Layered antiferromagnetic spin structures of expanded face-centered-tetragonal Mn(001) as an origin of exchange bias coupling to the magnetic Co layer

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Spin structures of an exchange-coupled-bilayer system of expanded-face-centered-tetragonal (e-fct) Mn(001) ultrathin films grown on Co/Cu(001) were resolved by means of spin-polarized scanning-tunneling microscopy. With an in-plane spin-sensitive probe, a layered antiferromagnetic-spin ordering of Mn overlayers was evidenced directly. In addition, the spin frustration across the same Mn layer creating a narrow domain wall down to nanometer scale was also observed along the buried step of Co underlayers. According to the micromagnetic simulation, the step-induced domain-wall width is in agreement with the experimental results. Such in-plane layered antiferromagnetic-spin structures of e-fct Mn(001) provide uncompensated spins at the interface with Co underlayers and elucidate the mechanism of the corresponding exchange-bias field observed in the previous studies.

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Exchange coupling between adjacent antiferromagnetic (AFM) and ferromagnetic (FM) layers has drawn much attention with regards to both fundamental magnetic physics and the application of modern spintronic devices. Typically, in the AFM/FM-bilayer systems, the exchange-coupling behavior could contribute the coercivity enhancement and the shift from the zero point of the field, which is the so-called exchange bias to the magnetic-hysteresis loops. According to previous studies, two kinds of AFM-spin configurations, i.e., uncompensated and compensated, were proposed to explain such exchange-coupling behavior observed in the AFM/FM-bilayer systems. In the uncompensated-AFM-spin configuration, which provides the pinning effect of FM spins at the interface, the unidirectional anisotropy would be created to have FM magnetization rotated more easily in one direction. On the contrary, for the AFM layer with compensated-spin configuration in contact with the FM layer at the interface, different models, such as those for the formation of domains of the AFM layer, noncollinear coupling at the interface, and residual uncompensated spin from interfacial roughness, etc., were reported. However, in these models, an interfacial-AFM-moment imbalance due to roughness or disorder, creating a certain number of uncompensated spins at the interface such that the interfacial spins of the Co layer can be pinned to possess unidirectional anisotropy resulting in an exchange-bias field. Therefore, it is needed to experimentally verify the proposed compensated-spin structure of e-fct Mn(001), the direct, advanced spin-mapping technique of spin-polarized scanning-tunneling microscopy (SP-STM) is required.

In contrast to the previous studies on body-centered-tetragonal (bct) Mn/Fe(001), the e-fct-Mn/Cu(001) system represents the important coercivity enhancement and prominent exchange-bias behavior due to interfacial coupling in the traditional AFM/FM ultrathin films, which is not observed in the bct-Mn/Fe(001) system. In order to understand the open question on the surface-spin structures of a few monolayers of e-fct Mn coupled to Co/Cu(001) and also have a general understanding of the physical origin of the exchange-bias field, a comprehensive study providing information on the connection to microscopic exchange-bias coupling and macroscopic magnetic behavior is significantly essential. Therefore, in this paper, we applied the SP-STM technique to resolve the spin structures of e-fct Mn(001) grown on Co/Cu(001), and the in-plane layered antiferromagnetic (LAF) spin arrangements have been observed. Besides, the AFM-coupling behavior of the Mn-capping layers was demonstrated to be connected with the determination of the coercivity enhancement observed in the thickness- and temperature-dependent-MOKE measurements. Furthermore, across the same Mn layer, the spin frustration accompanied with a sharp domain wall has been also observed in connection with hidden Co steps. The micromagnetic simulation for this AFM/FM-bilayer system further supports the picture of the LAF-spin structure of e-fct Mn(001).

The experiment was performed in an ultrahigh vacuum (UHV) multifunctional preparation chamber with a base pressure of 1×10−10 Torr, and the sample was mounted on a highly polished Cu(001) substrate that was maintained at room temperature. Spin-polarized scanning-tunneling microscopy measurements were performed in an ultrahigh vacuum chamber equipped with a standard ultrahigh vacuum (UHV) system, and the sample temperature was continuously monitored by a chromel-alumel thermocouple. The sample temperature was maintained at room temperature throughout the experiment. Spin-polarized scanning-tunneling microscopy measurements were performed in an ultrahigh vacuum chamber equipped with a standard ultrahigh vacuum (UHV) system, and the sample temperature was continuously monitored by a chromel-alumel thermocouple. The sample temperature was maintained at room temperature throughout the experiment.
pressure of about $3 \times 10^{-11}$ mbar. The clean Cu(001) substrate was prepared by cycles of Ar$^+$ sputtering and annealing at 850 K. Both Mn and Co films were deposited at room temperature with a deposition rate of 60 ~ 80 s/mL calibrated from STM. The measurement of low-energy-electron diffraction (LEED) was carried out to characterize the crystalline structure. From LEED-I/V curves (not shown here), the average vertical interlayer distance of the films was also determined using kinematic approximation.\textsuperscript{20} Magnetic properties of the films were characterized by the in situ magneto-optical Kerr effect in the longitudinal geometry with a modulation and lock-in technique. As for the SP-STM measurements, the sample was transferred into a low temperature (LT)-STM chamber, which was cooled to 77.5 K, and the tungsten tip coated with 40-mL Fe was applied to provide in-plane spin sensitivity.\textsuperscript{18,21} Furthermore, by adding a voltage modulation of 10 mV\textsubscript{rms} to the sample bias, the conductance spectra can be obtained from the first harmonic signals detected by the lock-in amplifier.

In Fig. 1(a), the STM morphology of 5-mL Co grown on Cu(001) as well as the corresponding LEED patterns are shown. The surface morphology of Co films and $p(1 \times 1)$ diffraction pattern both illustrate the good epitaxial growth of the Co films. After 1.5 mL of Mn capped on 5-mL Co/Cu(001), not only the uncompleted first layer but also the start of the second Mn layer were observed from the STM morphology in Fig. 1(b). In addition, due to the room-temperature growth of Mn films, the first layer of the Mn-Co(001)-surface alloy was formed\textsuperscript{22,23} according to the $c(2 \times 2)$ superstructures in appearance but only the $p(1 \times 1)$ layer left in the LEED patterns shown in both insets. This could be due to the fully outward buckling relaxation of Mn atoms after the completion of the first Mn layer, and no further interdiffusion of Co underlayers takes place at higher coverages of Mn films.\textsuperscript{22,23} The STM images point out the smooth surface morphology of Mn films with respect to the two layers exposed to the top of the surface and give an indication of the two-dimensional layer-by-layer growth mode of Mn epitaxial films, also supporting the consistency reported previously.\textsuperscript{22–24} For the vertical-interlayer-distance expansion of the e-fct-Mn films, a $c/a$ ratio of $\sim 1.045$ as the thickness of covered Mn layers of up to 3.5 mL has been confirmed and determined by either x-ray photoelectron-diffraction or LEED-I/V measurements.\textsuperscript{8,9}

After we have realized the growth and crystalline structures of Mn films on Co/Cu(001), the SP-STM experiments at 77.5 K for resolving Mn surface-spin structures on this exchange-coupled AFM/FM-bilayer system are illustrated in the following. The topography and spin-resolved conductance-mapping measurements. Nevertheless, in the STM images of Figs. 1(c) and 1(d) with further Mn capping layers of 3.5 and 5.5 mL on 5-mL Co/Cu(001), there are no $c(2 \times 2)$ superstructures in appearance but only the $p(1 \times 1)$ layer left in the LEED patterns shown in both insets. This could be due to the fully outward buckling relaxation of Mn atoms after the completion of the first Mn layer, and no further interdiffusion of Co underlayers takes place at higher coverages of Mn films.\textsuperscript{22,23} The STM images point out the smooth surface morphology of Mn films with respect to the two layers exposed to the top of the surface and give an indication of the two-dimensional layer-by-layer growth mode of Mn epitaxial films, also supporting the consistency reported previously.\textsuperscript{22–24} For the vertical-interlayer-distance expansion of the e-fct-Mn films, a $c/a$ ratio of $\sim 1.045$ as the thickness of covered Mn layers of up to 3.5 mL has been confirmed and determined by either x-ray photoelectron-diffraction or LEED-I/V measurements.\textsuperscript{8,9}

In order to characterize the exchange-coupling behavior between the Mn and Co layers, the MOKE measurements were applied to investigate the temperature dependence of the coercivity on 5-mL Co/Cu(001) covered with Mn films. From Fig. 2(d), the coercivity field of 5-mL Co films as a function of temperature was indeed obviously enhanced after capping with 5.5-mL-Mn layers. This demonstrates the antiferromagnetic property of e-fct-Mn films through the pinning effect on the interfacial spins of Co underlayers. Besides, in the reduced thickness of 3.5-mL Mn, the coercivity enhancement of 5-mL
layer at the bias voltage of 0.68 V above, surface-spin structures of 3.5-mL e-fct-Mn films are shown in the inset of Fig. 3(c). The fitted domain-wall width from this formula is around $15 \pm 48$ nm.

According to the topography and simultaneously obtained spin-mapping image of 3.5-mL Mn on 5-mL Co/Cu(001) in Figs. 3(a) and 3(b), not only the LAF-spin structures but also the striking phenomenon of spin frustration across the same Mn layer. Similar to the e-bct-Mn films grown on the Fe(001) system, the LAF-spin configuration can construct a prototypical model system to study topologically induced spin frustrations regarding the competition between domain-wall energy in AFM- and exchange-coupling energy in the interface of antiferromagnetism and ferromagnetism. As the region framed by the white-dashed square in Fig. 3(b), we show the averaged spin-resolved conductance-line profile in Fig. 3(c). The corresponding domain-wall width from spin frustration is able to be extracted through the standard wall-profile-fitting method for uniaxial systems:
The material parameters of exchange stiffness ($A_{\text{ex}}$) and magnetocrystalline anisotropy ($K_a$) used in the simulation with the mesh unit cell of $0.2 \times 0.2 \times 0.2$ nm$^3$ are set in the following. $A_{\text{ex}} = 1 \times 10^{-11}$ J/m and $K_a = 4.1 \times 10^5$ J/m$^3$ were for Co (Ref. 32), and $A_{\text{ex}} = -1 \times 10^{-11}$ J/m and $K_a = 6 \times 10^4$ J/m$^3$ were for Mn. The magnetocrystalline anisotropy of Mn was deduced from the domain-wall width fitted by $2\sqrt{A_{\text{ex}}/K_a}$, and the uniaxial-anisotropy direction was parallel to the [110] easy-axis direction of the Co layers on Cu(001).

The simulated results are shown in the top and side views of Figs. 4(a) and 4(b), respectively. First of all, the LAF-spin structures of the Mn films can only be stabilized by coupling with the FM Co underlayers and cannot reach the equilibrium state if the Mn films are free standing without being pinned by Co underneath. Besides, the Co hidden step, indicated by the white arrow in Fig. 4(b), inducing spin frustration and thus creating the domain-wall width of $\sim 3.2$ nm, which is consistent with the value measured in the experiments, has been demonstrated in the top view of Fig. 4(a). We found the value of the domain-wall width is strongly correlated with the exchange-coupling strength between the Mn and Co layers and displays a broadening effect as the thicknesses of the Mn films increase. Such micromagnetic simulation illustrates the significance of the Co underlayers, which give rise to not only the LAF-spin structures of the Mn films through the magnetic direct-exchange coupling but also the spin-frustration phenomenon due to the buried steps. These recognize the good agreement with the observed experimental results and provide deeper understanding for the spin structure of the e-fct-Mn films coupled with the Co underlayers.

In conclusion, the in-plane LAF-spin structures of e-fct-Mn films grown on Co/Cu(001) have been resolved by SP-STM at 77.5 K. From the MOKE measurements, the coercivity enhancement as a result of the pinning effect on the interfacial spins of Co underlayers illustrates the AFM properties of e-fct-Mn films. In addition, the spin frustration across the same Mn layer induced by hidden Co steps not only supports the LAF-spin configuration but also indicates the magnetic-coupling competition between the domain-wall energy of the Mn layers and the exchange-coupling energy of the Mn/Co interface. The micromagnetic simulation recognizes the equilibrium state of the LAF magnetic structures of the Mn films coupled by the Co layers underneath and also the thickness-dependent domain-wall width created by buried Co steps, both of which are in agreement with the experimental measurements. Our findings demonstrate the exchange bias arising from the AFM/FM-exchange coupling instead of uncompensated spins from the interfacial roughness between the Mn and Co layers. This directly connects the microscopic AFM/FM-exchange coupling with the macroscopic-exchange-bias phenomenon, which can be taken as a significant step toward the general interpretation and can also shed light on the application of fabricating high-quality spintronic devices in the future.

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31The Object Oriented Micromagnetic Framework (OOMMF) Project at NIST. We used the OOMMF program Ver.1.2a3 [http://math.nist.gov/oommf/].