Proceedings of the European Conference Physics of Magnetism, Poznań 2017

# Interlayer Exchange Coupling and Proximity Effect in V-Fe Multilayers

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We have studied interlayer exchange coupling (IEC) in (110) oriented V/Fe multilayers with ultrathin sublayers up to 7 monolayers (ML). Results showed that IEC energy depends on both vanadium and iron layer thicknesses. The local maxima of the antiferromagnetic coupling were found for V(7 ML)/Fe(4 ML) and V(3 ML)/Fe(3 ML) multilayers (MLs). The strongest AFM coupling energy of about 1.0 mJ/m$^2$ was measured at 5 K for the V(7 ML)/Fe(4 ML) multilayer. The position of the AFM peak for V(X ML)/Fe(3 ML) MLs near 3 ML of V spacer was also revealed by *ab-initio* calculations. Furthermore, theoretical calculations show an induced negative magnetic moment on V atoms near the V–Fe and Fe–V interfaces due to the proximity effect.

DOI: 10.12693/APhysPolA.133.597

PACS/topics: 75.70.–i, 68.55.–a

## 1. Introduction

Fe/V multilayers (MLs) have been used recently as a model system in studies of interlayer exchange coupling (IEC) [1–3], proximity effect [4–6], and hydrogen absorption [7–8]. The experiments on IEC performed previously have been limited to the second and third antiferromagnetic (AFM) maxima [1] or measurements at room temperature [3]. The oscillatory IEC across V(001) spacer showed in Ref. [3] was based on a Fe layer thickness of 7 monolayers. The authors illustrated the existence of three AFM regions as well as the presence of magnetic proximity effects at the interfaces.

It has been shown that the oscillatory exchange coupling is a general phenomenon for most transition-metal and noble metal spacer [9]. The experimentally determined oscillation periods are in agreement with the theory based on the interplay between the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction and the discrete spacer thickness [10]. The same behaviour of the oscillatory exchange coupling was achieved in another picture: quantum wells in the spacer produced by the different spin states of the electrons in the ferromagnets [11]. Furthermore, it has been shown that IEC energy depends not only on the spacer layer thickness but also on the FM layer thickness [12].

Metallic multilayers composed of alternating sublayers of ferromagnetic and non-magnetic metals have attracted great interest over the past years because of the successful application of these materials as ultrasensitive hard disc reading heads and magnetic sensors [13].

Interlayer exchange coupling through the vanadium spacer in epitaxial Fe/V(001) superlattices was detected and characterized in Refs. [1] and [3]. It was found that AFM coupling oscillates with a period of about 6 ÷ 7 monolayers (ML). However, the first AFM peak was observed between 13 ML [1] and 14 ML [3] instead of expected $d_V \sim 7$ ML. On the other hand, recently we have observed three AFM peaks [14] in the (110) oriented V/Fe MLs [15] for vanadium sublayer thickness greater than 5 monolayers (ML). Furthermore, we have reported in Refs. [16–17] that hydrogen could modify reversibly IEC energy value in Fe/V/Fe trilayers. In this paper, we report on the interlayer exchange coupling in V/Fe MLs as a function of Fe and V sublayer thicknesses.

## 2. Experimental and calculation details

Two series of (110) oriented V-Fe MLs with either constant Fe (3 ML) and variable V sublayer thickness or constant V (7 ML) and variable Fe sublayer (see Fig. 1) thickness were prepared by UHV magnetron sputtering. The number of repetitions was equal to 25. Details of preparation method can be found in Refs. [18–20].

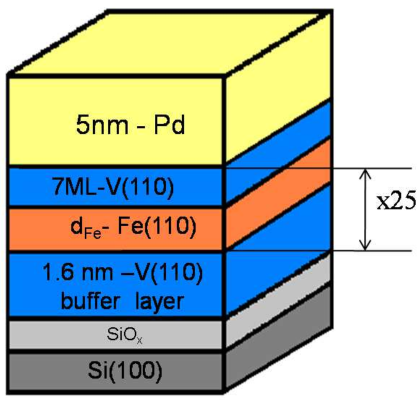


Fig. 1. Schematic description of Fe/V multilayers with constant V (7 ML) and variable Fe sublayer thickness.

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The structure of the multilayered samples was examined using the standard $\theta-2\theta$ low- and high-angle X-ray diffraction. The modulation wavelengths were calculated from the spacing between the satellites peaks and the central Bragg peak (CBP). The results were consistent with the values obtained from the total thickness divided by the number of repetition. A strong CBP was detected only between the positions expected for pure V(110) and Fe(110) reflections. The above behaviour revealed the (110) orientation of the V/Fe multilayers. The results were recently published in Ref. [15].

The chemical composition and the cleanness of all layers was checked *in situ*, immediately after deposition, transferring the samples to an UHV ($4 \times 10^{-11}$ mbar) analysis chamber equipped with X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES) and ion gun etching system. Details of the XPS measurements can be found in Refs. [21–22].

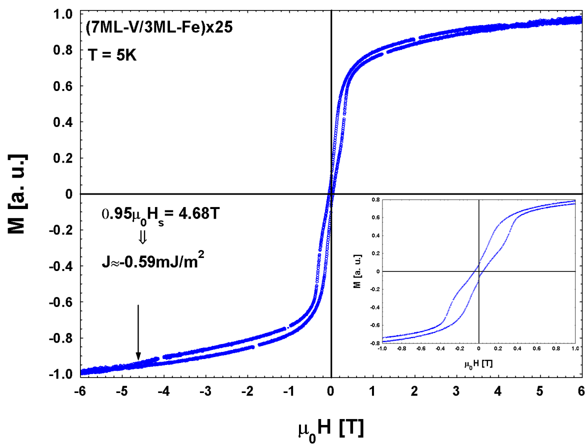


Fig. 2. In plane hysteresis loop near local maximum of AFM coupling for (7ML-V/3ML-Fe)x25 multilayer at 5 K.

The magnetic characterisation of the samples with constant-thickness sublayers was carried out using a vibrating sample magnetometer (VSM) in the temperature range of 4 - 350 K in a magnetic field up to 9 T. The coercive ($H_c$) and saturation ($H_s$) fields were determined from the in-plane hysteresis loop measurements.

The calculations of the theoretical IEC and magnetic moment distribution in the V/Fe MLs with constant Fe (3 ML) and variable V sublayer thickness ($d_{\mathrm{V}}$) were also carried out. We have used the projector-augmented-wave (PAW) implementation of the Density Functional Theory (DFT) method of pseudopotentials (VASP code - Vienna *ab-initio* simulation package) [23–25]. The exchange-correlation energy was chosen in the local spin density approximation (LSDA) as well as in the generalized gradient approximation (GGA). The exchange-correlation functionals were based on the formulation of Perdew-Zunger (LSDA) [26] and Perdew-Burke-Ernzerhof (GGA) [27]. The calculations of the total energies of AFM and FM states of the system were performed for fully relaxed Fe(3 ML)/V($d_{\mathrm{V}}$)/Fe(3 ML) layers stacked along the (110) direction with ferromagnetic and antiferromagnetic coupled magnetic slabs of Fe. The Hellmann-Feynman forces acting on the atoms have been used to perform a structural optimization of the systems. The plane-wave basis set used contained components with energies up to 400 eV. The presented results were obtained assuming the convergence threshold of $10^{-6}$ eV in the total energies. The IEC was calculated in terms of the difference in total energy of the system in the two magnetic configurations - FM and AFM coupled magnetic slabs: $J(d_{\mathrm{V}}) = E_{FM}(d_{\mathrm{V}}) - E_{AFM}(d_{\mathrm{V}})$.

## 3. Results and discussion

In Fig. 2 we show the hysteresis loop measured for the 7 ML V/3 ML Fe multilayer. As could be observed, the sample shows practically zero remanence value and 95% of the saturation field (denoted by arrow) of about 4.68 T. The saturation magnetization $M_s$ of the Fe sublayers was strongly reduced ($M_s = 1.1$ T) due to magnetic proximity effect [1, 3] and for $d_{\mathrm{Fe}} = 3$ ML was measured at 5 K as $\sim$ 1.1 T. The interlayer exchange coupling per unit surface $J$ is equal to:

$$J = -(1/4)M_s\mu_0 H_s d_{\mathrm{Fe}}. \quad (1)$$

According to Eq. (1), the IEC energy for $d_{\mathrm{V}} = 7$ ML is $\sim -0.59$ mJ/m$^2$. The above result confirms the AFM coupling across vanadium spacer.

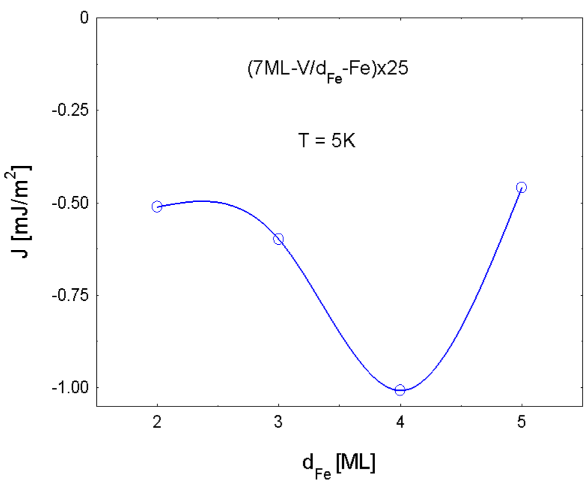


Fig. 3. The interlayer exchange coupling energy as a function of Fe layer thickness for V(7 ML)/Fe($d_{Fe}$) multilayers measured at 5 K.

Experimental results on the IEC energy as a function of the Fe layer thickness for a constant V spacer thickness (7 ML) are shown in Fig. 3. As can be observed in Fig. 3, IEC energy shows a clear minimum of the AFM coupling for Fe layer thickness equal to 4 ML. To observe an influence of the magnetic polarisation of the V atoms (proximity effect) on the IEC coupling across the vanadium spacer we have prepared the second series of the

V/Fe MLs with a constant thickness of the Fe sublayers of about 3 ML and a variable V sublayer thickness. Results on IEC as a function of the ultra-thin V thickness are shown in Fig. 4 (open circles). Despite the ultra-thin V spacer (few monolayers) we have observed a clear first minimum of IEC (maximum of AFM coupling) located near $d_V \approx 3$ ML.

The results of theoretical calculations with LSDA (open squares) and GGA (open triangle) are also shown in Fig. 4. The theoretical results for both LSDA and GGA approximation show a minimum of IEC energy (maximum of AFM coupling) for 3 ML V spacer thickness in very good agreement with the experiment (see Fig. 4).

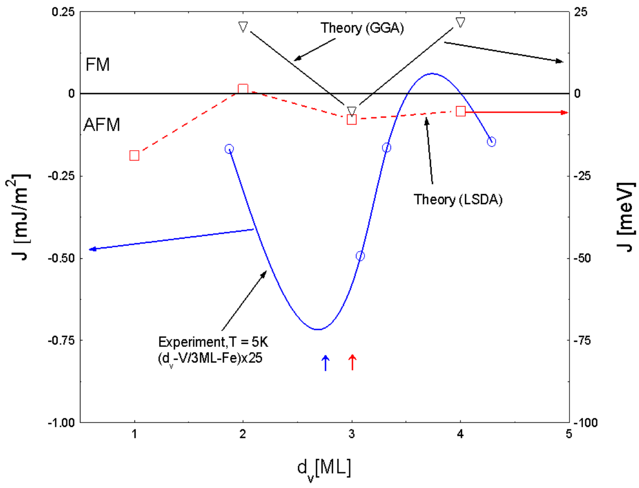


Fig. 4. Experimental results of the interlayer exchange coupling energy (left hand scale) as a function of V layer thickness determined for V/Fe MLs at 5 K (open circles). Results on theoretical calculations with LSDA (open squares) and GGA (open triangle) approximations are also shown (right hand scale).

The observed difference of the IEC presented in Fig. 4 and Refs. [1, 3] could be explained not only by different growth conditions and crystallographic orientations but also by the specific polarization of the vanadium spacer near the V–Fe and Fe–V interfaces. Note, that after hydrogenation process [16–17] we have observed an increase of the total magnetic moment of V/Fe MLs. Such behaviour reveals rather negative polarization of the interface V atoms due to proximity effect. In Fig. 5 we show the theoretical distribution of the magnetic moments on Fe and V atoms in V/Fe (3 ML) MLs with V spacer thickness equal to 2 ML (top), 3 ML (middle), and 4 ML (bottom). The magnetic moment on the Fe atoms is reduced compared to that measured for bulk material, especially at the interface Fe layer. Furthermore, a small negative (antiparallel to Fe) moment on the V atoms (up to $-0.3\mu_B$) is induced near the V–Fe interface. Magnetic moment calculated for (110) oriented V/Fe MLs revealed a reduction of the total magnetic moment in V/Fe MLs, as it was observed experimentally.

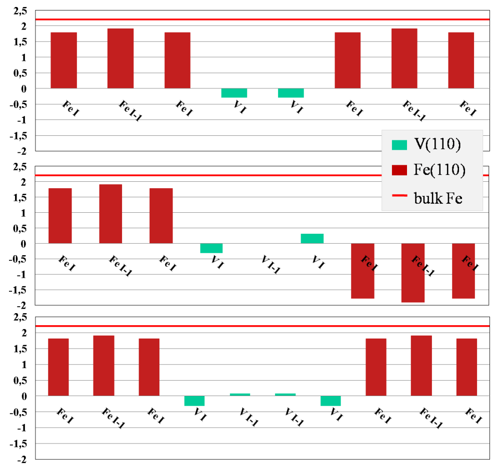


Fig. 5. Theoretical distributions of magnetic moments calculated with CGA approximation for $V(d_V)/Fe(3\ ML)$ multilayers with $d_V = 2$ ML (top), 3 ML (middle), and 4 ML (bottom).

In conclusion, we have found experimentally that the interlayer exchange coupling energy in the V/Fe MLs depends on both the vanadium and iron sublayer thicknesses. AFM coupling for the V(3 ML)/Fe(3 ML) multilayer was revealed also by the *ab-initio* calculations.

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