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Interlayer Exchange Coupling in Nb/Fe Multilayers

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The (110) oriented Nb-Fe multilayers (MLs) with constant Fe and variable Nb sublayer thicknesses were prepared at room temperature using UHV magnetron sputtering. The artificial periodicity was revealed by intense satellite peaks in the low- and high-angle X-ray diffraction patterns. Magnetic hysteresis loop measurements at 5 K revealed antiferromagnetic (AF) exchange coupling of the Fe sublayers for Nb spacer thickness of about 3 monolayers. The corresponding AF coupling energy is equal to about –1.36 mJ/m^2. The Nb spacer thickness corresponding to the position of the AF peak is in good agreement with *ab-initio* calculations within localized spin density approximations of exchange-correlation potential.

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1. Introduction

Oscillating ferromagnetic (F)/antiferromagnetic (AF) exchange coupling has been observed in various layered magnetic systems [1, 2], and has stimulated a large activity both in fundamental and applied research. Applications are based on the giant magnetoresistance of magnetic multilayers (MLs) which can be used as various sensors [3]. Widely accepted theories in explaining the oscillating exchange coupling are Ruderman-Kittel-Kasuya-Yoshida (RKKY) - like models and a model which is based on quantum interferences in the spacer layer electron system. In RKKY-like models [4] as well as in the quantum interference model [5] the coupling energy J oscillates approximately as: $J \sim (1/(2k_{\mathrm{F}} \cdot d_{NM}) \cdot \sin(2k_{\mathrm{F}} \cdot d_{NM})$, where k_{F} and d_{NM} are the Fermi wave vector and the thickness of the nonmagnetic layer, respectively. Up to now, the dependence of the exchange energy on the spacer layer thickness has been extensively studied in many magnetic layered structures. However, only few papers exist in the literature dealing with a manipulation of the Fermi wave vector [6]. In order to understand this phenomenon, first principles techniques have also been employed which are more transparent and parameter free but require considerable computational effort.

Nb/Fe multilayers (MLs) are an interesting magnetic system because it provides a possibility to study the coexistence of ferromagnetism and superconductivity. For instance, in Ref. [7] it was found a strong dependence of the superconducting transition temperature T_c on Fe layer thickness. A problem in experimental as well as theoretical studies on interlayer exchange coupling in Nb/Fe MLs is a relatively big difference in the lattice parameter of Fe and Nb ($\sim$ 13%). On the other hand, the Nb/Fe MLs showed oscillatory exchange coupling with a period of about 0.9 nm at room temperature [8–9]. Furthermore, it was shown in Ref. [10] that the interlayer exchange coupling could be changed in a continuous and reversible way by introducing hydrogen into the Nb sublayers.

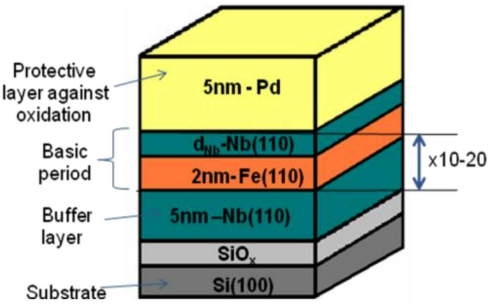

Fig. 1. Schematic presentation of the construction of the prepared Nb/Fe multilayers.

In this paper we report on low temperature interlayer exchange coupling in Nb/Fe MLs with ultrathin Nb sublayer ($d_{\mathrm{Nb}} < 5$ monolayers).

2. Experimental procedure

The Nb/Fe multilayers were prepared at room temperature using UHV (5×1^{-10} mbar) magnetron sputtering [11–14]. The number of repetition of the base period varied from 10 to 25. A capping layer of 5 nm Pd was used to allow a fast uptake and release of hydrogen at a temperature of less than 370 K and to avoid oxidation of the MLs. As a substrate we have used Si(100) wafers with an oxidised surface to prevent a silicide formation [15–17]. The constant thickness Fe-layers with $d_{\mathrm{Fe}} = 10$ monolayers (denoted as Fe(10)) were deposited using a DC source. For preparation of the Nb-layers a RF source was used. Before the deposition of Nb/Fe MLs a 5 nm Nb buffer layer was first deposited to enhance the (110) growth.

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In Fig. 1 we show schematic description of the construction of the multilayered samples. The chemical composition and the cleanness of all layers was checked *in-situ*, immediately after deposition, transferring the samples to an UHV (4×10^{-11} mbar) analysis chamber equipped with X-ray photoelectron spectroscopy (XPS). Details of the XPS measurements can be found in Ref. [18–20].

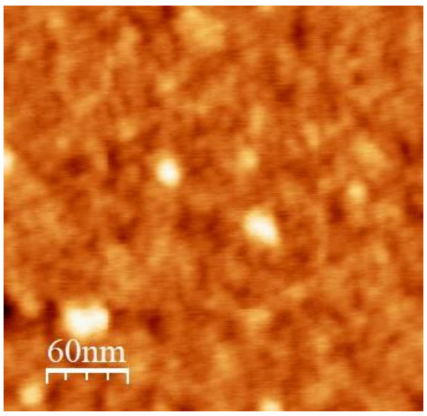

Fig. 2. AFM image for (Nb(6)/Fe(10)) × 10 multilayer covered by a 5 nm Pd protective layer. Average roughness parameter R_a was about 0.3 nm.

The morphology and roughness of the MLs were studied *ex-situ* by atomic force microscopy (AFM). The structure of the Nb/Fe MLs was examined by standard $\theta-2\theta$ X-ray diffraction with Cu-K$_\alpha$ radiation. The modulation wavelength was determined from the spacing between satellite peaks in the high- and low-angle X-ray diffraction patterns. The thicknesses of individual Fe and Nb sublayers were also determined using X-ray fluorescence analysis (XRF) and X-ray reflectivity (XRR).

The magnetic characterisation of the samples was carried out using a vibrating sample magnetometer (VSM) at 5 K. The saturation magnetisation (M_s) and saturation fields (H_s) were determined from the in-plane hysteresis loop measurements in magnetic fields up to 9 T.

The calculations were carried out using the projector-augmentedwave implementation of the Density Functional Theory (DFT) method of pseudopotentials (VASP code — Vienna *ab-initio* simulation package) [21]. The exchange-correlation (XC) energy was chosen in the local spin density approximation (LSDA). The other details of XC-energy, and a structural optimization of the systems can be found in Ref. [22]. The calculations of the total energies of AF and F states of the system were performed for fully relaxed Fe(10)/Nb(n)/Fe(10) layers stacked along the (110) direction with F and AF coupled magnetic slabs of Fe. The interlayer exchange coupling (IEC) energy is calculated in terms of the difference in total energy of the system in the two magnetic configurations: F and AF coupled magnetic slabs: $J(n) = E_{\mathrm{F}}(n) - E_{AF}(n)$, where n is the thickness of the spacer layer.

3. Results and discussion

In Fig. 2 we show AFM image obtained for the (Nb(6)/Fe(10)) × 10 multilayer covered by a 5 nm Pd protective layer. The estimated roughness parameter R_a measured for 2 μm × 2 μm area was about 0.3 nm. The relatively low values of the roughness parameters revealed planar growth of the multilayered sample.

The composition modulation of the Nb/Fe MLs was confirmed in the high- (Fig. 3a) and low-angle (Fig. 3b) X-ray diffraction patterns by intense satellite peaks. The wavelengths of modulation calculated from these peaks were in agreement with those values determined from XRF. In the high-angle XRD patterns (Fig. 3a) we have observed central Bragg peak located between positions expected for reflections of bcc-Fe(110) and bcc-Nb(110) and satellites up to 3rd order. Due to very similar thicknesses of the Nb and Fe sublayers the expected S2 satellite peak between S1 and S3 satellites in the low-angle diffraction patterns disappear (see Fig. 3b). The estimated roughness parameter from the XRD data was between 0.3 –0.4 nm, which is in agreement with AFM measurements.

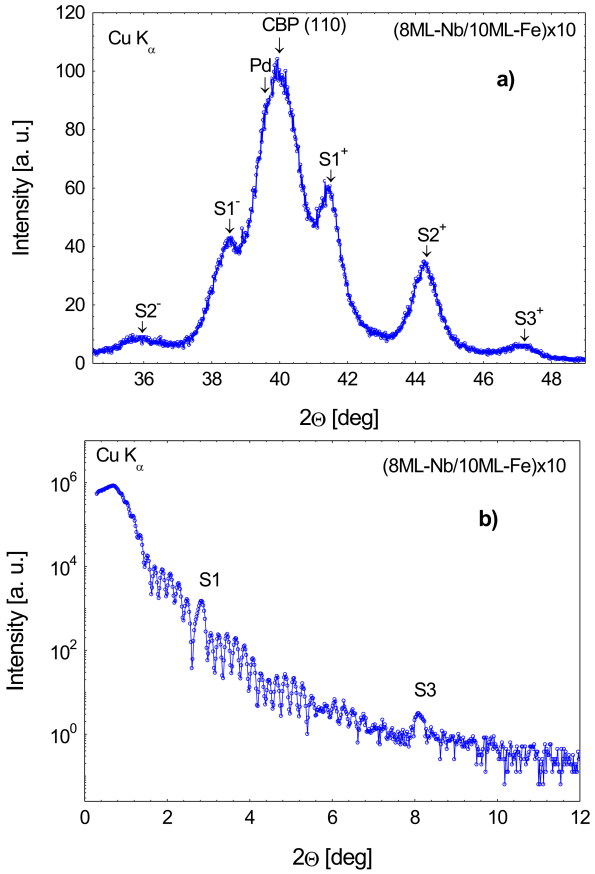

Fig. 3. High– (a) and low–angle (b) X-Ray diffraction (Cu–K$_\alpha$) pattern for (Nb(8)/Fe(10)) × 10 multilayer.

In the XPS experiment we have studied the Nb layer growth on a 2 nm - Fe underlayer. The freshly deposited

2 nm Fe/d_o–Nb bilayer was *in-situ* transferred from the preparation chamber to the analysis chamber, where the XPS Fe–$2p_{3/2}$ and Nb-$3d_{5/2}$ core level spectra were immediately measured in vacuum of 8×10^{-11} mbar. Then the bilayer was transferred back to the preparation chamber and the deposition process of the Nb overlayer was continued. The above procedure (overlayer deposition and XPS core level measurements) was repeated until the Fe-$2p_{3/2}$ and Nb-$3d_{5/2}$ integral intensities were saturated. Practically no trace of oxygen (or any other contaminations) adsorption or surface oxide formation was detected during the transfer operation or XPS measurements ($\sim$ 10 min). From the exponential variation of the XPS Fe-$2p$ and Nb-$3d$ integral intensities with increasing overlayer Nb thickness up to 5 nm we conclude that the Fe and Nb sublayers grow homogeneously in the planar mode. Very similar growth mode we have previously observed for the Fe/V [23], Fe/Ti [24] and Fe/Zr [25] bilayers.

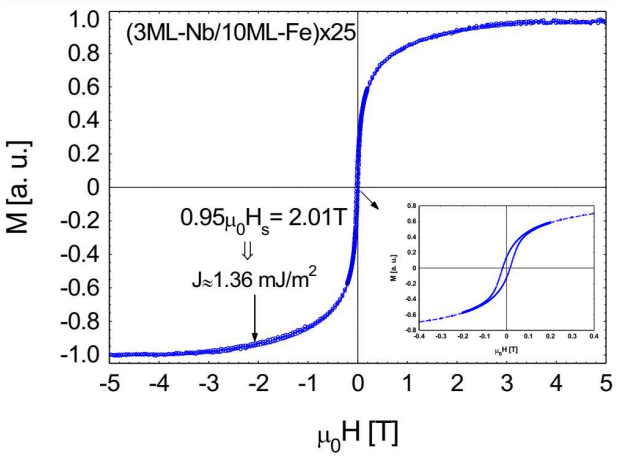

Fig. 4. In-plane hysteresis loop of 3 ML Nb/10 ML Fe multilayer measured at 5 K.

In Fig. 4 we show the hysteresis loop measured for the Nb(3)/Fe(10) multilayer at 5 K. As can be observed, the sample shows approximately zero remanence value and saturation field of about 2 T. The above result confirms the AF coupling across 3 monolayers of Nb spacer. The saturation magnetization M_s of the Fe sublayers was practically equal to the bulk value. The IEC per unit surface J is equal to: $J = -(1/4)M_s\mu_0 H_s d_{\mathrm{Fe}}$. According to the above equation, the estimated IEC energy for 3 monolayers of Nb is equal to about –1.36 mJ/m^2. Results on IEC as a function of the ultrathin Nb spacer are shown in Fig. 5 (open circles). Despite the ultra-thin Nb spacer (few monolayers) we have observed a clear first minimum of IEC energy (maximum of AF coupling) located near $d_{\mathrm{Nb}} \approx 3$ monolayers. Similar IEC AF coupling we have observed recently in V/Fe multilayers [26]. The results of theoretical calculations within LSDA (open squares) are also shown in Fig. 5. The theoretical results show also a minimum of IEC energy (maximum of AF coupling) for

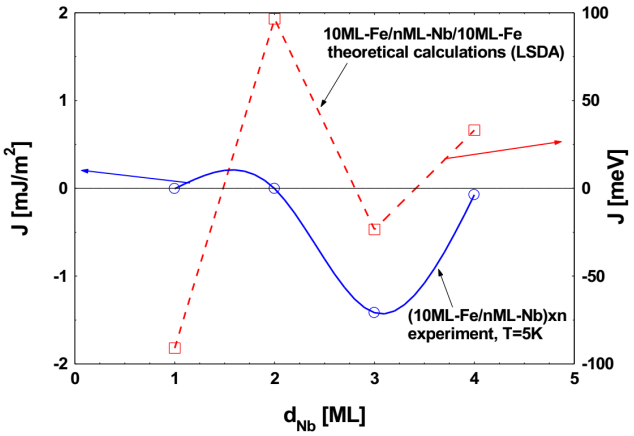

Fig. 5. Theoretical calculations (LSDA) and low temperature experimental results of the interlayer exchange coupling as a function of Nb layer thickness.

3 monolayers of Nb spacer in very good agreement with the experiment. On the other hand, the position of the first AF peak calculated for (001) oriented Nb/Fe MLs [27] was equal to 2 monolayers.

In conclusion, we have experimentally observed antiferromagnetic interlayer exchange coupling with zero remanence value in Nb/Fe multilayers for Nb layer thickness of about 3 monolayers. The experimental findings were also confirmed by *ab-initio* calculations within local spin density approximation.

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