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Construction of FeN alloy films with ultra-strong magnetism and tunable magnetic anisotropy for spintronic application

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ABSTRACT

FeN alloy film is a promising spintronic material with the theoretically ultra-strong magnetism (saturation magnetization M_S and magnetic anisotropy K_{eff}) and high spin polarization, which relies on the degree of N ordering interstice occupancy (S). However, due to the high activation energy for N ordering, the S value of an actual FeN film is mostly lower than 35% and this restricts the achievable magnetism and transportation property. Thus, the construction of a FeN alloy film with well-controlled magnetism and efficient electronic transportation remains a long-standing challenge. Here, we tackle the problem by strain engineering. Using an Fe/Cr underlayer, we introduced a considerable epitaxial strain in the FeN lattice. The strain is proven to effectively promote the S value to over 60%, resulting in remarkable enhancement of M_S value from 2.18T to 2.81T (30% increment) and effective tunability of K_{eff} value ranging 1.3~2.2 $\times$ 10^6 J/m^3. Besides, the matched energy band symmetry ($\Delta 5$) between Cr and $Fe_{16}N_2$ facilitates the efficient electronic transportation for spintronic applications. By simulating interstice distribution with the first-principles calculations, the lattice strain is found to decrease the activation energy for N interstitial migration, which serves as a thermodynamic driving force for the magnetism tunability.

1. Introduction

Recently, the discovery of spin-related effects has intrigued a wide variety of functionalized spintronic devices [1–6]. The saturation magnetization (M_S) and the magnetic anisotropy (K_{eff}) of core ferromagnetic materials are deterministic to the device performance as the miniaturization of the devices. For example, high M_S is beneficial for increasing anomalous hall signal, magnetic proximity effect, and permanent magnetic performance [4,5,7]. High K_{eff} is critical for enhancing thermal stability and lowering energy consumption of devices [8]. Thus, researchers have been pursuing the ferromagnetic material with ultrahigh magnetism (M_S and K_{eff}) to ensure strong signal output, good thermal stability, and low energy cost of spintronic devices in nanoscale.

The α''-$Fe_{16}N_2$ alloy [9], which was theoretically predicted to bear extremely high magnetism (M_S~2.9 T, K_{eff}~10^7 J/m^3) [10] and high spin polarization (0.52), is a promising candidate of the expected spintronic materials. However, the unique properties strongly rely on N ordered occupancy in octahedral interstitial sites. Due to the high activation energy for N ordering, N atoms prefer the disordered occupancy of the octahedral interstitial sites, forming an α'-Fe_8N phase and vanishing the peculiar properties of the α'' phase. Tremendous efforts have been made to increase the degree of N ordering (S) by promoting the phase transition from α'-Fe_8N to α''-$Fe_{16}N_2$, such as varying depositing kinetic energy [11–13], modulating crystal structures [14–16], and stabilizing α''-$Fe_{16}N_2$

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phase [17–21]. Unfortunately, the *S* value in these methods is mostly lower than 35% and this leads to a disappointing M_S value ranging 2.2–2.5T which is still far from the theoretical upper limit. In fact, the magnetism of FeN alloy is also sensitively dependent on the lattice volume [22,23]. Thus, a lattice strain is expected to be effective in tuning the magnetism of α''-$Fe_{16}N_2$ films. Ji et al. and Yang et al. achieved the lattice strain control of magnetism in FeN alloy by using Fe and Ag underlayers [24–26], respectively. However, due to the small in-plane lattice mismatch between FeN and Fe or Ag underlayer (−0.8%), the introduced lattice strain is limited to yield a satisfying effect on magnetism tunability with a maximal M_S value only 2.47 T. Moreover, the large mismatch of the energy band symmetry between Ag and $Fe_{16}N_2$ (Fig. 8) will block the interfacial electronic transportation and restrict the spintronic application. Thus, it is of great importance to able to generate a significant lattice strain in the FeN heterostructures with a matched energy band symmetry so that the magnetic/electronic properties can be tuned in a more noticeable way.

In this paper, we proposed to tackle the problem by lattice strain engineering with a Chromium underlayer. Cr possesses the same body-centered-cubic structure and similar lattice parameters as Fe matrix of the FeN lattice. The noticeable lattice mismatch (about 1.7% in Fig. 1) between Cr (002) and FeN (002) planes can be expected to provide an appreciable epitaxial strain in the FeN layer and generate an appropriate elastic energy in the film, possibly tuning the energy barrier for N ordering occupancy. Inspired by this idea, an Fe/Cr composite underlayer was utilized to introduce a tunable lattice strain in the FeN layer. The lattice strain is found to substantially decrease the activation energy for N interstitial migration and ordering occupancy in the FeN lattice by as much as of 38%. Under such driving force, the *S* value is effectively promoted to over 60%, resulting in remarkable enhancement of M_S value to 2.81 T and tunable K_{eff} value of 1.3~2.2 × 10^6 J/m^3. Besides, the matched energy band symmetry between Cr and $Fe_{16}N_2$ facilitates the interfacial electronic transportation in the Cr/FeN heterostructure for potential spintronic applications.

2. Experiment

2.1. Sample preparations

The Fe seed layer (10 nm)/Cr buffer layer/FeN/Cr protection layer

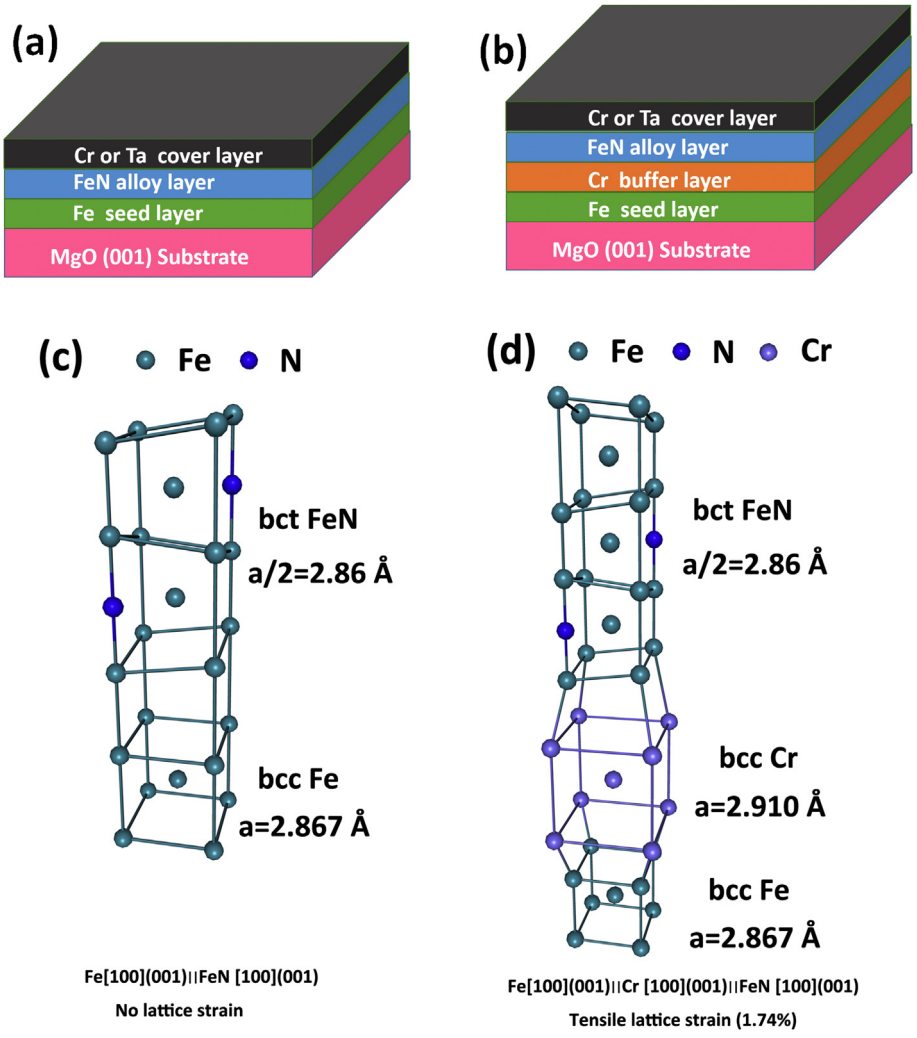

Fig. 1. Schematics of sample structure, epitaxial growth relationship, and lattice strain. (a) and (c) MgO/Fe seed layer/FeN layer/Cover layer heterostructures with the epitaxial growth of Fe[100](001)||FeN[100](001), representing a strain-free sample. (b) and (d) MgO/Fe seed layer/Cr buffer layer/FeN layer/Cover layer heterostructures with the epitaxial growth of Fe[100](001)||Cr[100](001)||FeN[100](001), representing a tensile strain treated sample.