Dargam, R.B. Capaz, B. Koiller, *Braz. J. Phys.* 27/A (1997) 299–304.
- [27] L. Bellaiche, D. Vanderbilt, *Phys. Rev. B* 61 (2000) 7877.
- [28] B. Bourahla, A. Khater, R. Tigrine, M. Abou Ghantous, *J. Phys.: Cond. Matter* 19 (2007) 266208.
- [29] A. Khater, B. Bourahla, M. Abou Ghantous, R. Tigrine, R. Chadli, *J. Eur. Phys. B* 82 (2011) 53.
- [30] M. Przybylski, S. Chakraborty, J. Kirschner, *J. Mag. Mag. Mater.* 234 (2001) 505.
- [31] Y. Li, C. Polaczky, D. Riegel, *J. Mag. Mag. Mater.* 165 (1997) 227–229.
- [32] L. Yichun, Z. Jiamin, Y. Jikang, D. Jinjhong, G. Guoyou, Y. Jianhong, *Rare Metal Mat. Eng.* 43 (2014) 2966–2968.
- [33] T.Y. Tashiro, M. Mizuguchi, T. Kojima, T. Koganezawa, M. Kotsugi, T. Ohtsuki, K. Takanashi, *J. Appl. Phys.* 117 (2015) 17E309.
- [34] G.-F. Li, S. Liu, S. Yang, Y. Du, *J. Nanomater.* 3 (2015) 1–5.
- [35] D. Spišák, J. Hafner, *J. Mag. Mag. Mater.* 272–276 (2004) 1184.
- [36] E.A. Smirnova, I.A. Abrikosov, B. Johansson, Yu.Kh. Vekilov, A.N. Baranov, V.S. Stepanyuk, W. Hergert, P.H. Dederichs, *Phys. Rev. B* 59 (1999) 14417–14423.
- [37] A. Al-Zubi, *Ab Initio Investigations of Magnetic Properties of Ultrathin Transition Metal Films on 4d Substrates vol. 16*, Forschungszentrum Jülich, Jülich, 2010.
- [38] J.F. Albersen, G.B. Jensen, J.M. Knudsen, *Nature* 273 (1978) 453.
- [39] R.S. Clarke Jr., E.R.D. Scott, *Am. Mineral.* 65 (1980) 624.
- [40] C.-W. Yang, D.B. Williams, J.I. Goldstein, *Geochim. Cosmochim. Acta* 61 (1997) 2943.
- [41] H. Ebert, D. Kodderitzsch, J. Minar, *Rep. Prog. Phys.* 74 (2011) 096501.
- [42] H. Ebert, *SPR-KKR package Version 7.7* on <http://ebert.cup.unimuenchen.de>.
- [43] C.G. Broyden, *Math. Comp.* 19 (1965) 577.
- [44] S.H. Vosko, L. Wilk, M. Nusair, *Can. J. Phys.* 58 (1980) 1200.
- [45] A.I. Liechtenstein, M.I. Katsnelson, V.P. Antropov, V.A. Gubanov, *J. Mag. Mag. Mater.* 67 (1987) 65.
- [46] D. Ghader, V. Ashokan, A. Khater, M. Abou Ghantous, *J. Eur. Phys. B* 86 (2013) 180–181.
- [47] A. Khater, M. Abou Ghantous, *Surface Sci. Lett.* 498 (2002) L97.
- [48] A. Khater Zerirgui, B. Bourahla, *J. Appl. Phys.* 111 (2012) 044907.
- [49] R. Chadli, A. Khater, R. Tigrine, *Eur. Phys. J. Appl. Phys.* 57 (2012) 21303.
- [50] D. Ghader, A. Khater, *J. Mag. Mag. Mater.* 482 (2019) 88–98.