Magnetic moments and exchange interactions in $Fe_{0.82}Ni_{0.18}$/V bcc (001) multilayers

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The magnetic ordering and average magnetization of multilayers are greatly affected by the interface structure of the system. In this paper, interface effects are discussed, and their impact on the amplitude and period of the interlayer exchange coupling and the magnetic moments are investigated for the $Fe_{0.82}Ni_{0.18}$/V body-centered-cubic (001) system. By modeling these effects by first principles calculations we find good agreement with experiments over the whole investigated range of layer thicknesses. In addition, as different interface effects give different fingerprints on the interlayer exchange coupling and magnetization, we are able to make an estimate of the interface structure of the different experimental samples by comparing experiment to theory.

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I. INTRODUCTION

During the past 15 years, experimental and theoretical studies on a class of magnetic materials—metallic multilayers—have drawn a great deal of attention[1,2] partly due to the applicative potential of such materials in industry, and partly due to the intriguing phenomena which appear in these systems, such as the giant magneto resistance (GMR) and the interlayer exchange coupling (IEC)—the coupling between two ferromagnetic layers separated by a spacer layer. A common goal of these studies is to investigate the dependence of the overall magnetization and IEC on the constituent materials, their structure and thickness, etc. A multilayered system is naturally characterized by a modulation of chemical composition and, thus, the appearance of transition zones, or interfaces, between the constitutive elements. Considerations of the interface structure are particularly important when analyzing the experimental results on magnetization and IEC.[3] In general the interface topology of a multilayer depends on the constituent structures and growth conditions and is described in terms of interface defects, such as interface roughness and intermixing, misfit dislocations and strain, etc. The effects of strain and misfit dislocations are possible to estimate by relaxing the multilayer structure and introducing a *k*-point dependent cutoff of the oscillations.[4] The effects of roughness[4–6] are easy to model by averaging the IEC over several spacer thicknesses and intermixing[7–9] by introducing an alloy in the interface region. Both effects can also be modeled simultaneously.[10] There are also many experimental studies on the interface qualities in multilayers but the main problem is usually that correlated and uncorrelated roughness are indistinguishable from each other and from interface alloying.[3,11,12] A third way of obtaining information about interface qualities is to model the growth process itself by means of kinetic Monte Carlo simulations.[13–15]

The Fe/V multilayer system, which is closely related to $Fe_{0.82}Ni_{0.18}$/V (from now on referred to as FeNi/V), has been shown to be difficult to understand theoretically[16–19] because of structural interface effects that are problematic to model. For epitaxial Fe/V (001) films, the strength of the IEC varies with the V thickness and has been investigated for, e.g., 3 monolayers (ML), 7 ML, and 15 ML of Fe.[11,20,21] The results show that the IEC is substantially affected by the growth mode (strain, etc.). The strain induced by the lattice mismatch at the interface between the two materials in a multilayer/superlattice is related to the growth mode of the superlattice in the force balance theory.[22] In Fe/V (001) superlattices the lattice mismatch between Fe and V is rather large (5%), and experiments have shown that the growth becomes incoherent at $\sim$15–16 ML of V.[23] Above this critical thickness the strain is relaxed by the introduction of misfit dislocations, which results in incoherent interfaces. Misfit dislocations affect the coupling periods in the asymptotic limit of large spacer widths by damping the amplitudes that correspond to extremal spanning vectors on the Fermi surface where the angle between the Fermi velocity and the out of plane direction is large.[4] Below the critical thickness the film is strained by the substrate lattice and coherent, pseudomorphic interfaces are formed between the two metals.

Replacing Fe with an $Fe_{0.82}Ni_{0.18}$ alloy leads to two important changes. First of all the magnetic anisotropy is lowered and this simplifies the interpretation of the experiments and the comparison to the theoretical results. The anisotropy constant, *K*, at 10 K for bulk FeNi has been estimated to be a factor of 3 lower than for Fe at the same temperature.[3] Second, the strain in the interface is relieved and the structural properties are improved. Consequently, the system is an example where the constituent materials are such that the effects of strain and misfit dislocations are small and in order to make precise comparisons with experiments only roughness and intermixing need to be modeled.[23] The scope of this paper is to demonstrate the crucial importance and success of modeling the growth related effects such as interface rough-

ness and interface intermixing in order to reproduce experimental findings.

As we shall see later, interface roughness and interface intermixing affect the IEC and average magnetic moments differently. By first studying the effect of roughness and intermixing on the magnetization and coupling we can later use this information to characterize the interface structure of a system. By comparing the behavior of the theoretically calculated IEC and magnetic moments for perfect structures to the experimental results and investigating to which extent they are modified when the interface structure is changed, we aim to show that it is possible to identify quantitatively the extent and nature of the interface structure.

II. THEORY

A. Method of calculations

The IEC, here defined as the energy difference between the antiferromagnetic (AFM) and the ferromagnetic (FM) configuration, $J=E_{\mathrm{AFM}}-E_{\mathrm{FM}}$, was obtained by total energy calculations. These first principles, self-consistent electronic structure calculations were performed by means of the spin-polarized interface Green's function technique, based on the linear muffin-tin orbitals (LMTO) method within the tight-binding, frozen core and atomic sphere approximations. The method was developed by Skriver and Rosengaard.[24] Furthermore, we have used the local spin-density approximation as parametrized by Perdew-Wang[25] and the principal layer technique.[26] The alloys were treated within the coherent potential approximation (CPA).[27–29] Great care was taken to converge all calculations both in total energy and *k*-space sampling. We found that 528 *k*-points in the irreducible Brillouin zone were sufficient to obtain convergence in all considered cases.

B. Modeling interface structure

In a superlattice, the multilayer structure is in general distorted at the interfaces due to the lattice mismatch. When two metals are forced to grow with the same in-plane lattice constant the resulting contraction or expansion is compensated by a change in the interplanar distances. This lattice relaxation has mainly an effect on the phase of the IEC[30] but may also affect the spin polarization of the magnetic layers[17] and thus indirectly the amplitude of the IEC. In order to estimate the influence of lattice relaxations on the magnetic layers we compared total magnetic moments for relaxed and unrelaxed calculations of Fe/V multilayers, that are very similar to our system. We observe that full potential LMTO calculations on multilayers with experimentally obtained structures from Refs. 31 and 32 and results from Ref. 10 where the structure was assumed to be ideal, agree within 5% regarding total magnetizations of the samples. In terms of layer magnetizations the differences are somewhat larger but we conclude that relaxations have a small effect on the total magnetization. Additionally, Ni is introduced in our system in order to reduce the strain in the multilayer and our assumption is then that structure relaxations will play an even less important role in the FeNi/V system.

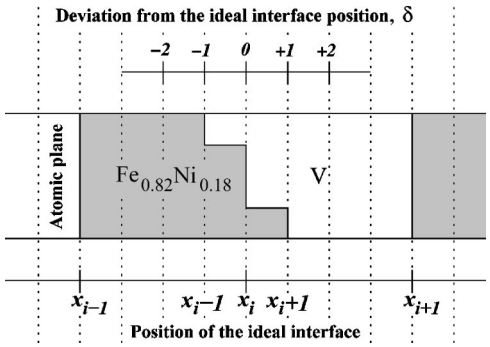

FIG. 1. Schematic model of an FeNi/V multilayer. Each interface between FeNi and V is labeled by a number *i*. The ideal position for this interface in terms of atomic planes is labeled x_i.

Considering effects where we neglect all types of distortions to the general underlying structure of the superlattice, all defects are associated with the arrangement of different kinds of atoms with respect to their positions in an ideal multilayer structure. Consequently, at an interface there may be corrugations with varying height, size, and density. This introduces a wide span of possible configurations to be modeled. The large range of possible interface structures can for simplicity be reduced to two different effects that are of main importance: interface roughness and interface intermixing. Interface roughness denotes formation of extended protrusions and depletions of a specific atom species at the interface, while interface intermixing represents formation of an alloy around the interface. When combined, interface roughness and interface intermixing are believed to capture most of the effects of the real structural disorder.[10]

The current approach is to create simple models that characterize the most significant parts of the deviations from ideal multilayers in terms of the effects on the IEC and the magnetization. For both interface roughness and intermixing we use models that, as we shall see later, permit us to specify the deviation in terms of a single parameter, giving in total two independent parameters.

C. Model for interface roughness

A scheme for incorporating roughness into general multilayer properties, such as interlayer exchange coupling or magnetic moment, will be derived. The main idea follows the models outlined in Refs. 7 and 10. For simplicity we assume that the quality of one individual interface is independent of the other interfaces (i.e., no correlated roughness). However, correlated roughness does not affect the thickness of the layers and does thus not influence the magnetic moment or IEC in our model. Correlated roughness has been shown to affect the IEC by the interaction of magnetic dipoles on the interfaces resulting in the orange peel coupling.[33]

Some terminology needs to be introduced in connection to our model. For each interface between two materials in a multilayer we define an intended, ideal position x_i, where *i* is the label of the interface as shown in Fig. 1. In a multilayer with perfect interfaces, x_i is the position of the interface.

TABLE I. Probabilities for the whole configuration space of roughness deviations for $FeNi_4/V_{15}/FeNi_4$ with $\sigma=0.2$.

	n_{FeNi}	2	3	4	5	6
$n_V=13$	2	0	0	0	0	0
	3	0	0	0	0	0
	4	0	0	0.16	0.48	0.16
	5	0	0	0.48	1.44	0.48
	6	0	0	0.16	0.48	0.16
$n_V=14$	2	0	0	0	0	0
	3	0	0	0.48	1.44	0.48
	4	0	0.48	2.88	4.80	1.44
	5	0	1.44	4.80	2.88	0.48
	6	0	0.48	1.44	0.48	0
$n_V=15$	2	0	0	0.16	0.48	0.16
	3	0	1.44	4.80	2.88	0.48
	4	0.16	4.80	13.28	4.80	0.16
	5	0.48	2.88	4.80	1.44	0
	6	0.16	0.48	0.16	0	0
$n_V=16$	2	0	0.48	1.44	0.48	0
	3	0.48	2.88	4.80	1.44	0
	4	1.44	4.80	2.88	0.48	0
	5	0.48	1.44	0.48	0	0
	6	0	0	0	0	0
$n_V=17$	2	0.16	0.48	0.16	0	0
	3	0.48	1.44	0.48	0	0
	4	0.16	0.48	0.16	0	0
	5	0	0	0	0	0
	6	0	0	0	0	0

Deviations of the interface by the distance δ is described in terms of a probability function $p_i(\delta)$.

If the roughness is symmetric across the interface and the same for all interfaces, and if roughness only extends ±1 layer from the intended interface, we can uniquely specify the probability function of the interface deviation with just one parameter, σ. This parameter then describes the quality of all the interfaces in our sample with respect to roughness, as follows:

$$p_i(-1)=\sigma,$$

$$p_i(0)=1-2\sigma,$$

$$p_i(1)=\sigma. \tag{1}$$

The layer thickness of layer i is defined as $N_i=x_{i+1}-x_i$. For a system with M interfaces the probability of a configuration with layer thicknesses $N_1, N_2, \ldots, N_{M-1}$ deviating from the ideal thickness configuration $n_1, n_2, \ldots, n_{M-1}$, may be written as

$$P(N_1,N_2,\ldots,N_{M-1})=\sum_{\delta=-1}^{\delta=1} p_1(\delta)\prod_{i=2}^{M} p_i\Big(\delta+\sum_{j=1}^{i-1}N_j-n_j\Big). \tag{2}$$

With *ab initio* calculations, properties such as layer magnetic moment and exchange energy are calculated for a set of perfect layer thicknesses. To get a quantity which can be compared to experiments, we have to perform a weighted average over configurations (cf. Table I) that deviate from the intended ideal structure. The calculated property (e.g., magnetic moment) is denoted Ω and the average is calculated as

$$\hat{\Omega}(n_1,n_2,\ldots,n_{M-1})=\sum_{\delta_1\delta_2\cdots\delta_{M-1}} P(n_1+\delta_1,n_2+\delta_2,\ldots,n_{M-1}+\delta_{M-1})\Omega(n_1+\delta_1,n_2+\delta_2,\ldots,n_{M-1}+\delta_{M-1}). \tag{3}$$

Table I is an illustration of the function $P(n_{FeNi},n_V,n_{FeNi})$ specifically for $FeNi_4/V_{15}/FeNi_4$, with roughness $\sigma=0.2$. When calculating a property for this geometry, including the effect of roughness, we perform a configurational sum of the property over all relevant configurations. Since the example is for a trilayer system, a configuration is represented by three numbers, i.e., the layer thicknesses of the three regions of the trilayer. The table gives one probability for each combination of these three numbers, specifying the weight with

which the configuration enters the configurational sum. The probability is indicated in percentage, and hence, it adds up to 100% for all the numbers listed in the table. The V thickness, n_V, divides the table in sections. Within each section the probabilities for a certain V thickness is constant and the thicknesses of the two FeNi layers are listed on the horizontal and vertical axis. The table gives an indication of the amount of configurations one is dealing with when introducing roughness to any property of a multilayer. It should be noted that, the nominal configuration ($FeNi_4/V_{15}/FeNi_4$) is found in the center of the table ($n_{FeNi}=4$, $n_V=15$), and this configuration is seen to have the highest probability. Furthermore, the weight of this nominal configuration is only about 13% for this particular value of the interface roughness.

In the present work the considered structure consists of trilayers embedded in a V host with four interfaces and in order to reduce the number of calculations needed for calculating $\hat{\Omega}$ we introduce some approximations. In the sum over different configurations, there might be several configurations for which the property Ω is roughly equal, then Ω only needs to be calculated for one of these configurations. Two approximations of this kind have been tested for our system. The first approximation consists of replacing all Ω for configurations with different thicknesses of the two FeNi layers with Ω for a symmetric calculation with the same number of total FeNi layers (i.e., assuming that $FeNi_3/V_{15}/FeNi_5$ has the same property as $FeNi_4/V_{15}/FeNi_4$). Using this approximation we only need to perform calculations on trilayers with equal thicknesses of the magnetic layers.

The second approximation is used for properties that do not depend strongly on the thickness of the magnetic layers. Ω is here assumed to be equal for samples with different magnetic layer thicknesses. The approach has been tested and proved to be good for the interlayer exchange coupling in FeNi/V. The approximation is in general not good for the total magnetic moments of multilayers since this depends on the thickness of the magnetic layers. When treating the total magnetic moments we use only the first approximation.

D. Model for interface intermixing

The modeled intermixing at the interfaces was calculated by using the CPA. For the majority of the calculations in this work we treat intermixing extending only in one layer in both directions from the interface. Under these assumptions two parameters are needed to characterize the intermixing uniquely. As a first parameter we use the fraction of V which has crossed the ideal interface and migrated into the FeNi layer. This specifies the extent of the intermixing. A second parameter is needed to specify the composition of the FeNi alloy which has crossed the interface, which may differ from the ideal alloy composition in the magnetic layers. Calculations were done in order to give an indication about the second parameter. These were done for a system consisting of a single FeNi layer embedded in V. The first parameter was fixed, somewhat arbitrary, at values between 3% and 10% and the second parameter was varied between 0 (only Ni migrates into the V layer) and 1 (only Fe migrates). The calculated differences in energy for different configurations are extremely small in the μ Ry range. Since these films are grown at finite temperatures, entropy contributions then dominate the free energy, which motivates using the same concentration of Fe and Ni atoms migrating into V as found in the magnetic layer, i.e., 82% and 18%, respectively. The total extent of the intermixing is thereby specified by only the first parameter, the fraction of V that migrates into the FeNi layer (or vice versa), denoted m in our calculations.

A few calculations were done treating interface intermixing over more layers than the interface layers. The intermixing has in these cases been modeled by the following expression for the concentration

$$C(X,\Gamma_C) = \sum_{i\neq 0} -1^{(|i|+1)}\Lambda_i[\mathrm{sgn}(i)X,\Gamma_C], \tag{4}$$

where Λ_i is a general normal cumulative distribution function centered at interface i with standard deviation Γ_C and X is the distance from the interface in the direction of growth. Note that the parameters m and Γ_C are not related since m belongs to a model of intermixing where the mixing occurs within two layers at each interface, whereas Γ_C belongs to a model where the parameter defines the width of the alloying region around each interface. For a detailed description of this expression, see Refs. 34 and 10.

III. EXPERIMENTAL METHODS AND RESULTS

A. Growth

A series of samples with 25 repetitions of $[Fe_{0.82}Ni_{0.18}/V]$ was grown on one-sided polished $10\times10\times0.5$ mm^3 MgO(001) substrates by direct current magnetron sputtering at 150 °C in an ultrahigh vacuum chamber.[23] The thicknesses used for the FeNi layer and the V layer were 0.4–1.7 nm (3–12 ML, 1 ML$\approx$0.145 nm) and 0.7–2.4 nm (5–17 ML), respectively. The samples were covered with a 4-nm-thick V layer that was partly oxidized on air exposure. Details on substrate preparation and growth parameters are presented in Ref. 12.

B. Structural characterization

The structural quality of the films was investigated with conventional Bragg-Brentano low- and high-angle x-ray diffraction, as well as reciprocal space mapping, using Cu $K\alpha$ x rays. For technical details on all x-ray measurements and general facts on the structure of FeNi/V (001) superlattices, see Ref. 12. The results from that study that are relevant here were the following: The films have a body-centered-tetragonal structure since the FeNi and V layers are biaxially strained to decrease the misfit to the MgO substrate. They all show high interface sharpness and good crystalline quality. The overall crystalline coherence length is for all samples more than one order of magnitude longer than the nominal bilayer thickness and falls in the interval 10–30 nm. The root-mean-square interfacial roughness was estimated by means of a simulation of the low angle x-ray reflectivity measurements and a value of 0.22 nm was obtained.

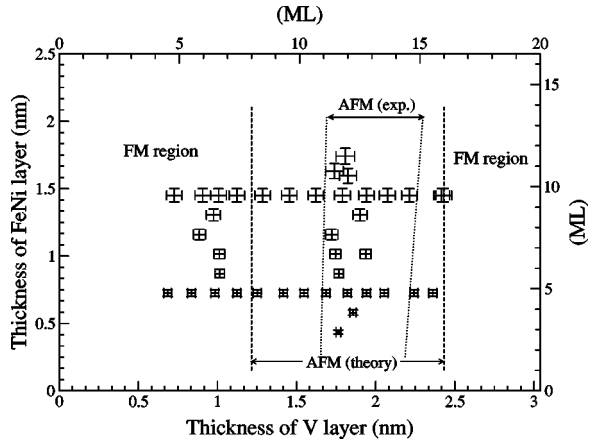

FIG. 2. The measured magnetic phase diagram of the $[\mathrm{FeNi/V}]\times 25$ superlattice films together with the calculated diagram modeling interface roughness (using $\sigma=0.18$). The thickness of the experimental samples is displayed in the graph with error bars corresponding to the uncertainty in layer thickness. The AFM regions for experiment and theory are indicated by the vertical lines. The thickness of the experimental samples was measured in the nanometer scale. The ML scale in the figure was obtained by a simple conversion using the experimental bulk V lattice constant (0.303 nm).

C. Magnetic measurements

All samples besides one (3 ML FeNi) had their T_c above room temperature. The type of interlayer coupling, FM or AFM, was deduced from room temperature longitudinal magneto-optic Kerr effect hysteresis loops.[3] A phase diagram, describing the interlayer exchange couplings, for the samples is shown in Fig. 2. The error bars reflect the uncertainty in the precision of the individual FeNi and V layer thicknesses (3.4%). However, the uncertainty in the bilayer thickness determination done by x-ray measurement is much smaller (±0.005 nm, less than 0.3%). Four-probe current-in-plane magnetoresistance measurements were done at room temperature and at low temperatures (21–27 K), as described in Ref. 3.

A Quantum Design MPMS 5.5 superconducting quantum interference device magnetometer was used for absolute magnetization measurements of the films at 10 and 300 K. The external magnetic field was applied in the film plane and the magnetization was measured along the [100] and [110] in-plane directions. For these experiments the films were cut into 5×5 mm^2 pieces.

Full experimental results on the magnetic properties are published in Ref. 35 and only a brief overview is given here. Below FeNi thicknesses of 6 ML the films appear to be more or less isotropic in-plane at room temperature, while a four-fold in-plane anisotropy with [100] as the easy axis increases with thicker FeNi layers. Moreover, the magnetic moment increases (see later) while the saturation field (H_s) decreases with the FeNi thickness as previously seen in the Fe/V system.[36] The negative slope in magnetoresistance within the studied thickness region is very small compared to the rapid decrease in the Fe/V system. Among the measured AFM coupled samples, we obtained a maximum GMR value of 2.5% at low temperature.

IV. RESULTS AND DISCUSSION

A. Perfect interfaces

Ab initio calculations were done for a set of multilayer structures with perfect interfaces where the FeNi layer thicknesses were 3–8 ML and the V layer thicknesses 1–20 ML.

In our calculations we are restricted to using the same atomic volume for all atoms in the multilayer. Since the volume of V is larger than that of FeNi we expect V in the FeNi/V system to be compressed in plane and expanded out of plane while the reverse should occur for FeNi. For calculations of the IEC we have found it reasonable to use the larger volume of V in order to model the multilayer spacer width correctly, while calculations of magnetic moments probably are more accurate using the Fe volume. In order to investigate the influence of the global volume on the magnetic moments, calculations were performed both in the experimental volume of Fe and V. We observed that a decrease in volume from V to Fe, reduces the moments with about 10%–20%.

If we neglect interface effects and assume ideal interfaces, we observed the normal disagreement between the calculated and experimental values of the magnetic moment and interlayer exchange coupling. The agreement between the calculated and measured (shown in Fig. 2) phase diagrams is then extremely poor, where the theoretical IEC curve changes sign with a period of about 2 ML (data not shown). The amplitudes of the calculated oscillations are in disagreement with the experiment by about two orders of magnitude and the magnetic moments are off by 60%. We will continue our discussion by showing first of all how interface roughness and mixing affect the magnetic moments and then how they affect the IEC.

B. The magnetic moment

The calculated magnetic moments of the FeNi/V superlattices depend greatly on the amount of interface intermixing. This is due to the fact that the moment of both Fe and Ni is greatly affected by the local chemical surrounding. The magnetic moment is in particular reduced by the presence of neighboring V atoms. Interface intermixing consequently leads to a lower magnetic moment, as is illustrated in Fig. 3. The magnetic moment is given by the total magnetic moment of a bilayer divided by the number of magnetic layers. There is a contribution to the magnetic moment from the V atoms of about $-0.6\mu_B$ per interface. Figure 3 also shows that when the V thickness becomes small, all theoretical curves seem to converge to a similar value, which is natural since in this limit there is a vanishingly small amount of V to mix, which results in a vanishing influence of mixing.

Interface roughness also affects the magnetic moments but to a much smaller extent. The effect is only noticeable for thin magnetic layers, mainly below the thicknesses that were investigated in this study. The effect originates from

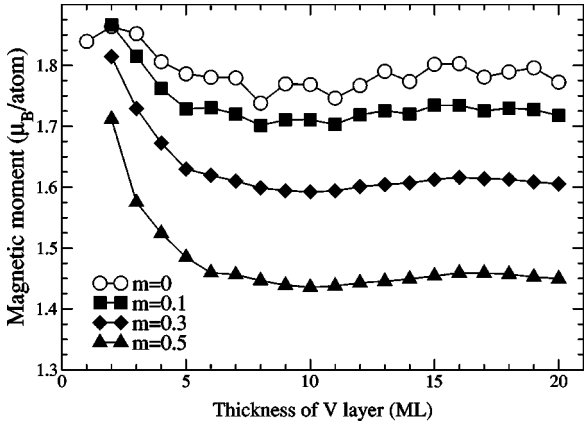

FIG. 3. Calculated average magnetic moment per atom in the magnetic layer, and for different V thickness and for different values of interface intermixing m (see Sec. II) in samples with 4 −ML-thick $Fe_{0.82}Ni_{0.18}$ layers.

how the magnetic moment depends on the thickness of the magnetic layer, even for sharp interfaces between V and the FeNi layer, shown in Fig. 4. As may be observed, the magnetic moment varies with the thickness of the magnetic layer. However, in order for roughness and thickness variation to affect the total magnetic moment of a system, the magnetic moment as function of layer thickness has to show a pronounced nonlinear behavior.

Since the thickness variation affects the magnetic moments very little (at most about $0.05\mu_B$) the intermixing may be estimated by measuring the magnetic moment of a multilayer sample and comparing it to theory. A study of the interface structure for $Fe_{0.82}Ni_{0.18}/V$ superlattices grown at different temperatures was done by Andersson[3] where it was shown that the evolution of interface sharpness could be monitored in detail by employing this method.

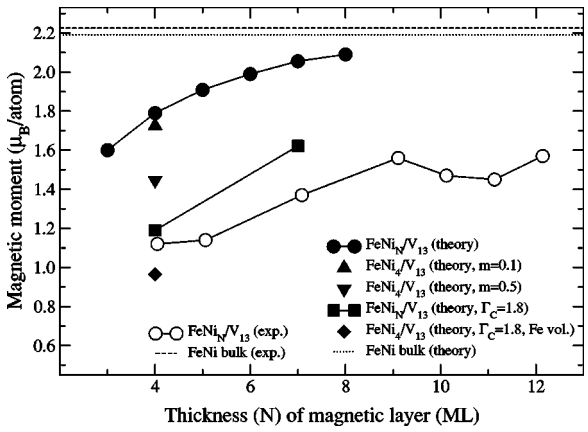

FIG. 4. Total magnetic moments per magnetic layer for different thicknesses of the magnetic layer. Both experimental (open symbols) and theoretical data (filled symbols) are shown. The V lattice constant has been used in all calculations except for the data marked with a diamond where the Fe lattice constant was used. Filled circles denote theoretical data using sharp interfaces.

In Fig. 4 both the measured and calculated magnetic moment per magnetic monolayer are shown as function of magnetic layer thickness. The difference between the theoretical values for ideal interfaces and experiment is typically about 60%, or $0.7\mu_B$. This error is larger than one normally expects from first principles calculations. Part of this difference can be explained by interface intermixing and part of the difference can be explained by a volume effect as discussed earlier.

From Fig. 4 it is evident that the simple model for interface intermixing treating alloying in only the first layer close to the interface is not sufficient for describing the detailed behavior of the magnetization of the experimental multilayers (see black symbols). For the maximum value of intermixing in this scheme ($m=0.5$) the magnetic moment is reduced by about $0.4\mu_B$. Since calculations were done for the V lattice constant we can expect a maximum additional reduction of the magnetic moment by 20% in calculations where the Fe lattice constant is used (according to the analysis presented earlier). This combined reduction is just barely sufficient to reach the experimental values. For that reason, a few calculations were performed for intermixing stretching further from the interface following the normal distribution function in Eq. (4). This was done for the $FeNi_4/V_{13}$ multilayer. Our chosen value of mixing profile results in a calculated spin moment that underestimates the total magnetization by about $0.2\mu_B$. This value is close to the expected one for the orbital moment, and our calculated spin moments are, hence, most likely in good agreement with the measured spin moment. Hence, taking into account the volume effect, an intermixing of $\Gamma_C=1.8$ gives a good description of the interfaces in the considered system.

In Fig. 4 we also compare the experimental and calculated moments of bulk FeNi alloys (81% Fe) and one may notice that theory reproduces experiment with an error that is less than a few percent. This indicates that the theoretical approximations (e.g., KKR-ASA and the local spin density approximation) used by us, are not the cause of the disagreement between theory and experiment for the multilayers, since these approximations are used with success for the bulk values.

Figure 4 also shows that the experimental thin film moments have not approached the bulk values even for largest measured thicknesses (13 ML FeNi). This shows that the region around the interfaces for which the magnetic moments deviate substantially compared to the bulk data is appreciable. This is consistent with our theoretical analysis given below, where we come to the conclusion that this region extends over several atomic layers on each side of the interface.

C. The interlayer exchange coupling

Interface roughness and interface intermixing have different effects on the IEC. This is clearly shown in Fig. 5. Assuming the coupling decays as $1/N^2$, where N is the V thickness, by Fourier transforming the quantity N^2J, the existence of two distinct peaks in the spectrum can be seen that correspond to two oscillation periods. The Fourier transforms for

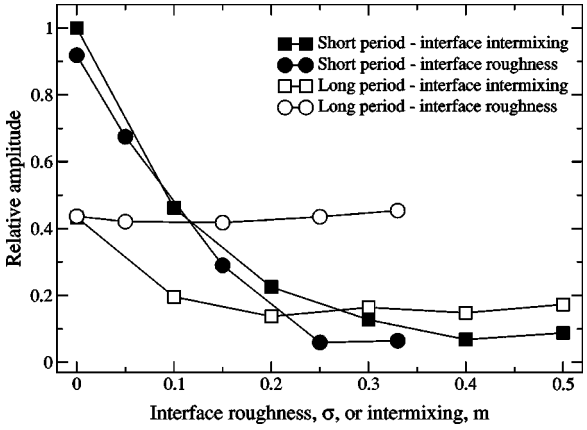

FIG. 5. Calculated amplitudes of the peaks in the Fourier transform of N^2J as a function of interface roughness or intermixing.

configurations with roughness and intermixing were made on sets of 21 and 25 points, respectively, which is somewhat less than used in the work in Ref. 7. We see that the amount of points used is still enough for a qualitative description of how coupling periods are affected by the interface structure. The intensities of these Fourier components are shown in Fig. 5 as a function of the roughness or intermixing parameters. Only the amplitude that is connected to the short period oscillation is damped by the interface roughness while both periods are damped by the intermixing.

Let us now discuss more in detail how interface roughness influences the coupling. In Fig. 6 we plot the calculated interlayer exchange interaction as a function of the V thickness. The interface roughness gives rise to thickness variation in the system, and it is evident that the short period oscillation is suppressed when the roughness parameter is increased. The fact that the long period oscillation survives produces a curve that agrees better with experiment. It is interesting to note that although the thickness variation affects the IEC strongly, it is only the thickness variation of the

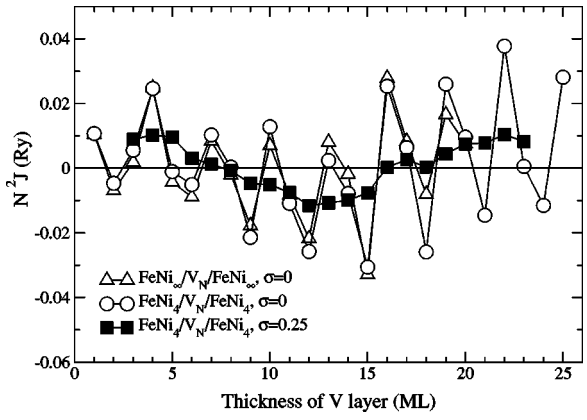

FIG. 6. Calculated interface exchange coupling times the layer-thickness squared, N^2J. Three different geometries were considered, a trilayer geometry (open triangles), a multilayer geometry (open circles), and a multilayer geometry with interface roughness (filled squares).

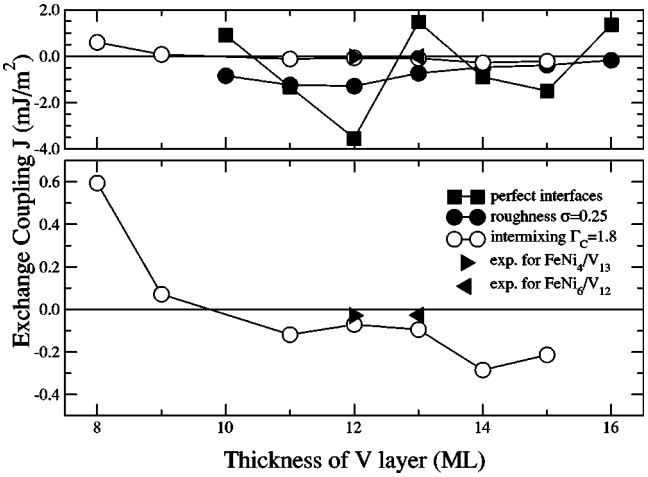

FIG. 7. Calculated exchange coupling of $FeNi_4/V_N/FeNi_4$ for different interface models. Both ideal interfaces, interfaces with roughness and interfaces with intermixing, are considered. The lower panel shows a blown up version of the data displayed in the upper panel.

spacer that plays an important part in our case. This is illustrated in Fig. 6 where a comparison of the IEC as calculated for semi-infinite magnetic layers with the IEC calculated for 4-ML-thick magnetic layers is made. All thicknesses for which the calculations were done are not shown but they all fall on top of each other and only one is plotted. It is well-known that quantum well states in the magnetic layers in general change with the thickness of the magnetic layer and thereby affect the coupling.[37] In our case the fact that the magnetic layer consists of an alloy may lead to a smearing of the quantum well states leading to negligible oscillations of the coupling with magnetic layer thickness.

From a full experimental determination of the IEC over the whole investigated range of the V thickness it is possible to make a precise calculation of the extent of interface roughness and interface intermixing in the samples based on our models. This full information on the coupling strengths is not available in the current study, but from the phase diagram which provides the sign of the coupling over the whole investigated range and from the coupling amplitudes for a few samples, we are still able to extract information on the interface structure.

Using the combined experimental information that we now have on the IEC and the magnetic moments we now come to the main result of this particular study. At zero interface roughness an interface intermixing of $\Gamma_C = 1.8$ reproduces the magnetic moments as seen in Fig. 4. This means that at the layers nearest the interface the mixing is approximately 40% and in the next nearest layers it is 20%. Since interface intermixing is the most important interface effect when it comes to reproducing the magnetic moments of this system, we use this value as the intermixing parameter for the continued analysis. The IEC is calculated including this interface intermixing, without the effects of roughness. We find that the magnetic phase diagram is reproduced as seen by inspection of Figs. 2 and 7. The actual coupling strength

was determined experimentally for a few of the AFM samples and the order of magnitude of these was found to agree with our calculations (see Fig. 7). Since the calculated IEC can be made to agree with experimental data by assuming only intermixing, the extent of interface roughness is undetermined.

Considering the phase diagrams more in detail we see that the theoretical AFM region is somewhat wider compared to the experiment. The calculated AFM region is centered very close to 13 ML which is in agreement with experimental results. The small discrepancy in width could be a result of effects of concentration profiles or tetragonal distortions in the magnetic layers that we have not taken into account in theory. The effect of roughness could also explain the discrepancy assuming the fact that we have used the approximation previously described, where the whole phase space of configurations in Table I are approximated from calculation of about 30% of the configurations. It is also possible that there is correlated roughness in the experiment that results in a positive bias of the IEC. In fact an upward shift of the theory curve by about +0.01 Ry in Fig. 6, corresponding to a shift in the coupling energy of 0.1 mRy at the 10 ML V thickness, would reproduce the experimental phase diagram in Fig. 2 perfectly. It is worth noting that in this case both the calculated periodicity and the phase of the IEC agrees with observations. This implies that lattice relaxations (omitted in the calculations) do not have a major influence of the IEC in the FeNi/V system.

The amplitude of the IEC has in general proved to be very difficult to reproduce by theory[7–9] and the obstacle is in most cases the lack of detailed information of the interface structure. One must be careful in making detailed comparisons of single point values of the IEC due to the possible presence of the short period oscillation that is suppressed but of unknown strength. The existence of a slight phase shift in this oscillation will have an impact on the coupling value. However, we can still get a rough idea of the agreement by comparing the orders of magnitude of the experimental IEC values with those found in calculations. In Fig. 7 we show the obtained calculated values together with the experiment for a series of $(Fe_{0.82}Ni_{0.18})_4/V_N$ samples, and we note that where a comparison can be made, the agreement between experiment and theory is good when intermixing is considered.

D. Interface phase space and experiments

The earlier analysis can be applied in a more general sense to characterize other FeNi/V samples and it can be applied to various other systems to extract information on the interfaces. Figure 8 illustrates schematically how different experiments are related to the phase space of the interface structure in our case.

From a full experimental determination of the IEC and magnetic moments it would be possible to specify a small region where the interface model is close to the true interface structure. This is indicated by the dashed lines in Fig. 8 for two different experimental outcomes. The ellipse corresponds to the case that the short period oscillation is visible

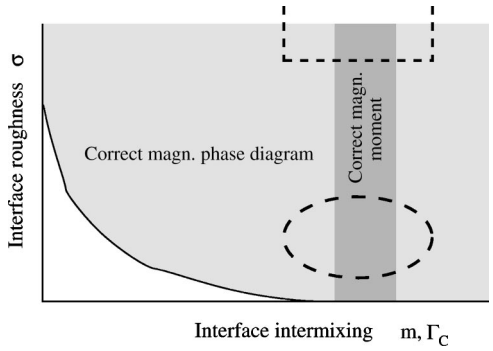

FIG. 8. The phase space of the interface structure is shown schematically. Shaded regions indicate the area of the phase space where a the magnetic phase diagram is reproduced. The dark shaded region indicates the area where the experimental magnetic moments are reproduced. From further experimental studies the possible interface structure could be narrowed down further as indicated by the dashed lines. Two possible outcomes are shown.

in the IEC implying that we can determine the interface roughness. If the short period oscillation is not visible we are left with a lower bound for the roughness. From the experimental magnetic phase diagram found in the current study there is a region in the interface phase space where there is agreement. With agreement we here mean it in a more approximate sense, where we neglect the fact that the widths of different regions in experiment and theory do not fully agree. We have performed calculations for various cases of intermixing at the interfaces and calculated the extent of roughness necessary to reproduce the experimental phase diagram giving us the border line of this region. For no intermixing a roughness larger than $\sigma=0.18$ reproduces the experimental phase diagram in Fig. 2 with good accuracy. For calculations with intermixing of $m=0.3$ the necessary amount of interface roughness reduces to $\sigma=0.15$, while for $m=0.5$ it reduces to $\sigma=0.05$. From the experimental magnetic moments found in the current study there is a thin slice of the interface phase space where experiments are reproduced. By compiling information from different experiments in this way it is possible to extract information on the interface structure.

V. SUMMARY AND CONCLUSIONS

We have found that neglecting interface roughness and intermixing in multilayers results in a large disagreement between experiment and theory, that can be condensed to the following three issues. First of all, the magnetic moment found from first principles calculations deviate from experiments. Second, the rapid oscillation of the IEC is in strong contrast to the experimental phase diagram where a more long-range oscillation is seen. Finally, the amplitude of the calculated IEC is much higher than the values deduced from the experimental samples.

We address all of these issues and show that the measured IEC may be reproduced by first principles calculations if one

assumes that both interface roughness and alloying in the interfaces are present. The two effects are shown to be partially distinguishable, since they lead to different effects on the different oscillation periods of the interlayer exchange coupling and on the total magnetic moment of the samples. When the interface roughness and intermixing of the system are included in the theory we find good agreement with the measured amplitudes of the interlayer exchange coupling. In addition the theoretical description of the magnetic moments is improved substantially.

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