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High Ms $Fe_{16}N_2$ thin film with Ag under layer on GaAs substrate

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(001) textured $Fe_{16}N_2$ thin film with Ag under layer is successfully grown on GaAs substrate using a facing target sputtering (FTS) system. After post annealing, chemically ordered $Fe_{16}N_2$ phase is formed and detected by X-ray diffraction (XRD). High saturation magnetization (Ms) is measured by a vibrating sample magnetometer (VSM). In comparison with $Fe_{16}N_2$ with Ag under layer on MgO substrate and $Fe_{16}N_2$ with Fe under layer on GaAs substrate, the current layer structure shows a higher Ms value, with a magnetically softer feature in contrast to the above cases. In addition, X-ray photoelectron spectroscopy (XPS) is performed to characterize the binding energy of N atoms. To verify the role of strain that the FeN layer experiences in the above three structures, Grazing Incidence X-ray Diffraction (GIXRD) is conducted to reveal a large in-plane lattice constant due to the in-plane biaxial tensile strain. [http://dx.doi.org/10.1063/1.4943236]

INTRODUCTION

It is well known that high saturation magnetization (Ms) material is in great need for both scientific research purpose and industry application. $Fe_{16}N_2$, as a high Ms material candidate, has been given intense focus in the past 50 years. Since its high Ms discovery,[1] many researchers have done substantial amount of research work in this material's fabrication and its physical property calculations,[2] resulting in a non-decisive conclusion that $Fe_{16}N_2$ does or does not possess high Ms property. With one decade efforts,[3] we have demonstrated that the partially ordered $Fe_{16}N_2$ thin film exhibit high Ms with the measurement of conventional magnetometry[4] and polarized neutron reflectivity.[5] To support our experiment result, we developed a "cluster+atom" model[6] to disclose the unique electronic structure of $Fe_{16}N_2$. We also discussed the relationship between the high Ms and the strain that the FeN layer experiences from the substrate or under layer.[7] In this report, a partially ordered $Fe_{16}N_2$ thin film with high Ms, which surpasses the previous report values, will be presented with the analysis of its nitrogen electronic state and the relationship between the high Ms and the tensile strain of the film.

EXPERIMENT

Partially ordered $Fe_{16}N_2$ thin films are grown by a facing target sputtering (FTS) system. The FeN layer grown on GaAs substrate and the FeN layer grown with Ag under layer on MgO substrate are both reported previously.[7] To further optimize the strain effect on the FeN layer, Ag under layer is developed on GaAs substrate and FeN layer is deposited on it subsequently. Prior to Ag growth,

a 5nm Fe layer is deposited on GaAs substrate, which is heated up to 250°C in advance, to promote the (001) texture. Ag under layer is grown at room temperature thereafter. Next, FeN layer is grown in the sputtering atmosphere of Ar and N_2 mixture. Finally, a 5nm Ru layer will be capped for protection purpose. Post annealing is carried right after in vacuum for 17hrs around 150°C.

$Fe_{16}N_2$ phase is detected by θ-2θ X-ray diffraction (XRD) using a Simens Bruker D5005 system with a Cu Kα radiation. Its MH-loop is characterized by a Princeton measurement vibrating sample magnetometer (VSM) with an external field up to 10kOe. The volume of the film is determined by the sample thickness and its surface area, which usually gives an estimation error 3%-5%. X-ray photoelectron spectroscopy (XPS) surface science SSX-100 is used to measure the nitrogen 1s electron binding energy. It is equipped with high efficiency large collection angle electron lens under monochromatic Al Kα X-ray. Grazing Incidence X-ray Diffraction (GIXRD) is performed by a Philips X'pert Pro X-ray diffractometer.

RESULTS AND DISCUSSION

To examine the crystallinity of the partially ordered $Fe_{16}N_2$ thin film, XRD is performed to explore the out of plane texture. In FIG 1, it is clearly shown that Ag (001) is developed although Fe (002) peak is hard to find due to its presence in the vicinity of single crystal substrate GaAs (004) peak. The Fe_8N (002) peak indicates that disordered phase with the right stoichiometry is formed at the as-deposit stage. Finally, the fingerprint peak at 2θ=28.5°, which can be indexed to $Fe_{16}N_2$ (002), can be observed with robust peak intensity. This proves the existence of ordered $Fe_{16}N_2$ phase, which arises due to the superlattice diffraction given by the ordered Fe-N planes as a result of the disorder-to-order transformation after the post annealing process. When FeN layer grows on top of the Ag under layer, FeN <100>will rotate 45° from Ag <100> to match the lattice constant of Ag. This is different from FeN growth on the Fe under layer.

VSM measurements are done at room temperature. To fully saturate the magnetization of the whole FeN thin film, an external field is applied in plane up to 10 kOe. To measure the thin film thickness, a cross section dark field TEM is taken as shown in FIG 2. The contrast of different layers corresponds to different average atomic numbers. We can clearly find the thickness of Fe and FeN layer around 5nm and 35nm, respectively. Different from previous FeN thin film results, the MH loop in FIG 3 indicates a softer FeN layer, which is shown by a lower saturation field (around 3500 Oe). This is most likely due to the anisotropy change of the FeN phase in the

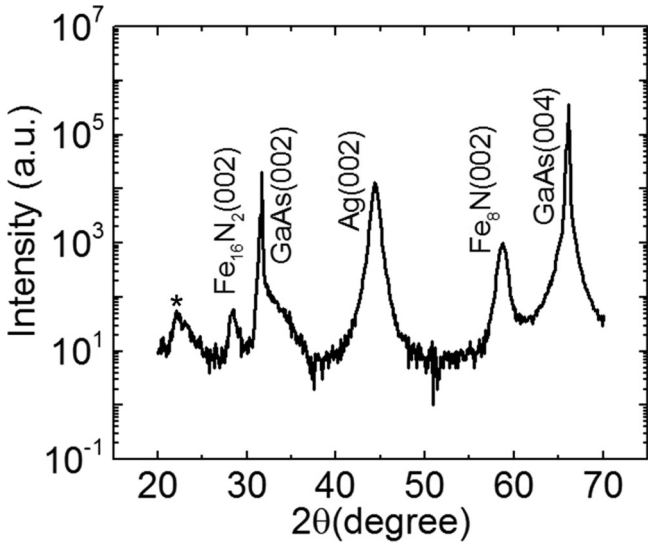

FIG. 1. X-ray diffraction pattern of (001) textured $Fe_{16}N_2$ grown on GaAs with Ag under layer. Finger print peak $Fe_{16}N_2$ (002) is observed after in-situ annealing at 150°C in vacuum for 17hrs. The peak indexed by (*) comes from the combination of Ag and FeN layer interface.

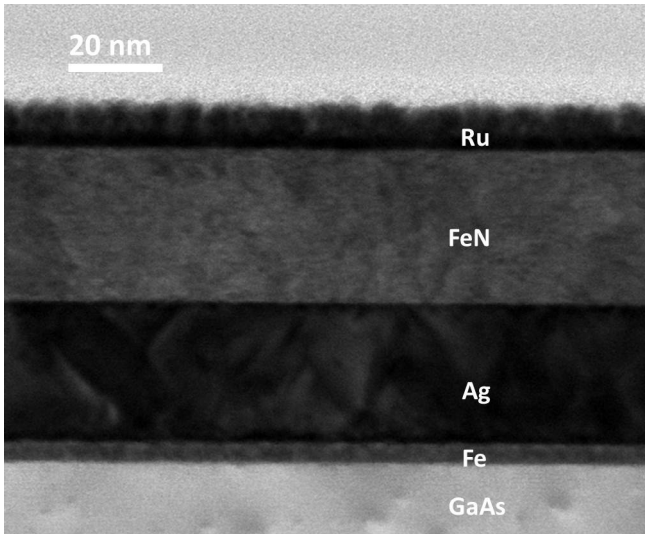

FIG. 2. Cross section dark field TEM image of FeN thin film with Ag underlayer on GaAs substrate.

thin film compared to previous FeN thin film structures. As shown by the previous results,[7] the first-rapid-and-then-slow increase of magnetization with applied field is due to the separation of hard $Fe_{16}N_2$ phase and soft Fe layer by Ag under layer. However, a zoom-in look in lower field range reveals a two-step magnetization increase during the soft phase switching with external field. This is most likely due to a soft phase moment reverse process in the FeN layer in addition to the soft Fe under layer. Therefore, we can conclude that the perpendicular magnetic anisotropy of the film is lowered with Ag under layer on GaAs substrate than that on MgO substrate. After saturation, the Ms reaches 1860 emu/cc for the whole film. The Ms of the FeN layer after subtracting that of Fe under layer yields a value of 1910 emu/cc, which is higher than both previously reported cases,[7] namely FeN/Ag/MgO and FeN/GaAs samples. The large Ms value should be associated with the combination of both Ag under layer and GaAs substrate since other growth conditions do not differentiate from the other two structures.

To better understand the high Ms result, nitrogen 1s electron binding energy is investigated with XPS. To make a comparison, FeN/Ag/MgO and FeN/GaAs structures are tested as well. After

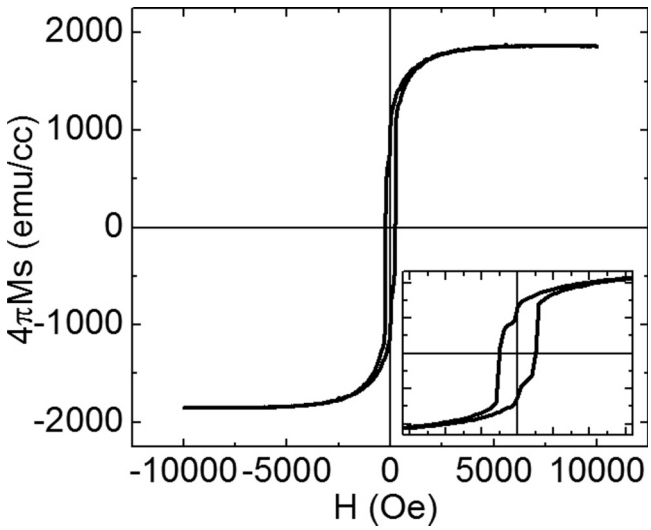

FIG. 3. Hysteresis loop of FeN on GaAs substrate with Ag under layer. The Ms value of the whole film reaches about 1860 emu/cc.

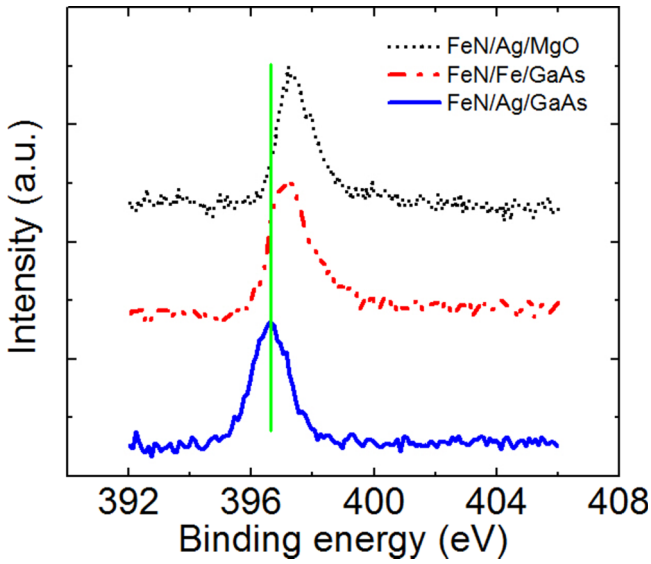

FIG. 4. XPS result on nitrogen 1s binding energy of three FeN thin film structures. An obvious shift of FeN/Ag/GaAs structure can be observed.

carbon energy calibration, a high resolution scan is performed with the binding energy from 392eV to 406eV. As seen in FIG 4, FeN/Ag/GaAs sample nitrogen 1s electron binding energy peak shifts to left compared to the other two samples. This shows a higher energy case due to a more negatively charged environment for nitrogen atom. Thus the local electrons for the surrounding iron atoms will be reduced and therefore it is more likely to exhibit higher Ms.

Since compared to the FeN/Ag/MgO structure, the only difference here is the change of substrate, we examine the relationship between the high Ms and strain effect by conducting GIXRD. Sample is placed with the out of plane direction perpendicular to the film plane. After aligning the GaAs (220) plane, a θ-2θ scan is performed in the vicinity of GaAs (220) peak. In FIG 5, the peak around $2\theta = 43.4^\circ$ is shown, which indicates one specific layer or phase follows the epitaxy of substrate and Fe under layer but apparently with a weaker intensity due to imperfect crystal growth.

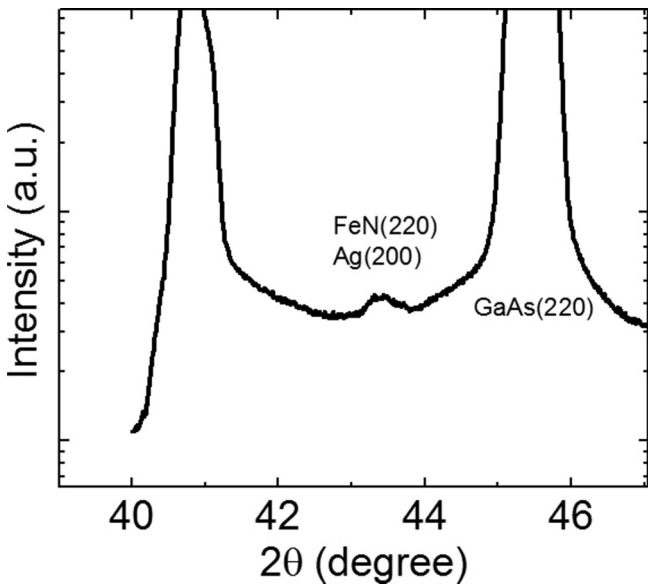

FIG. 5. GIXRD result of FeN thin film aligning GaAs (220) plane. The contribution from FeN and Ag (200) peak suggests a larger in plane constant as a result of using Ag under layer on GaAs substrate.

Since textured Ag (200) peak and FeN (220) can be hardly differentiated, it is safe to assume that part of the contribution of the interest peak comes from FeN (220) phase, corresponding to an in plane lattice constant 5.9Å, which is also larger than the FeN in plane lattice constant of the other two structures. As the nominal $Fe_{16}N_2$ in plane lattice is 5.72Å, this ~3% lattice constant increase should have a big impact on its electronic structure. In addition, this observation is consistent with previous results[5] that an in plane tensile strain is correlated with a high Ms of $Fe_{16}N_2$ phase. Since XPS results show a more negatively charged nitrogen atomic environment, it is intuitive to relate the charge transfer to the lattice distortion. The high Ms result of the current FeN thin film can be understood by the charge transfer between iron and nitrogen atoms,[6] which originates from the lattice distortion of the unit cell. Also, the anisotropy of the thin film is reduced for this sample, which can also be related to the lattice distortion. Since the out of plane lattice constant of $Fe_{16}N_2$ phase, which is determined from the out of plane XRD scan, does not vary much from FeN/Ag/MgO structure and only in plane lattice constant increases, this leads to a decrease in c/a ratio, which in turn results in a lower tetragonal crystalline anisotropy.

CONCLUSIONS

In conclusion, FeN/Ag/GaAs was successfully developed by a FTS system and partially ordered $Fe_{16}N_2$ thin film was obtained. The FeN layer of this structure was measured to possess Ms value of 1910 emu/cc (3%-5% error), which surpasses the previous structures of sputtered FeN thin film. XPS measurement confirms the higher nitrogen binding energy of the sample, which indicates a more negatively charged nitrogen environment. An enlarged in plane lattice constant was detected by the GIXRD, which helps to understand the electronic environment of FeN layer and its crystalline anisotropy.

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