

Growth and Kerr magnetometry of Mn_2Au on a gold-capped Nb(001) substrate

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We report on the epitaxial growth of antiferromagnetic Mn_2Au on a Nb(001) substrate capped with a pseudomorphic layer of gold. We observe a layer-by-layer growth by means of medium-energy electron diffraction and confirm stoichiometry and surface structure by Auger electron spectroscopy and low-energy electron diffraction. Evaporation of 15 ML of ferromagnetic Fe on 12–17 ML of Mn_2Au results in an exchange-coupled bilayer system with an exchange-bias shift that can be set by field-cooling from 400 K. Areas with and without exchange bias, with domain sizes in the range of tens of μm , are identified by Kerr microscopy. Postannealing the sample at or above 450 K after Mn_2Au layer growth decreases the fraction of areas where Fe magnetically couples to Mn_2Au . We suggest that exchange coupling to an interfacial Fe layer depends on the interface termination of Mn_2Au or on the chemical order in the Mn_2Au layer. Our findings provide insight into the growth process of Mn_2Au and the coupling to an Fe layer. Our results point out the importance of growth, interface quality, and termination for the magnetic properties of a $\text{Mn}_2\text{Au}/\text{Fe}$ bilayer, which may help to improve material properties for spintronic applications.

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I. INTRODUCTION

In the last decade, antiferromagnetic (AFM) materials have seen a rise in interest for spintronic applications [1–4]. Because of their faster dynamics in the THz range [5] compared with the GHz range of ferromagnetic (FM) materials, as well as their robustness against perturbations from external magnetic fields and absence of stray fields, AFMs are promising materials not only for fast and energy-efficient data storage but also for applications beyond storage, like THz emitters and detectors or spin-current generators [2,6–10]. One way to achieve electric switching of the AFM order parameter, without the use of an interfacial heavy-metal layer, is by using current-induced staggered N el spin-orbit torques (SOTs). So far, only Mn_2Au and CuMnAs are known to possess the required centrosymmetric lattice with locally broken inversion symmetry to generate these torques. After its theoretical prediction, several groups have demonstrated current-induced switching in these materials (even though it is not quite clear whether magnetostriction or SOT-switching was observed)

[11–14]. Recently, a reorientation of the AFM order parameter in Mn_2Au has been observed by strong exchange coupling to an FM Permalloy (Py) layer at the interface [15,16].

Mn_2Au is a metallic collinear AFM with a bulk N el temperature above 1000 K [17] and a body-centered tetragonal crystal structure with $a = 3.32 \text{ \AA}$ and $c = 8.53 \text{ \AA}$ as lattice parameters [18]. For layers grown in the (001) plane, the magnetic easy axes are parallel to the [110] directions. It has been shown that the quality of the layer growth is essential for its (magnetic) properties [18,19] and that the N el temperature can be lowered in proximity to Fe [20]. So far, not many substrates are available for the epitaxial growth of Mn_2Au (001) layers, often requiring reliance on a sputter-deposited buffer layer, like Ta, to accommodate the large lattice mismatch with the substrate [13,18,21,22]. For well-ordered and defect-free layer-by-layer growth of Mn_2Au (001), it would thus be ideal to use a single-crystalline substrate with lattice parameters similar to those of Mn_2Au .

In this paper, we report on the epitaxial growth of Mn_2Au directly on a metallic Nb(001) substrate capped with a pseudomorphic layer of Au. Nb, like Ta, has a very close lattice match to Mn_2Au , with a bcc lattice and a lattice constant of $a = 3.30 \text{ \AA}$. To our knowledge, this kind of single-crystal substrate has not been used before for the growth of Mn_2Au . Medium-energy electron diffraction (MEED) reveals a layer-by-layer growth of Mn_2Au . After evaporation of 15 monolayers (ML) of ferromagnetic Fe on top of the Mn_2Au films, a two-step magnetization reversal is observed in longitudinal magneto-optical Kerr effect (L-MOKE) measurements, where the second step exhibits an exchange-bias (EB) shift of the magnetization loop as well as a

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temperature-dependent coercivity, indicating a coupling between FM Fe and AFM Mn_2Au . We conclude that the first step of the magnetization reversal belongs to areas of the sample where Fe and Mn_2Au do not couple at the interface, while the second step belongs to areas where they do. Postannealing the Mn_2Au layer to ≥ 450 K, prior to Fe evaporation, reduces the coupled areas while simultaneously increasing their EB and coercivity. Utilizing Kerr microscopy, we identify coupled and uncoupled areas on the sample as well as magnetization reversal mechanisms. Our findings highlight the feasibility of expanding the range of available substrates to metal single crystals for the growth of Mn_2Au layers, as well as providing a better understanding of the coupling between Mn_2Au and Fe at the interface.

II. EXPERIMENTAL DETAILS

Samples were grown on a Nb(001) substrate with molecular beam epitaxy in UHV. The base pressure of the chamber was around 7×10^{-10} mbar while the pressure was kept in the lower 10^{-9} range during (co)evaporation of Mn, Au, and Fe.

The layer system of our samples consists of Nb(001)/NbAu/12–17 ML $\text{Mn}_2\text{Au}/t_F$ Fe, with the Nb(001) single crystal capped by one ML of Au, as explained in the following. Achieving an oxygen-free Nb surface is quite challenging, requiring repeated flash annealing at temperatures close to the melting point of Nb with excellent chamber pressure conditions [23–25]. Still, oxygen may segregate from the bulk to the surface, contaminating the surface and altering the lattice structure. To avoid this, we employed the substrate-cleaning protocol from Hüger *et al.* [26]. The Nb(001) single crystal was first cleaned by repeated Ar^+ sputtering and flash annealing at around 1900 K for a few minutes. To prevent oxygen segregation, 10 ML of Au was evaporated on Nb and subsequently flash-annealed to 1200–1300 K for 70 s. At these parameters, all the Au in excess of 1 ML diffuses into the bulk of the Nb but remains close enough to the surface [26]. This results in the formation of a near-surface Au–Nb alloy, which acts as a barrier to oxygen segregation, leading to an inert, flat surface with metallic character while still preserving the Nb lattice parameters. Auger electron spectroscopy (AES) at 3 keV confirmed successful flash annealing of Au by monitoring the presence of Nb and Au peaks and the absence of C and O contamination. Additionally, low-energy electron diffraction (LEED) was employed to check for a clean, flat surface with a (001) orientation without an oxygen superstructure. LEED images, taken at electron energies of 140–148 eV, are shown in Fig. 1 after flash annealing of Nb(001) at 1900 K (a) and after flash annealing of 10 ML of Au (b) on Nb(001). In (a), additional LEED spots indicate an oxygen superstructure on the Nb(001) surface, which was confirmed by AES measurements, while in (b) clear (001) spots correspond to a flat surface with long-range crystallographic order.

Deposition of Mn_2Au was achieved at a substrate temperature of 380–390 K (or 350 K) by coevaporation of Mn flakes in a Ta-crucible and Au from a rod wrapped in a W filament. During evaporation, a quartz crystal microbalance (QCM) was used to monitor the evaporation rates of Mn and Au,

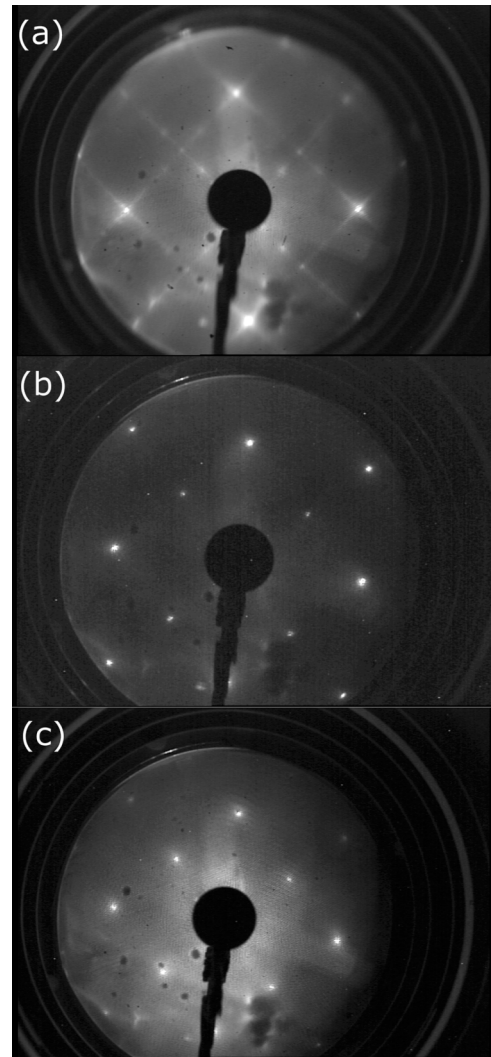


FIG. 1. LEED images of surface-oxidized Nb (a), after flash annealing of Au (b), and after evaporation of 15 ML of Mn_2Au (c) at electron energies of 140–148 eV. Additional LEED spots in (a) indicate an oxygen superstructure, while (b) and (c) show clear (001) spots corresponding to a flat surface with long-range crystallographic order.

while MEED oscillations were used to observe layer-by-layer growth of Mn_2Au *in situ*.

After evaporation, the atomic composition of the deposited Mn_2Au layer was checked by AES. Surface quality, lattice orientation, and lattice parameters were checked by LEED. Figure 1(c) shows a LEED image of the sample after evaporation of 15 ML of Mn_2Au . The intensity of the LEED spots is reduced compared to the Au/Nb(001)-like surface, however, clear (001) spots can be seen at the same positions. Thus, the horizontal lattice parameters of the grown Mn_2Au layer match those of the Nb(001)/NbAu substrate.

A 15-ML film of Fe was subsequently evaporated from a rod with the sample kept at room temperature, and its magnetic properties were checked by measuring the magnetization loop via *in situ* L-MOKE magnetometry. The azimuth of the Nb(001) single crystal was turned by 45° to apply the external magnetic field parallel to the [110] direction of the Mn spins

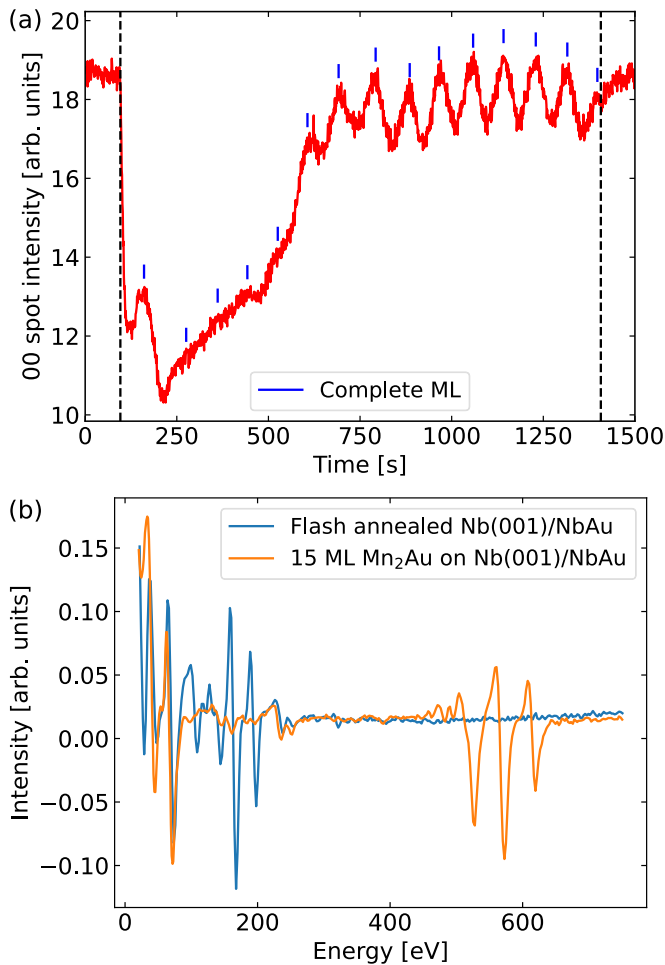


FIG. 2. (a) MEED oscillations measured *in situ* during deposition. Black dotted lines indicate the start and end of deposition. Blue dashes indicate a complete ML, with the second and third ML marked at likely positions interpolated from the other peaks. (b) Auger electron spectra of the clean flash-annealed Nb(001)/NbAu substrate and after deposition of 15 ML of Mn_2Au .

in the Mn_2Au layer. For the field-cooling (FC) process, the sample temperature was increased to 400 K for 10 min, and an external magnetic field of 100 mT was applied in the [110] direction before cooling with liquid helium to 40–50 K to set the direction of the EB.

For the *ex situ* Kerr microscopy measurements, the sample was capped with at least 15 ML of Cu before being taken out into air to prevent oxidation of Fe and Mn_2Au . Magnetic domains were imaged at room temperature by a wide-field Kerr microscope from Evico Magnetics arranged in the Köhler illumination scheme [27,28]. Images were subsequently drift-corrected by a software-based approach according to [29] to enhance domain contrast.

III. RESULTS

Figure 2(a) shows the intensity of the (00)-MEED spot during evaporation of 15 ML of Mn_2Au . The intensity first decreases with a local maximum (marked by a blue line) after deposition of 1 ML. Between 1.5 and 7 ML, the

intensity of the (00) spot increases to approximately the initial value. Strong oscillations after 6 ML indicate a well-ordered layer-by-layer epitaxial growth. The surface roughness of the finished layer appears to be minimal. Maxima of the MEED oscillations are in good agreement with multiples of the deposited amount measured by the QCM.

The Auger electron spectrum of 15 ML of Mn_2Au on Nb(001)/NbAu is displayed in Fig. 2(b). Calculating the ratio of the Auger peaks (see the Supplemental Material [30]) yields a composition of $\text{Mn}_{67}\text{Au}_{33}$ (67:33) indicating a deposition of Mn_2Au in a 2:1 ratio. Deposition of a $\text{Mn}_{1-x}\text{Au}_x$ layer with a composition other than 2:1 results in a lower intensity of the MEED spots and no or only a few weak oscillations, since the lattice parameters do not match those of the Nb substrate.

LEED images, taken at electron energies of 140–148 eV both for the clean Au/Nb(001) substrate [Fig. 1(b)] and after deposition of 15 ML of Mn_2Au [Fig. 1(c)], show clear (001) spots at similar positions, though the intensity of the LEED spots is slightly decreased and the spots are more diffuse after Mn_2Au deposition. This is probably because of an increased surface roughness or reduced crystallinity throughout the whole layer.

The LEED pattern after evaporation of Mn_2Au suggests epitaxial (001)-oriented growth with the in-plane lattice constant of Nb(001). This is consistent with the ordered bulk phase of Mn_2Au . However, we cannot exclude chemical disorder in the films. A LEED intensity vs beam energy (LEED-IV) measurement of the (00) spot does not yield conclusive information about the chemical order [30].

Figure 3 shows magnetization loops measured by *in situ* L-MOKE after the deposition of 15 ML of Fe. While heating from room temperature to 400 K, shown in Fig. 3(a), the coercivity of the Fe layer decreases from 22.5 mT at room temperature to about 11 mT at 400 K. This temperature-dependent coercivity suggests a coupling of FM Fe to the AFM Mn_2Au . Since no FC process has yet been performed, the Néel vector orientation in the AFM domains is randomly distributed and averages out within the beam spot. Hence, no EB shift can be measured.

After a FC process from 400 K down to about 50 K, magnetization loops were measured at different temperatures while heating back up to 348 K and are depicted in Fig. 3(b). Now, one part of the hysteresis loop is shifted horizontally towards larger negative fields, opposite to the setting field during the FC process. A second part of the hysteresis loop is not shifted, resulting in a two-step magnetization reversal. Here, the coercivity of the unshifted part of around 12.5 mT is comparable to that of a pure Fe layer on Nb(001). Looking at the temperature dependence, the unshifted part of the hysteresis loop shows no change with temperature, while both the coercivity and the horizontal shift of the shifted part decrease with increasing temperature. The absolute horizontal shift decreases from around 16.4 mT at 53 K to 7.6 mT at room temperature and approaches zero at 348 K. The coercivity decreases from 39.0 mT at 53 K to 24.9 mT at 348 K. From these measurements, we conjecture that the evaporated Mn_2Au layer is antiferromagnetic and that we were able to set, at least partially, the direction of its moments at the interface with Fe by field cooling from 400 K,

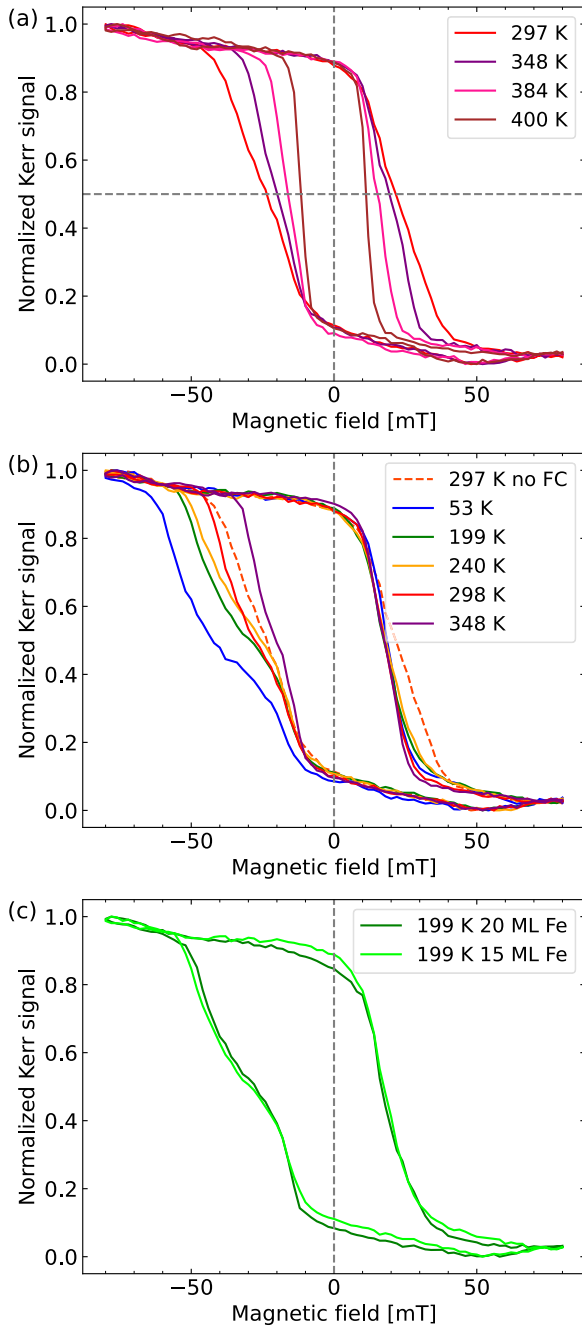


FIG. 3. Temperature dependence of the hysteresis loops of Nb(001)/NbAu/15 ML Mn₂Au/15 ML Fe before (a) and after (b) FC, together with the original hysteresis loop measured at room temperature for reference. (c) Comparison of hysteresis loops for 15 ML and 20 ML of Fe after FC.

resulting in an EB shift and increased coercivity of the shifted part.

For 15 ML of Mn₂Au, the ordering temperature appears to be between 348 K and 400 K, since otherwise the EB could not be set. This value is similar to the results from Wu *et al.* [20] for 10 nm of Mn₂Au(101) grown on Fe/MgO(001). This means that the Néel temperature of Mn₂Au is significantly reduced in the thin film compared with that in the bulk, where it should be above 1000 K. Reasons for this could be the

finite-size effect as well as the interface and exchange interaction with the Fe layer [20,31–34].

Aside from the ordering temperature, the EB shift and increased coercivity of the shifted part, as well as their temperature dependence, are further indications for a magnetic coupling between the FM Fe and the AFM Mn₂Au. Consequently, there are two possibilities for the two-step remagnetization: (1) only the interfacial Fe moments magnetically couple to the Mn₂Au moments while the bulk Fe moments do not couple; or (2) there are coupled and uncoupled areas between Fe and Mn₂Au laterally on the sample. To test these two hypotheses, we evaporated an additional 5 ML of Fe on top for a total of 20 ML of Fe. The comparison between the L-MOKE hysteresis loops of Nb(001)/NbAu/15 ML Mn₂Au/15 ML Fe and those with 20 ML of Fe is presented in Fig. 3(c). As a result, the uncoupled part remained unchanged, while the horizontal shift (EB) of the coupled part decreased. This reduction in EB is likely caused by its inverse dependence on FM layer thickness. The relative amplitude, defined as the ratio of the amplitudes of the shifted part and the unshifted part in the L-MOKE signal, did not change, which means that we can exclude their assignment to interfacial and bulk Fe, respectively. Instead, this confirms the presence of coupling and non-coupling areas on the sample.

These areas could depend on the interface roughness between Fe and Mn₂Au, with a flatter interface resulting in a larger coupling area. To investigate this, another sample was postannealed at 450 K for 30 min after Mn₂Au evaporation but before Fe deposition. This should reduce the surface roughness of the Mn₂Au layer before Fe evaporation and, consequently, reduce the interface roughness. Figure 4(a) shows the temperature-dependent magnetization loops of the 450 K postannealed sample after FC from 400 K to 52 K. Interestingly, the portion of the shifted part decreased from 0.6 without postannealing to about 0.42, compared with Fig. 3(b), meaning that a smaller area of Mn₂Au and Fe is coupled than without the extra postannealing. Additionally, the second sample was field-cooled again, this time from 450 K down to 41 K with an external magnetic field of 100 mT in the opposite direction to that of the first FC step. As a result, the shifted part of the hysteresis loops in Fig. 4(b) changes the sign of its EB from negative to positive. The ratio between the shifted and unshifted parts is again the same, so the coupled and uncoupled areas are the same as before. Therefore, increasing the field-cooling temperature seems to have no effect, indicating that the EB can already be set at 400 K for all coupling areas. Nevertheless, this demonstrates that the shifted part is indeed an EB shift, the direction of which can be reset by another FC process.

To better understand the effect of the postannealing step after Mn₂Au evaporation, we studied several samples with different postannealing temperatures ranging from room temperature (300 K) up to 475 K. Temperature-dependent hysteresis loops of samples with postannealing temperatures of 350 K, 400 K, and 475 K are plotted in Figs. 4(c)–4(e). Higher postannealing temperatures were not studied, since annealing at or above 500 K shows a noticeable change in the Mn:Au ratio in the AES measurements (with an increased Mn portion because of diffusion). Additionally, samples with

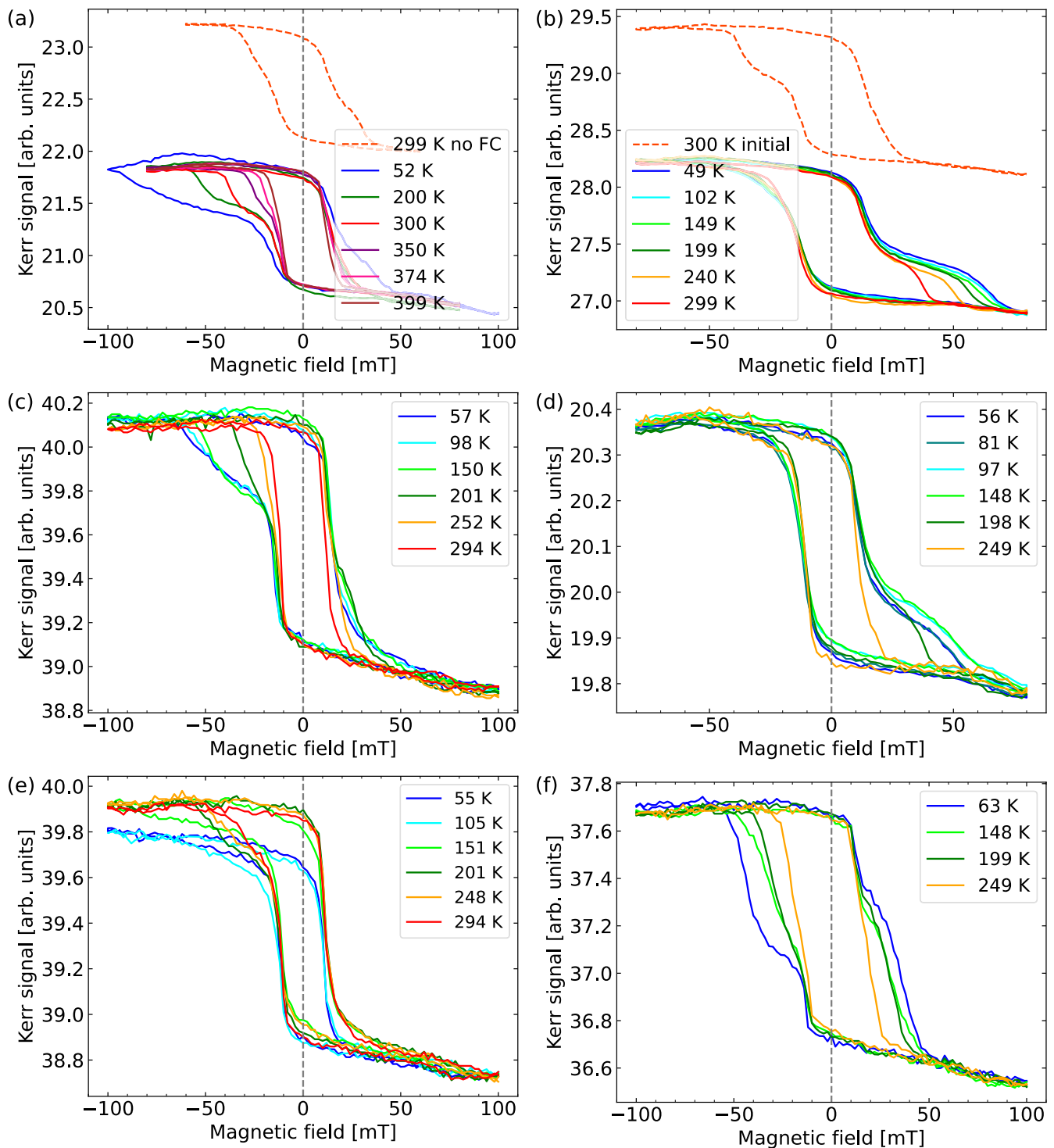


FIG. 4. (a) Temperature-dependent magnetization loops of a 450 K postannealed sample after FC. (b) Hysteresis loops after a second FC process in a reversed field, compared with the initial hysteresis loop at 300 K after the first FC process. (c)–(e) Hysteresis loops for different postannealing temperatures: (c) 350 K, (d) 400 K (FC field applied in the negative direction, 17 ML of Mn_2Au), and (e) 475 K. (f) Hysteresis loops after FC for a sample with only 12 ML of Mn_2Au , postannealed at 350 K.

12 and 17 ML as well as 20 ML of Mn_2Au were grown to study the influence of Mn_2Au thickness. Figure 5(a) plots the temperature-dependent coercivity and EB shift after FC for different postannealing temperatures, measured while heating up. All samples show a two-step remagnetization with a temperature-dependent coercivity and EB shift. The 350 K

postannealed sample with only 12 ML of Mn_2Au [Fig. 4(f)] shows a small EB shift below 100 K as well as an increased coercivity below 249 K in both directions, indicating a reset of the EB during the hysteresis loop measurement. The sample with 15 ML of Mn_2Au at the same postannealing temperature shows an EB shift at higher temperatures, up to 201 K, but also

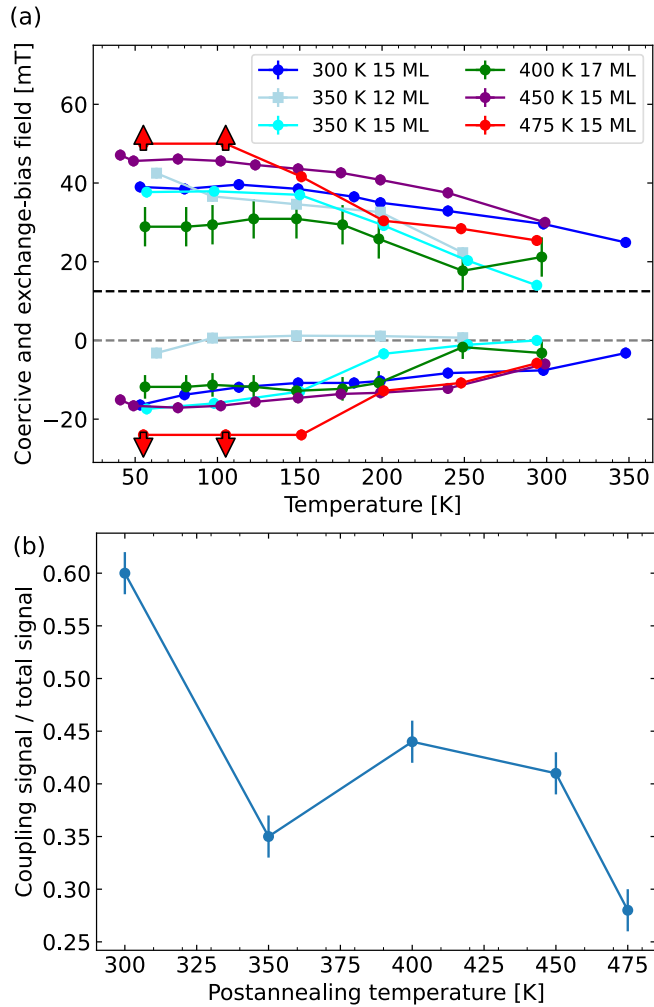


FIG. 5. (a) Plot of the temperature dependence of the coercive field (top) and EB shift (bottom), taken after a FC process, for different postannealing temperatures ranging from 300 K to 475 K. The black dashed horizontal line at 12.5 mT indicates the coercivity of the unshifted part. The red arrows at 55 and 105 K indicate data points for which the coercive or exchange-bias field exceeds the maximum measurable field range. (b) Ratio of the Kerr signal amplitude of the exchange-bias-shifted part of the hysteresis loop to the total amplitude of the saturated hysteresis loops for samples with 15–17 ML of Mn₂Au.

a small increase in coercivity in the positive field direction, which is not present at lower temperatures, indicating a partial reset of the EB. At 252 K, there is no EB shift but still an increased coercivity, while at 300 K only a single-step hysteresis remains. The other samples with a larger Mn₂Au thickness still have an EB shift below 300 K or at even higher temperatures. Therefore, increasing the Mn₂Au thickness results in an increased blocking temperature. For 20 ML of Mn₂Au, no EB shift but a temperature dependence of the increased coercivity can be observed (see the Supplemental Material [30]). This indicates that field cooling at 400 K was not sufficient to reach the blocking temperature in that sample. In general, samples with a postannealing temperature of 450 K and above show a trend toward larger values of EB shift and coercivity. It should be noted that for the sample with a 475 K postannealing

temperature, only a lower limit for the coercivity and the absolute EB shift can be determined below 150 K, indicated by arrows in Fig. 5(a), since an external field of 100 mT does not saturate the sample.

The relative coupling area of the sample, i.e., the ratio between the amplitude of the shifted part of the hysteresis loop and its total amplitude (sum of the shifted and unshifted parts), is plotted in Fig. 5(b). Here, it seems that the increased EB shift and coercivity come with a reduction of coupling area, as the amplitude of the second step decreases with higher postannealing temperatures. Sapozhnik *et al.* [19] observed something similar for their sputter-deposited samples, where they explained their findings by different crystallite sizes depending on the sample temperature during sputtering.

Kerr microscopy

To get a closer look at the coupled and uncoupled areas of our 450 K postannealed sample, it was capped with 15 ML of Cu to prevent oxidation and imaged by Kerr microscopy in air. Figure 6(a) shows the hysteresis loop of a (220 × 130) μm² sample area, measured in longitudinal geometry with 0.4 mT field steps [27,28]. It shows a two-step magnetization curve, similar to the one taken with the in situ L-MOKE in UHV. Figures 6(c)–6(f) show Kerr images taken at different external magnetic fields to access different states during magnetization reversal. Images are background-subtracted using an image taken at a positive saturating field. Dark and bright areas indicate alignment of Fe domains in the positive or negative field direction, respectively. Comparing the images at different fields in the hysteresis loop, Figs. 6(c) and 6(d), taken at –12.4 mT and 11.6 mT, respectively, show that the same magnetic domain patterns arise, meaning that the same regions on the sample that switch at small negative fields also switch at small positive fields. These dark areas in (c) and bright areas in (d) are the uncoupled areas of the sample, while the regions that did not switch are the coupled areas. Kerr images Figs. 6(e) and 6(f) were taken at –28.2 mT and 17.2 mT, respectively, and show the domain patterns when the coupled areas are partially switched. This means that an additional field of 10.5 mT is needed to reach the same state in the negative field direction, which is caused by the exchange bias. For the uncoupled areas, about the same field strength is needed in both directions to switch their magnetization direction. The size of the domains is surprisingly large, as they are in the μm range. Additionally, the sample was measured at the same position in polar and transverse geometries to identify the magnetization reversal mechanisms of the Fe layer.

In polar geometry with an in-plane field (see the Supplemental Material [30]), the signal did not change during the magnetization reversal, meaning that the Fe domains do not rotate out of plane. Figure 6(b) shows the signal taken in transversal geometry. A change in signal, beyond the background slope, can only be observed during the magnetization reversal of the uncoupled areas. This means that these domains switch by a coherent in-plane rotation. On the other hand, the switching mechanism of the coupled areas seems to be domain-wall nucleation and propagation.

In the next step, Kerr images (2 mT steps) were quantitatively analyzed by fitting the magnetization loop of each

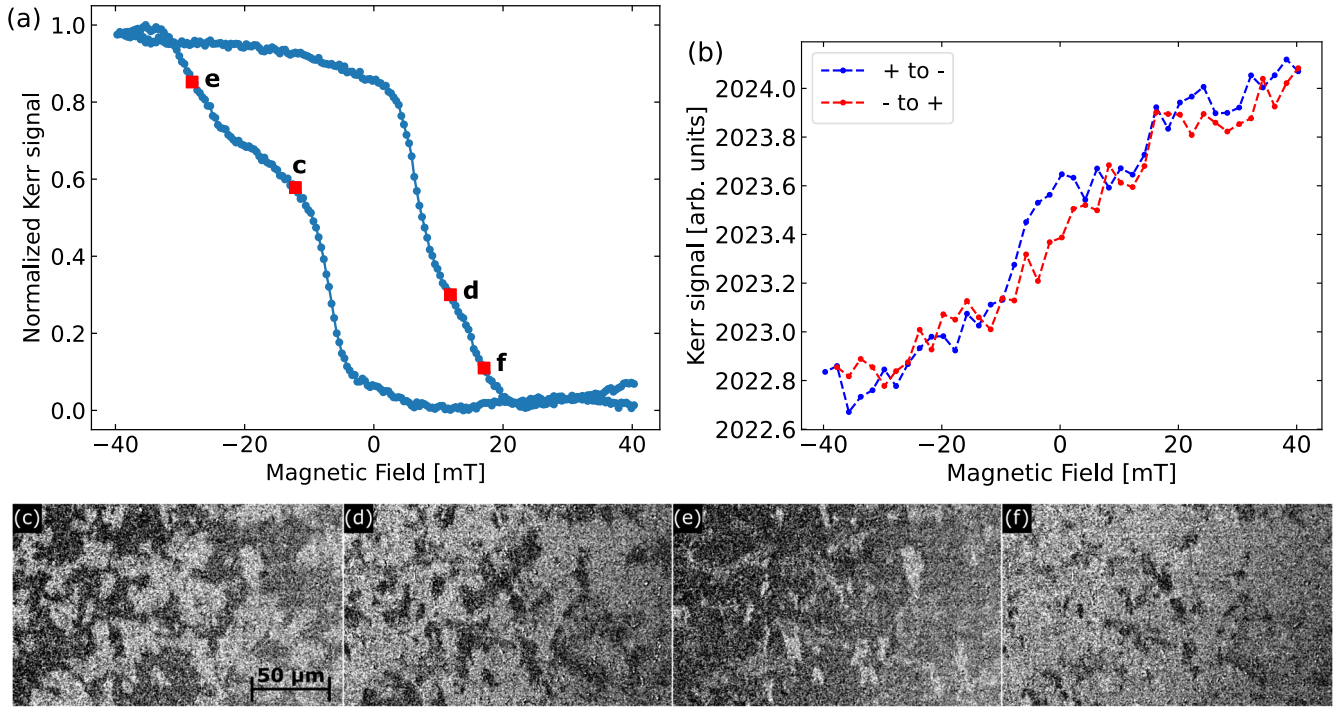


FIG. 6. Hysteresis loops measured by Kerr microscopy in longitudinal (a) (0.4 mT steps) and transverse (b) (2 mT steps) geometries. (c)–(f) Background-subtracted and drift-corrected longitudinal Kerr microscopy images taken during magnetization reversal at different external magnetic fields: after the first remagnetization step at -12.4 mT (c) and 11.6 mT (d), as well as close to saturation at -28.2 mT (e) and 17.2 mT (f), respectively.

pixel with an EB-shifted magnetization curve based on two branches of horizontally shifted arctan functions, one for each step of the magnetization reversal, with the equation $y_{\pm} = a + (2/\pi)b \cdot \arctan(c \cdot (x - d \pm e))$. Here, a is a vertical shift in case there are differences in the average Kerr signal between pixels, b is the amplitude, c describes the steepness of the magnetization reversal step, and d is the horizontal shift, i.e., H_{EB} , of the hysteresis loop, while e is a branch-dependent shift with its absolute value being H_C . The intensity at each pixel position was averaged by a Gaussian with a FWHM of six pixels to reduce noise. The Gaussian filter represents a compromise between achieving a sufficient signal-to-noise ratio for the fits without losing too much local information. The resulting color map and histogram for the EB shift H_{EB} and the coercivity H_C are depicted in Figs. 7(a) and 7(b). In Fig. 7(c), four regions of interest (ROIs) (light brown, dark brown, light blue, and dark blue) within the Kerr image can be identified that exhibit different behaviors of the magnetization reversal and are marked by black squares (1–4) for illustration. For each black square, the corresponding average Kerr signal is normalized and plotted as a function of the applied magnetic field in Figs. 7(d)–7(g). Dark brown (ROI 2) and light blue (ROI 3) regions belong to coupled and uncoupled areas, respectively. The dark brown region exhibits a single-step EB-shifted hysteresis loop with large H_C , while the light blue region shows an unshifted hysteresis loop with small H_C . From the magnetization loop of the light brown region (ROI 1), it is evident that this area is not saturated by the applied field of 40 mT. As a result, the fit function returns a rather large H_{EB} and a small H_C . It can be assumed that if these areas were completely saturated, they would also belong to coupled areas

exhibiting both a large H_{EB} and a large H_C . Finally, dark blue regions (ROI 4) show a large H_C but no H_{EB} . One reason for this behavior could be a noisy hysteresis loop, for which the fit function partially fails and returns unreasonable values, which can also be seen as purple spots in Fig. 7(a). The origin of the large noise may be defects or inhomogeneous illumination of the sample. Another reason could be a coupling area without an EB shift, which is marked by black square 4, with the corresponding hysteresis loop plotted in Fig. 7(g). For this region, the direction of the EB could not be set, which could be either because of a very large magnetic anisotropy of the Mn_2Au domain, preventing the FC process from setting the direction, or because the magnetic anisotropy of the Mn_2Au domain is actually small enough that the whole domain follows the Fe during the magnetization reversal, as has been shown in the literature for polycrystalline systems [35,36]. Since all dark blue regions are rather small, the latter explanation seems to be more likely.

Setting aside dark blue regions, it is evident that sample areas exhibiting a large H_C also exhibit a significant H_{EB} . Additionally, it can be concluded that the two-step hysteresis loop from the L-MOKE measurements results from two single hysteresis loops belonging to either coupled or uncoupled areas. The histogram of the color map exhibits two peaks each for H_{EB} and H_C , corresponding to coupled and uncoupled areas, with the larger peak belonging to the uncoupled areas. Fitting a Gaussian to each peak, as is shown in Figs. 7(a) and 7(b), and taking the area ratio between the two Gaussian functions results in an uncoupled:coupled ratio of 1.74:1 for the H_{EB} and a ratio of 1.47:1 for the H_C histogram. Here, some of the difference may be explained by the dark blue regions

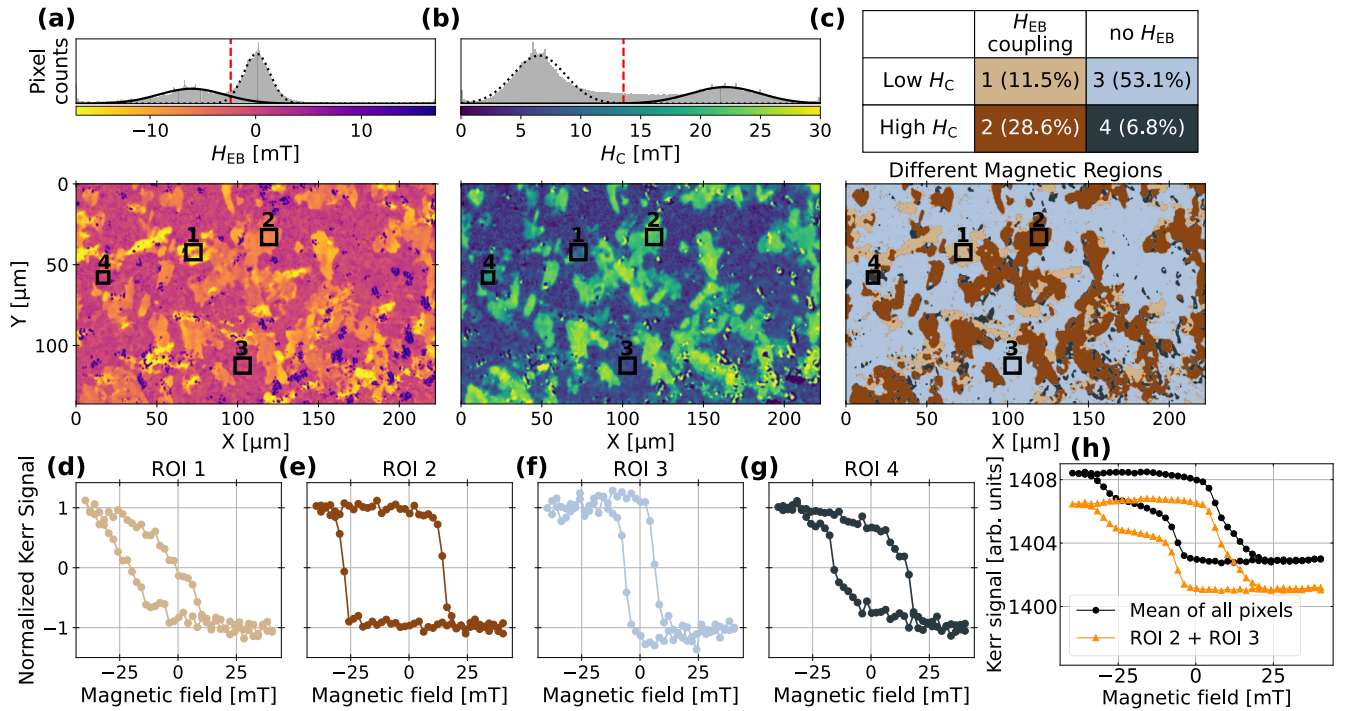


FIG. 7. Pixel-by-pixel analysis of Kerr microscope images (2 mT steps). Each pixel's magnetization loop was fitted with an EB-shifted magnetization curve based on arctan functions [$y_{\pm} = a + (2/\pi)b \cdot \arctan(c \cdot (x - d \pm e))$]. (a)(b) Color map and corresponding histogram of the local, pixel-wise EB shift (H_{EB}) and coercivity (H_C). The two peaks within both histograms, corresponding to coupled and uncoupled areas of the sample, are fitted by Gaussians (black solid and dotted lines). (c) Depending on the value of H_C and the absolute value of H_{EB} , four magnetic regions of interest (ROIs) can be identified, which are colored in light brown, dark brown, light blue, and dark blue. The table shows the relative amount of each ROI within the image. Example areas for each ROI are marked by a black square (1–4) within the images in (a)–(c). (d)–(g) Plot of the normalized average Kerr signal as a function of the applied magnetic field for each square. The light brown ROI corresponds to magnetically coupled sample areas that are not saturated by the magnetic field, leading to larger H_{EB} and smaller H_C values. Dark brown and light blue ROIs correspond to coupled and uncoupled areas, respectively, while the dark blue ROI represents areas where either the fitting function failed to accurately model the data, returning unreasonably large values, or the sample exhibits a magnetic coupling without an EB, resulting in a large value of H_C without an EB shift. (h) Reconstructed loops for the mean Kerr signal over all pixels (black) and for pixels identified as regions of interest (ROIs) 2 and 3 (orange).

exhibiting no EB shift. Not only are these area ratios quite similar, but they are also very close to the 1.41:1 ratio between the two hysteresis loop steps observed in the L-MOKE measurement. Differences may arise from an imperfect Gaussian fit as well as local variations in the amount of coupled areas, since Kerr images and L-MOKE measurements were taken in different sample regions. It should also be noted that the classification into four distinct magnetic ROIs represents a relatively simplistic approach and may not fully capture the complexity of the sample. However, a hysteresis loop was reconstructed using only the pixels from ROIs 2 and 3 [orange curve, Fig. 7(h)]. This loop exhibits a shape consistent with the loop generated from the mean intensity of all pixels (black curve), confirming the accurate identification of these ROIs. More importantly, the pixel-wise analysis further confirms the connection between H_{EB} and an increased H_C for coupled regions as well as the relative amounts of coupled and uncoupled regions.

IV. DISCUSSION

From the dependence on the postannealing temperature, it is clear that the annealing influences the coupling between Fe

and Mn_2Au . However, it does not clarify the physical origin of coupled and uncoupled areas. In the following, we will discuss different reasons for the occurrence of these areas.

Samples from Wu *et al.* [20] for an Fe/ Mn_2Au bilayer on MgO(001) show a two-step magnetization reversal as well, but they observe only coupled areas, i.e., both reversal steps are temperature dependent. Additionally, in contrast to our results, the relative amplitude of both steps depends on the Fe thickness with the unshifted part decreasing and the shifted part increasing with increasing Fe thickness. Here, it should be noted that Mn_2Au is grown on top of Fe and there is a small Au buffer layer on top of Fe, so the Fe– Mn_2Au interface is always Au. The asymmetric hysteresis loop is explained as the result of intergrain exchange coupling and different Mn_2Au domain configurations. Otherwise, the unshifted part should not decrease with temperature.

Since for our samples the unshifted part of the hysteresis loop shows no significant temperature dependence, we can discard different domain configurations within the Mn_2Au layer as an explanation. Oxidation of the Mn_2Au layer can be excluded as a cause, since AES measurements showed no oxygen peaks after the growth. Surface roughness of the Mn_2Au layer changes the interface with the Fe layer and

could lead to uncoupled areas by reducing the direct exchange interaction. However, MEED oscillations during growth and clearly visible LEED spots indicate a layer-by-layer growth with small surface roughness and long-range order. Also, Kerr microscopy images show domains for the coupled areas with sizes in the tens-of- μm range, larger than those that would be expected from roughness. In addition, increasing the postannealing temperature would then be expected to result in a larger EB-shifted amplitude, but here it shows the opposite effect. On the contrary, our postannealing temperature dependence would, in this case, indicate that a smaller amount of surface roughness actually results in a larger coupling area.

One other reason could be the growth of the Fe layer on top of Mn_2Au , which shows no MEED oscillations, since the lattice constant is quite different between both layers. Fe may not grow as a complete layer but instead exhibit an island-like growth, where only some areas have a good interface contact between Mn_2Au and Fe. However, this should not be influenced by the postannealing temperature of the Mn_2Au layer before Fe evaporation.

A change in the Mn_2Au crystallite size during the postannealing step could result in an increase or decrease in the Néel temperature T_N so that fewer or more crystallites can be oriented along the field-cooling direction. These crystallites should, however, still couple to Fe, leading to an unshifted part of the hysteresis loop with increased coercivity and temperature dependence, which we observe only in a minor portion of the sample (ROI 4).

Another reason could be the interface termination of the Mn_2Au layer with the Fe layer. During the growth of ordered Mn_2Au , there will either be Au or Mn atoms on the surface and an incomplete Mn_2Au layer should have both terminations. If we assume that only one species couples to Fe while the other does not, then this could lead to the two-step hysteresis loop that we observe. Bommanaboyena *et al.* [15] observed that a Mn_2Au layer with Au atoms at the interface couples very well to Py. Wu *et al.* [20] started the alternating deposition of Au and Mn with Au to create Mn_2Au on $\text{MgO}(001)/\text{Fe}$ and observed exchange bias. We can thus assume that a Au termination also leads to exchange bias in our samples. If Mn termination created no exchange bias, diffusion of Mn atoms to the surface after growth would lead to a reduction in the coupling area. Our AES measurements show a slightly Mn-rich Mn_2Au layer with a ratio close to 2:1, but with a slightly larger Mn portion. This points toward Mn surface diffusion and is in good agreement with our postannealing temperature dependence, where a higher postannealing temperature could mean more Mn surface diffusion and therefore a smaller coupling area. Agglomeration to Mn-rich and Au-rich areas at the interface would also explain the tens-of- μm -sized domains we observe in our Kerr images. In comparison, Bommanaboyena *et al.* and Sapozhnik *et al.* observed an average domain size around one magnitude smaller with a size of 1 to 3 μm for $\text{Mn}_2\text{Au}/\text{Py}$ and pure Mn_2Au layers grown on a Ta buffer layer, respectively [15,37].

In principle, one could also think of two different phases of Mn_2Au as the coupled and uncoupled areas if they exhibit the same in-plane lattice constant, for example, a chemically ordered and a chemically disordered phase. Sapozhnik *et al.*

have shown that decreasing the atomic order of Mn_2Au films enhances the exchange bias field in epitaxial (001) $\text{Mn}_2\text{Au}/\text{Fe}$ bilayers [19]. A slight deviation in overall stoichiometry could lead to a separation of ordered Mn_2Au areas and chemically disordered areas with a different stoichiometry. One would then need to assume that the chemically ordered areas are always terminated in such a way that they do not show magnetic coupling to the Fe layer in order to explain the temperature independence of the coercivity of the uncoupled areas. The effect of postannealing could be to enlarge areas with the bulk chemical order while at the same time moving the stoichiometry of the chemically disordered areas further away from the 2:1 ratio. This or an improved interface quality of these areas might then explain the experimental observation of enhanced exchange bias in the coupled areas.

Therefore, we suggest that coupled and uncoupled areas could result either from a different interface termination of the chemically ordered Mn_2Au layer, whereby only a Au termination results in magnetic coupling to Fe, or from areas of different chemical order in the Mn_2Au alloy. Cross-sectional TEM could give better insight into our $\text{Mn}_2\text{Au}/\text{Fe}$ interface, but this would go beyond the scope of this research. Additionally, changing the interface after Fe evaporation, without causing intermixing, would be interesting to carry out in future studies.

V. CONCLUSIONS

In summary, we achieved layer-by-layer growth of a room-temperature AFM Mn_2Au layer on a metallic Nb(001)-like substrate, extending the range of available substrates and giving more insight into the growth mode of Mn_2Au . Evaporation of Fe on top of Mn_2Au and subsequent FC results in a partial EB shift, which can be reset by another FC process, as well as a temperature-dependent coercivity for the shifted part. Both effects originate from the coexistence of coupled and uncoupled areas between the two layers. Kerr microscopy images reveal coupled areas with sizes in the tens-of- μm range. We observed a decrease in the coupled area with larger postannealing temperatures, which means that interface roughness is not the reason for the uncoupled areas. Instead, we conclude that either the interface termination of the Mn_2Au layer or the presence of two differently ordered areas of Mn_2Au causes the existence of coupled and uncoupled areas.

Our findings highlight the importance of high-quality Mn_2Au layer growth but also give rise to many more questions regarding the interface and the coupling between Mn_2Au and a ferromagnetic layer. Understanding the coupling behavior is crucial for applications in AFM spintronic devices.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [38].

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