

Energy of spin wave excitations in nickel monolayers

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1995 J. Phys.: Condens. Matter 7 3453

(<http://iopscience.iop.org/0953-8984/7/18/009>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.179

The article was downloaded on 13/05/2010 at 13:03

Please note that [terms and conditions apply](#).

Energy of spin wave excitations in nickel monolayers

M V Tovar Costa†, R B Muniz† and J d'Albuquerque e Castro‡§

† Instituto de Física - Universidade Federal Fluminense, Avenida Litorânea s/n Gragoatá, 24210-340 Niterói, RJ, Brazil

‡ Department of Mathematics, City University, Northampton Square, London EC1V 0HB, UK

Received 16 February 1995

Abstract. The spin wave stiffness constant $D(\hat{q})$ of unsupported fcc (100), (110), and (111) nickel monolayers are calculated for different directions, \hat{q} , of spin wave propagation. It is shown that D is isotropic for the (100) and (111) orientations, and highly anisotropic for the (110) orientation. Results indicate that the strength of the exchange coupling between nearest neighbour magnetic moments is quite sensitive to the effective space dimensionality as well as the crystalline structure of the system.

1. Introduction

Artificial metallic systems such as thin films and multilayers exhibit remarkable magnetic properties, which are of interest from both scientific and technological points of view. In particular, the magnetic properties of transition metal ultra-thin films have been intensively studied because of their potential applications in magnetic recording devices.

Regarding ferromagnetic films, special interest has been focused on the determination of the strength of exchange interactions between magnetic moments and the dependence of the magnetization, M , on the temperature, T , which can be measured by spin polarized electron spectroscopy [1]. It is known that the magnetic properties of metallic systems are intimately related to their atomic structures, hence to the dimensionality of the systems. For instance, it has been found recently [2] that at low temperatures, the surface magnetization of metallic overlayers obeys a pseudo- $T^{3/2}$ law, with a prefactor that strongly depends on the surface orientation. Such dependence arises because of the differences in the surface lattice structure for each crystalline orientation. Therefore, one can expect significant changes in the magnetic behaviour of the systems as the dimensionality is reduced from three to effectively two (ultra-thin films).

The low-temperature behaviour of $M(T)$ is controlled by long wavelength spin wave excitations. The energy a spin wave propagating with vector q is given by $\hbar\omega(\hat{q}) = D(\hat{q})q^2$, where the exchange stiffness constant $D(\hat{q})$ may, in general, depend on the direction $\hat{q} = q/|q|$. The magnitude of D depends on the strength of the exchange coupling between the magnetic moments in the system. Therefore, measurements of $M(T)$ in the low-temperature region may be used to estimate the value of those interactions [1, 5]. In previous theoretical works [3, 4, 5] the interpretation of such experiments was based on phenomenological exchange Hamiltonians. However, for the description metallic systems it is more appropriate to use the itinerant electron model, which relates the magnetic properties to the electronic structure of the material.

§ Permanent address: Instituto de Física, Universidade Federal Fluminense, 24210-340 Niterói, RJ, Brazil.

The present work is concerned with the study of the long-wavelength spin wave excitations in Ni unsupported monolayers. The approach is based on a multi-orbital tight-binding model and the RPA approximation, and the contributions to D coming from intra- and inter-band effects are investigated. Three different monolayer orientations are considered, namely FCC (100), (110), and (111). These three monolayers have different crystalline and electronic structures. As a consequence, the spectrum of long wavelength spin excitations differ significantly from one monolayer to another. In particular, for the (110) orientation the dispersion relation of magnons turns out to be highly anisotropic, i.e. strongly dependent on the direction of spin wave propagation. Comparison of the calculated results of D indicates that the magnitude of the effective exchange interaction, J , between nearest neighbour (NN) magnetic moments in those low-dimensional systems strongly depends on the crystalline structure, increasing considerably as the number of NN is reduced. This is an important point, which clearly illustrate the deep relation between the crystalline structure, the electronic structure, and the magnetic properties of metallic systems. In addition, it shows that the effective exchange interactions, J , that appear in phenomenological spin Hamiltonians, frequently used to describe the magnetic properties of metallic systems, cannot be taken as transferable parameters from one crystalline structure to another.

We have organized this paper as follows. In section 2 we discuss the basic theory used to calculate $D(\hat{q})$, and in section 3 we present our results and conclusions.

2. Theory

The electronic structure of the systems is described by a multi-orbital tight-binding model Hamiltonian given by

$$H = \sum_{\mathbf{k}} \sum_{\mu, \nu, \sigma} V_{\mu\nu}(\mathbf{k}) c_{\mu\mathbf{k}\sigma}^{\dagger} c_{\nu\mathbf{k}\sigma} + H_{\text{int}} \quad (1)$$

where the first term corresponds to the one-electron band energy and H_{int} represents the electron–electron effective interaction, which we assume contains only spin-invariant intra-atomic terms. $c_{\mu\mathbf{k}\sigma}^{\dagger}$ creates an electron with spin σ in a Bloch state $|\mu\mathbf{k}\sigma\rangle$ with orbital μ and wavevector \mathbf{k} . The ground state is treated in the Hartree–Fock (HF) approximation, and the one-electron energies $E_{n\mathbf{k}\sigma}$ associated with band n are the solutions of

$$\sum_{\nu} H_{\mu\nu}^{\sigma}(\mathbf{k}) a_{n\nu\sigma}(\mathbf{k}) = E_{n\mathbf{k}\sigma} a_{n\mu\sigma}(\mathbf{k}) \quad (2)$$

where

$$H_{\mu\nu}^{\sigma}(\mathbf{k}) = H_{\mu\nu}^0(\mathbf{k}) - \frac{1}{2} \Delta_{\mu} \delta_{\mu\nu} \sigma. \quad (3)$$

Here $\sigma = \pm 1$ for \uparrow and \downarrow spins, respectively, $H_{\mu\nu}^0(\mathbf{k})$ is equal to $V_{\mu\nu}(\mathbf{k})$ plus a \mathbf{k} -independent term of the form $\lambda_{\mu} \delta_{\mu\nu}$ and Δ_{μ} is also \mathbf{k} -independent. We consider d bands only, and assume that $\Delta_{\mu} = \Delta$ is independent of μ (rigid exchange splitting), which is a good approximation for Ni. $H_{\mu\nu}^0(\mathbf{k})$ is parametrized by canonical two-centre hopping integrals [6] $dd(\sigma, \pi, \delta) = (-6, 4, -1)(W/2.5)(S/R)^5$, where R is the interatomic distance, W is the canonical d band width parameter, and S is the Wigner–Seitz radius. Figure (1) shows the calculated density of states curves for one spin direction for; (a) FCC(100), (b) (110) and (c) (111) Ni monolayers. For the (110) orientation we have taken into account first and second NN hoppings. The shapes of the density of states curves are markedly different, reflecting the distinct atomic arrangements of the three structures. These correspond to the

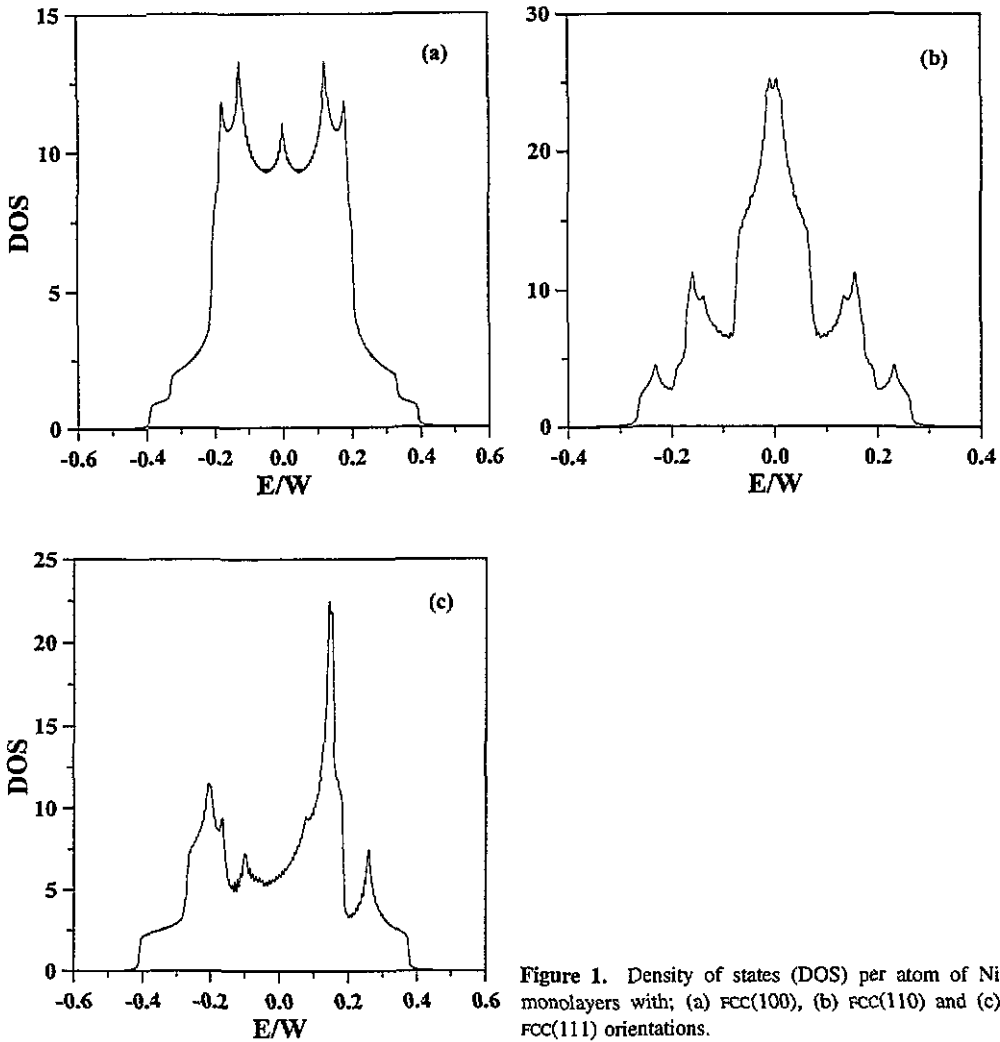


Figure 1. Density of states (DOS) per atom of Ni monolayers with; (a) FCC(100), (b) FCC(110) and (c) FCC(111) orientations.

square, rectangular, and honeycomb lattices for the FCC (100), (110), and (111) monolayers, respectively.

To calculate the long wavelength spin wave energies we start with the general and exact formula for D derived by Edwards and Fisher [7]. We follow Edwards and Muniz [8] and evaluate D within the random phase approximation. Here, however, we do not average D over the direction \hat{q} and end up with the expression

$$\begin{aligned}
 (N_{\uparrow} - N_{\downarrow}) D(\hat{q}) &= \sum_{n,k} [B_{n\uparrow}(\hat{q}, k) N_{nk\uparrow} + B_{n\downarrow}(\hat{q}, k) N_{nk\downarrow}] \\
 &\quad - \sum_{m,n,k} C_{mn}(\hat{q}, k) \frac{N_{nk\uparrow} - N_{mk\downarrow}}{E_{mk\downarrow} - E_{nk\uparrow}}
 \end{aligned}
 \tag{4}$$

where

$$B_{n\sigma}(\hat{q}, k) = \frac{1}{2} \sum_{\mu, \nu} [(\hat{q} \cdot \nabla)^2 V_{\mu\nu}(k)] a_{n\mu\sigma}^*(k) a_{n\nu\sigma}(k)
 \tag{5}$$

$$C_{mn}(\hat{q}, \mathbf{k}) = \left| \sum_{\mu, \nu} [(\hat{q} \cdot \nabla) V_{\mu\nu}(\mathbf{k})] a_{n\mu\downarrow}^*(\mathbf{k}) a_{n\nu\uparrow}(\mathbf{k}) \right|^2 \quad (6)$$

and $N_{nk\sigma} = a_{n\mu\sigma}(\mathbf{k}) a_{n\mu\sigma}^*(\mathbf{k})$ are the HF occupation numbers, with $a_{n\mu\sigma}(\mathbf{k})$ is given by equation (2).

As in [8], it is possible to separate the contributions from intra-band and inter-band terms in equation (4). In the rigid exchange splitting approximation we obtain, after some manipulations, that

$$(N_{\uparrow} - N_{\downarrow}) D(\hat{q}) = \frac{1}{2} [M(\hat{q}, E_{+}) + M(\hat{q}, E_{-})] - \frac{1}{\Delta} \int_{E_{-}}^{E_{+}} dE M(\hat{q}, E) \\ + \sum_{\substack{m, n, k \\ m \neq n}} C_{mn}(\hat{q}, \mathbf{k}) [N_{nk\uparrow} - N_{mk\downarrow}] \frac{\Delta}{(E_{mk} - E_{nk})(E_{mk} - E_{nk} + \Delta)} \quad (7)$$

where, for a two-dimensional system,

$$M(\hat{q}, E) = \frac{A}{(2\pi)^2} \sum_n \int_{E_{nk}=E} dl \frac{[(\hat{q} \cdot \nabla) E_{nk}]^2}{|\nabla E_{nk}|}. \quad (8)$$

Here E_{+} and E_{-} are the spin \uparrow and \downarrow Fermi energies, respectively, A is the area of the two-dimensional Brillouin zone, and the integral in equation (8) is over a contour of constant energy E . The last term on the right hand side of equation (7) contains the inter-band contributions to D . When this last term is neglected, a \hat{q} -dependent extension of the expression for D previously derived by Wakoh [9] for isotropic ferromagnetic systems is obtained.

On the basis of the results derived above we have calculated $D(\hat{q})$ for different Ni monolayers, corresponding to FCC(100), (110) and (111) orientations. In each case the relative importance of the contributions on D coming from inter-band terms is evaluated.

3. Results and conclusions

Within the rigid exchange splitting approximation, Δ is related to the magnetic moment per atom, m , and the effective intra-atomic interaction, U , by the equation $\Delta = Um$. Typical local spin density functional values of W and U for Ni are 3.89 eV and 1 eV, respectively [10, 11, 12]. Thus, for a fixed value of U , the values of Δ to be used in the calculation of D can be determined from the saturation magnetization of each monolayer. For the FCC(100) Ni we have taken the calculated magnetic moment per atom $m \simeq 1.0\mu_B$, [10, 11, 12] whereas for the other two orientations we estimate m as follows: In view of the quasi one dimensional character of the FCC(110) structure, we use in this case the calculated value of $m \simeq 1.1\mu_B$ for one dimensional (1D) Ni [13]. We also note that the values of m for bulk Ni, FCC(100) Ni monolayer, and 1D Ni when plotted against the number of NN sites (12, 4, and 2, respectively) lay on the straight line, as shown in figure (2). We use this fact to estimate m for the FCC(111) orientation (6 NN) as $0.9\mu_B$.

Figure (3) presents results for D as a function of the spin wave propagation direction \hat{q} for the three monolayer orientations, evaluated from equation (4). In all cases θ is the angle between \hat{q} and a line joining first NN sites. Calculations for the FCC(110) orientation include both first and second NN hoppings. The inclusion of second NN hoppings for the other two structures does not lead to any significant change in the results for D . We find that D is isotropic in the FCC(100) and (111) monolayers orientations, and highly anisotropic in the (110) case. The origin of such anisotropy lays on the crystalline structure of the

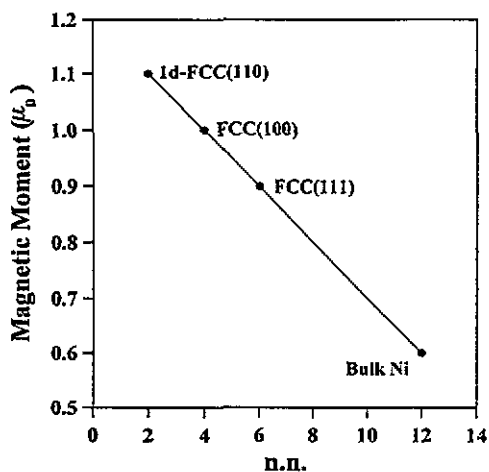


Figure 2. Magnetic moment as a function of the number of nearest neighbour (NN) atoms in bulk Ni, FCC(100), (110), and (111) Ni monolayers.

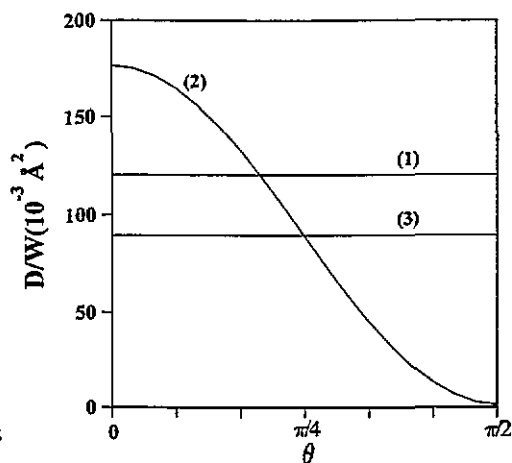


Figure 3. Exchange stiffness constant D as a function of the spin wave propagation direction θ for FCC(100) (curve 1), (110) (curve 2) and (111) (curve 3) Ni monolayers.

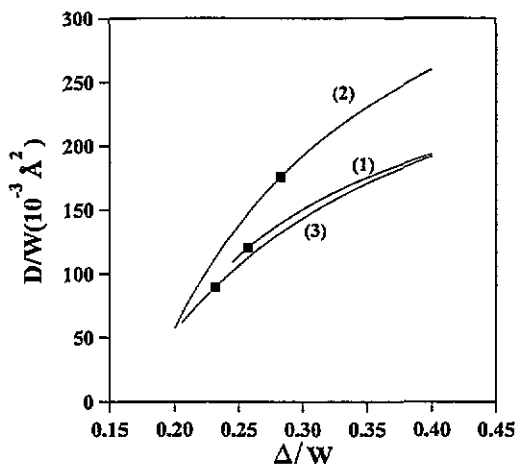


Figure 4. Exchange stiffness constant $D(\theta = 0)$ as a function of the exchange splitting Δ for FCC(100) (curve 1), (110) (curve 2), and (111) (curve 3) Ni monolayers. The values of Δ used in obtaining figure 3 are indicated on each curve.

FCC(110) monolayer. It consists of linear chains of NN sites, that are connected by second NN hoppings. As a consequence, the exchange interaction between the chains turns out to be rather weak, which makes it relatively easy to excite long wavelength spin waves propagating perpendicularly to the chains ($\theta = \pi/2$).

It is also interesting to investigate the dependence of D on the value of the exchange splitting. Figure (4) shows curves of $D(\theta = 0)$ as a function of Δ for the three monolayer orientations. The corresponding values of m are kept fixed and equal to those estimated

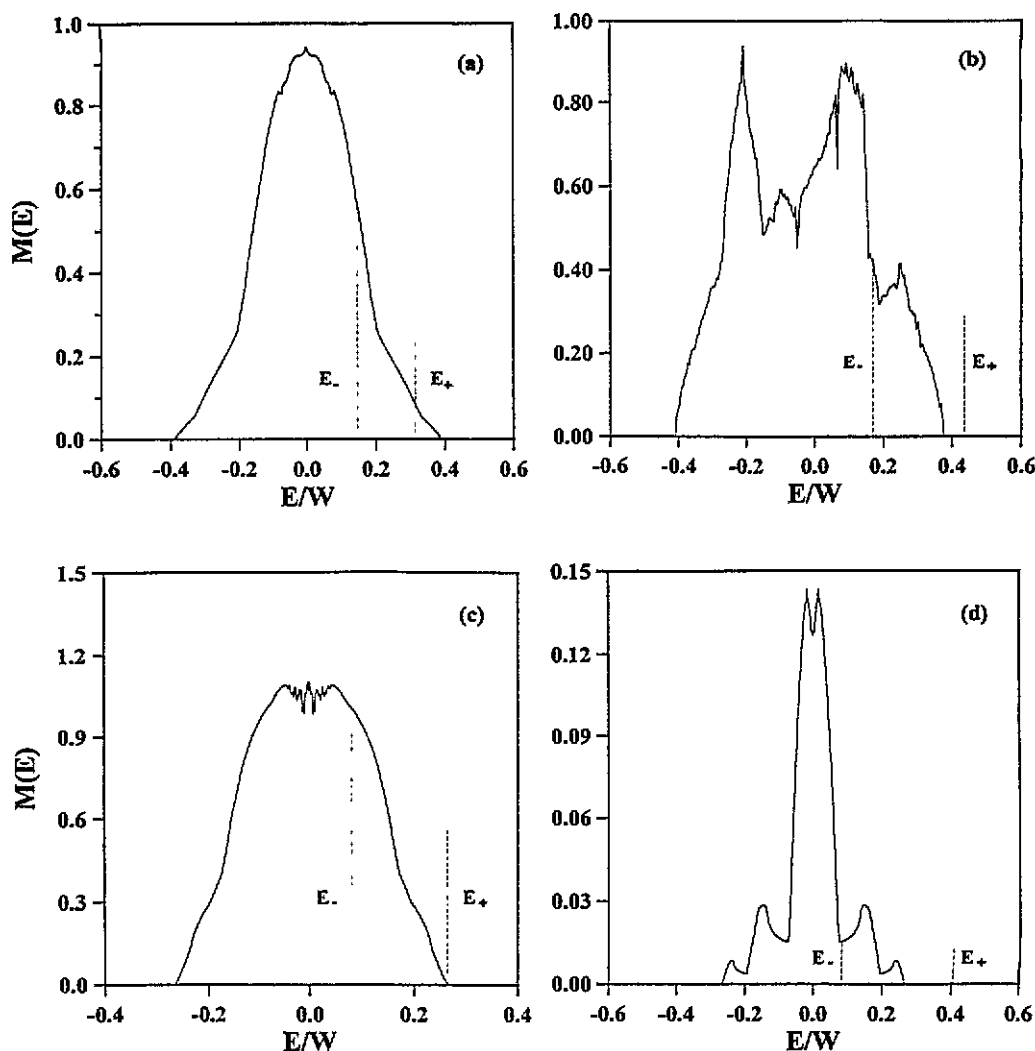


Figure 5. $M(\theta = 0, E)$ for FCC(100) (a) and (111) (b) Ni monolayers. Results of $M(\theta = 0, E)$ and $M(\theta = \pi/2, E)$ for FCC(110) Ni monolayer are shown in (c) and (d), respectively.

above, and hence a variation of Δ represents a variation of U . For comparison, the values of Δ used in obtaining figure (3) are indicated on each curve.

A remarkable point regarding the results in both figures (3) and (4) is the considerable difference between the values of $D(\theta = 0)$ for the three monolayers orientations. Since the magnetic moment in all cases is close to $1 \mu_B$ and the distance between NN is the same, this implies that the effective exchange interaction J between NN Ni atoms differs considerably from one monolayer to the other. In fact, from our results we conclude that for the three Ni monolayers we have that $(J_{111} < J_{100} < J_{110})$, in other words, the effective exchange coupling increases as the number of NN decreases. Therefore, contrary to what is usually assumed in Heisenberg-like model description of the low-temperature behaviour of metallic magnetic materials, our present calculation shows that J cannot be regarded as a transferable parameter. This is a clear manifestation of the intimate relation between the

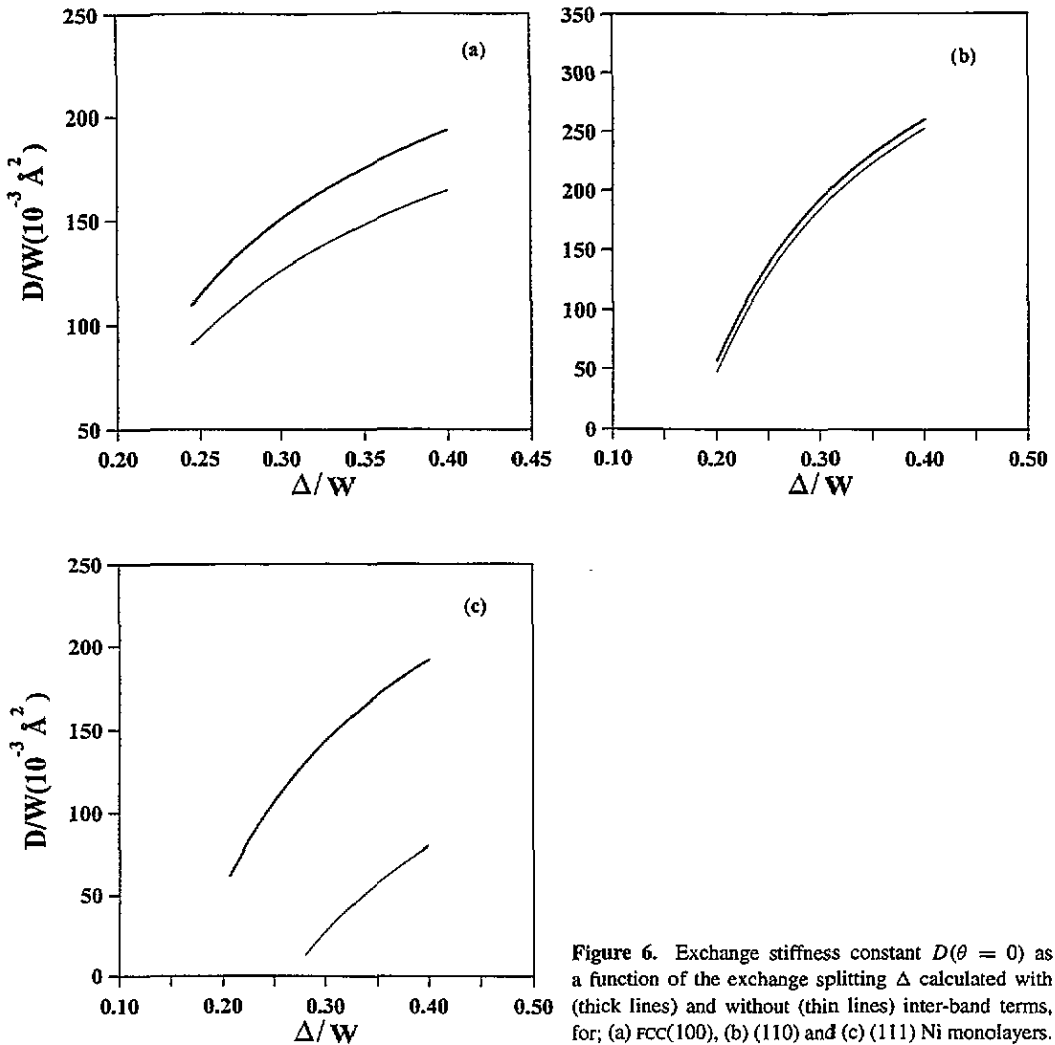


Figure 6. Exchange stiffness constant $D(\theta = 0)$ as a function of the exchange splitting Δ calculated with (thick lines) and without (thin lines) inter-band terms, for: (a) fcc(100), (b) (110) and (c) (111) Ni monolayers.

magnetic coupling in the ground state and the electronic structure of the system, which is quite different in the three cases under consideration here.

Finally, it is also interesting to investigate the importance of the contributions from inter-band effects to the value of D . It can be assessed in each case by considering just the first two terms on the RHS of equation (7). Figure (5) depicts the curves of $M(\hat{q}, E)$ for the three monolayers. For the isotropic cases, namely FCC(100) and (111), only the results for $\theta = 0$ are shown, whereas for FCC(110) calculations were performed for $\theta = 0$ and $\theta = \pi/2$. In the latter case we note that the shape of the $M(\hat{q}, E)$ curve is rather similar to the corresponding density of states. This fact can be understood by noticing that the dispersion in the band structure $E_{n,k}$ perpendicularly to the linear chains is quite small. Thus, to a first approximation, one can replace the numerator in the integrand in equation (8) for $\theta = \pi/2$ by its average value along the integration contour. Hence $M(\hat{q}, E)$ becomes proportional to the density of the states. Figure (6) shows results for $D(\theta = 0)$ as a function of Δ , for the three monolayer orientations, calculated with (thick lines) and without (thin

lines) inter-band terms. The difference between the results of the two calculations for the cases of the (100) and (111) orientations illustrates the importance of a proper multi-orbital description of the electronic structure and magnetic properties of metallic systems. Thus, it might seem surprisingly the fact of the contribution from the inter-band terms being so small for the (110) orientation. The reason for this, however, is the quasi-one-dimensional character of the atomic arrangement in the (110) monolayer and the fact that d orbitals with different symmetries on a linear chain almost do not hybridize.

In conclusion, we have investigated the spectrum of spin wave excitations in Ni monolayers. The calculation of the stiffness constant, D , for three monolayer orientations has revealed how sensitive to the crystalline structure the magnetic properties of those low-dimensional systems are. In particular, the strong anisotropy in the dispersion relation of magnons in FCC (110) monolayers can be easily understood in terms of the corresponding underlying crystalline structure. One of the most important conclusion that we draw from the results we have obtained is that the effective exchange interaction between NN Ni atoms in those systems strongly depends on the crystalline structure, and cannot be taken as a transferable parameter from one structure to another.

Acknowledgments

This work was partially supported by Conselho Nacional de Desenvolvimento Científico e Tecnológico /CNPq and Financiadora de Estudos e Projetos/Finep of Brazil.

References

- [1] Siegmann H C, Mauri D, Scholl D and Kay E 1988 *J. Physique Coll.* **49** C8
Mauri D, Siegmann H C, Scholl D and Kay E 1989 *Phys. Rev. Lett.* **62** 1900; 1989 *Appl. Phys. A* **49** 439
- [2] d'Albuquerque e Castro J, Mathon J, Muniz R B 1995 *J. Magn. Magn. Mater.* **140-144** at press
- [3] Mathon J 1990 *J. Magn. Magn. Mater.* **22** 168
- [4] Continentino M A and Lins de Mello E V 1990 *J. Phys.: Condens. Matter* **2** 3131
- [5] Scholl D, Donath M, Mauri D, Kay E, Mathon J, Muniz R B and Siegmann H C 1991 *Phys. Rev. B* **43** 13309
- [6] Pettifor D G 1977 *J. Phys F: Met. Phys.* **7** 613
- [7] Edwards D M and Fisher B 1971 *J. Physique Coll.* **32** C1
- [8] Edwards D M and Muniz R B 1985 *J. Phys. F: Met. Phys.* **15** 2339
- [9] Wakoh S, Edwards D M and Wohfarth E P 1971 *J. Physique Coll.* **32** C1 1073
- [10] Jepsen O, Madsen J and Andersen O K 1982 *Phys. Rev. B* **26** 2790
- [11] Zhu X and Hermanson J 1983 *Phys. Rev. B* **27** 2092
- [12] Norffke J and Fritsche L 1981 *J. Phys. C: Solid-State Phys.* **14** 89
- [13] Weinert M and Freeman A J 1983 *J. Magn. Magn. Mater.* **38** 23