# Role of interfaces in the exchange coupling of Fe/Cr/Fe(001) systems

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Exchange coupling has been studied in Fe whisker/Cr/Fe(001) systems that were grown in a perfect layer by layer mode. The exchange coupling through Cr was found to be very sensitive to alloying at the Fe whisker/Cr(001) interface. It will be shown that the observed reversed phase of the short wavelength oscillations compared to those predicted by *ab initio* calculations can be caused by alloying at the Fe whisker/Cr(001) interface. In order to test this point, we have grown samples with the Cr/Fe(001) interface intentionally alloyed by codepositing the Cr and Fe atoms during the formation of the last Cr atomic layer. The strength of the exchange coupling has also been investigated in systems fabricated with heterogeneous spacers using bcc Cu(001) and fcc Ag(001). Cu and Ag layers have been inserted between the Cr spacer and the Fe(001) film. The strength of the antiferromagnetic coupling was found to be substantially increased due to the presence of Cu at the Cr/Fe(001) interface. It will be argued that the observed increase in the exchange coupling is caused by an increased asymmetry in spin dependent reflectivity at the Cr/Cu/Fe interface.  [S0021-8979(97)45908-X]

## INTRODUCTION

We have carried out quantitative studies of the exchange coupling through Cr(001) using Fe whisker/Cr/Fe(001) samples.[1,2] Our objective was to grow samples having the best available interfaces, to measure quantitatively the strength of the exchange coupling, and to compare that coupling strength with *ab initio* calculations which included explicitly the presence of spin-density waves in Cr.[3]

Scanning electron microscopy with polarization analysis (SEMPA),[4] Brillouin light scattering (BLS), and magneto-optical Kerr effect (MOKE)[1] studies have shown that Fe whisker/Cr/Fe(001) systems possess well defined short wavelength oscillations in the exchange coupling. BLS and MOKE studies[1,2] have shown that the exchange coupling in Fe whisker/Cr/Fe samples can be well described by bilinear and biquadratic exchange coupling terms,

$$E = -J_1 \cos(\theta) + J_2 \cos^2(\theta), \tag{1}$$

where $\theta$ is the angle between the surface magnetic moments of the facing ferromagnetic layers. This is in agreement with early *ab initio* calculations by Stoeffler and Gautier.[5] However, the most recent calculation by Stoeffler's group[6] indicates that for samples with ideal interfaces the approach to saturation follows the Slonczewski's proximity magnetism model[7] in which the approach to saturation is asymptotical. There are even more profound differences between the experimental results and the theoretical predictions.[2] The coupling between the Fe and Cr atoms at the Fe/Cr interface is expected to be strongly antiferromagnetic[8] and since the period of the short wavelength oscillations is close to 2 ML one would expect antiferromagnetic (AF) coupling for an even number of Cr atomic layers and ferromagnetic (FM) coupling for an odd number of Cr atomic layers. For the period of $\lambda = 2.11$ ML, the first phase slip in the short wavelength coupling is predicted to occur at 24 ML.

Surprisingly, the SEMPA[9] and BLS[10] measurements showed that the phase of the short-wavelength oscillations is exactly opposite to that expected. It is also important to note that the measured strength of the exchange coupling $|J_{\max}| \sim 1.0$ ergs/cm$^2$,[1] was found to be much less than that obtained from first principals calculations, $|J_1| = 30$ ergs/cm.[5] These facts represent a significant disagreement between experiment and theory.

Recent quantitative BLS and MOKE studies[2,11,12] have shown that the origin of this behavior is closely linked with the structural properties of the Fe whisker/Cr(001) interface. The angular resolved Auger spectroscopy (ARAES),[2,11,12] STM,[13] and proton induced Auger electron spectroscopy[14] have shown that the formation of the Fe/Cr(001) interface is far more complicated than expected. The above studies revealed very clearly that the Cr undergoes interface mixing when the substrate temperature is adjusted for optimum growth. However, the quantitative conclusions based on the STM technique differ significantly from those based on Auger spectroscopy. The STM studies indicated that the atom exchange mechanism between Fe and Cr persists up to 5–6 atomic layers, and the atomic concentration of Cr in Fe does not exceed 10%. The ARAES and proton induced AES showed that the interface mixing was confined mostly to the two Fe interface atomic layers, and nearly 50% of Cr atoms were mixed with Fe at the substrate temperature of 300 °C. The proton AES studies[14] also showed that the atom exchange replacement process does not proceed appreciably beyond the Fe/Cr interface. This result is in agreement with recent x-ray diffraction studies using a tunable synchrotron radiation source.[15]

The results of our ARAES studies have shown that the Cr–Fe interface mixing depends on the substrate temperature during the initial stages of the Cr growth. But the interface mixing remains even at relatively low substrate temperatures, ~20% at $T_{\text{sub}} = 100$ °C. One should point out that interface alloying is an asymmetric effect:[16,17] it happens only when Cr is deposited on Fe; interface alloying does not occur when Fe is deposited on Cr, see further discussion in Ref. 2.

We have pointed out that the above differences between the experimental results and theoretical predictions of the exchange coupling through Cr(001) spacers can be caused by interface alloying.[2,12] *Ab initio* calculations by Stoeffler and Gautier showed that the exchange coupling through Cr(001)

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is significantly affected by interface alloying.[3] The calculations that were carried out using a 2 ML 75% Fe–25% Cr, 25% Fe–75% Cr ordered alloy which turned out to be particularly interesting. The orientation of the Cr atomic moments are magnetically frustrated by the lack of a sharply defined chemical environment. The fact that the mixed Fe layer (75% Fe–25% Cr) remains as a part of the ferromagnetic layer is not surprising, but a strong ferromagnetic coupling between the magnetic moments of the mixed Cr atomic layer (75% Cr–25% Fe) and the adjacent Fe moments are definitely unexpected. It is the second Cr atomic layer that has its magnetic moment oriented antiparallel to the Fe layer. Magnetically speaking the Cr spacer lost one atomic layer. Thus the parity is changed: an odd number of Cr atomic layers gives rise to AF coupling and an even number of Cr layers results in FM coupling. The calculated strength of the short wavelength coupling in the sample with intermixed interfaces was found to be close to that obtained in our measurements.

The purpose of the studies presented in this article is to shed further light on the role of heterogeneous interfaces in Fe/Cr/Fe(001) systems.

## RESULTS AND DISCUSSION

We have tried to avoid interface mixing by decreasing the substrate temperature during the growth of the first Cr atomic layer. We found that the quality of subsequent Cr layers was noticeably affected once the initial substrate temperature was decreased below 100 °C. The dependence of the exchange coupling on the parity of the number of Cr layers remained unchanged for samples that grew in a layer-by-layer mode. This result ought to be expected since the interface mixing was always present. Not being able to defeat interface mixing directly we decided to use heterogeneous Cr spacers.

(a) In the first series of experiments the last atomic layer of Cr(001) was prepared by codepositing Cr and Fe together. The reflection high energy electron diffraction (RHEED) intensity oscillations and RHEED patterns showed that the Cr–Fe alloyed layer was atomically flat. In our studies, we used the following concentrations: Cr 85%–15% Fe and Cr 65%–35% Fe. The BLS studies, see Fig. 1, together with the MOKE measurements showed that the sign of the exchange coupling was not changed by adding an alloyed atomic layer of Cr–Fe on the top of the already deposited Cr spacer. Therefore, it follows that an additional alloyed layer of Cr does not participate in the parity rule affecting the sign of the exchange coupling. This is consistent with the behavior of interface alloying at the Fe/Cr interface. Based on the Stoeffler and Gauthier calculations, one can expect that the magnetic moment of the alloyed atomic layer is oriented parallel to the adjacent Fe layer and consequently the sign of the exchange coupling is unaffected by it. (b) Another two heterogeneous Cr spacers were prepared for testing the effect of interface composition on the exchange coupling strength. Fe whisker/11 Cr/1–2 Cu/Fe(001) and Fe whisker/11 Cr/1–2 Ag/Fe specimens were grown, where the integers represent the number of MLs. The growth of Ag at $T_{sub}=105$ °C resulted in nearly perfect layer by layer growth. The growth of

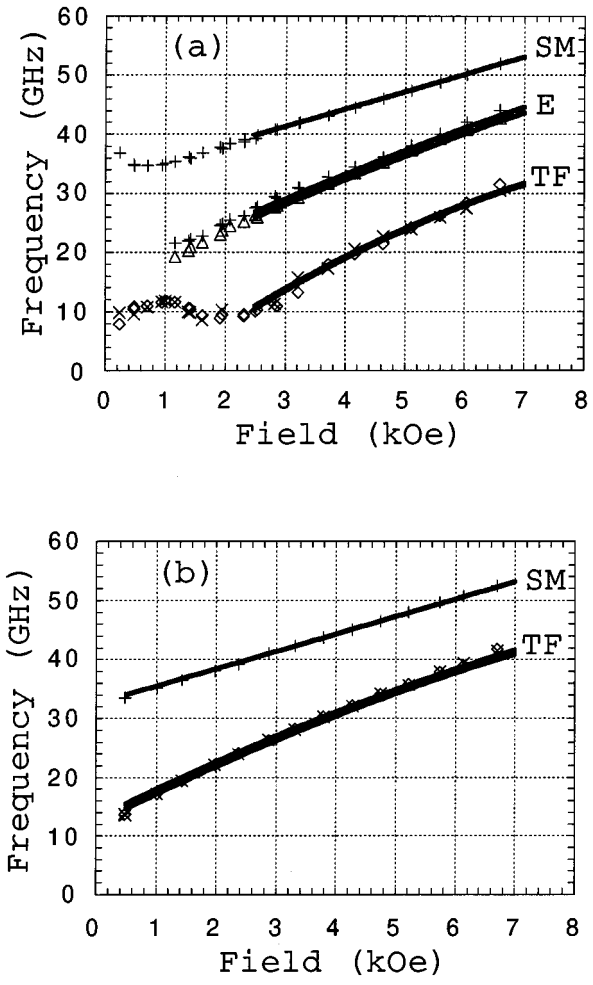


FIG. 1. Magnetic excitation frequency vs applied magnetic field for the system Fe whisker(001)/NCr/1 mixed/20 Fe/20 Au, where the integers denote the number of monolayers (ML). The mixed layer consisted of 65% Cr and 35% Fe. SM—surface mode; E—bulk edge modes; TF—Fe thin film modes. The solid lines were calculated using saturation magnetization densities $4\pi M_s=21.4$ kOe for both bulk Fe and the Fe thin film; cubic anisotropy constants $K_1=4.76\times10^5$ ergs/cc for bulk Fe and $K_1=3.5\times10^5$ ergs/cc for the Fe thin film; uniaxial surface anisotropy constants $K_u=0.5$ ergs/cm$^2$ for the bulk Fe and $K_u=1.0$ ergs/cm$^2$ for the Fe thin film. (a) $N=11$ ML Cr, $JEX=J_1-2J_2=-0.87$ ergs/cm$^2$. (b) $N=12$ ML Cr, $JEX=+0.25$ ergs/cm$^2$.

Cu at $T_{sub}=65$ °C was less perfect but still showed well defined RHEED oscillations, even for the second anti-Bragg condition, indicating that the atomic deposition of the Cu layers was reasonably smooth. The behavior of exchange coupling in both of Fe whisker/11 Cr/1–2 Cu/Fe(001) samples is most surprising, see Fig. 2. The strength of the exchange coupling in these samples was increased twofold compared to that observed in samples having simple Cr interfaces. This is an unexpected result. In all our previous studies, using Fe/Cu/Fe(001) structures with a wide range of heterogeneous Cu spacers, the exchange coupling was always decreased significantly due to the presence of alloyed atomic layers inside the nonmagnetic spacer.[18] This systematic behavior led us to conclude that atomic heterogeneity in the spacer leads to an additional electron scattering potential and results in a decreased spin transport between the ferro-

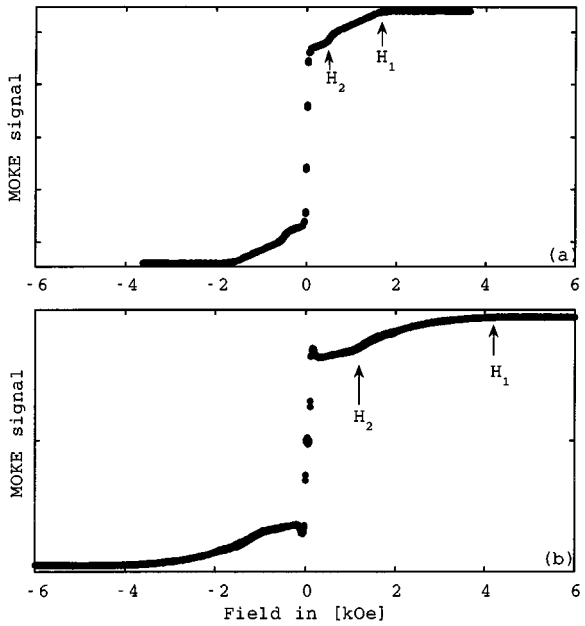


FIG. 2. Longitudinal MOKE studies of heterogeneous Cr spacers. (a) Fe whisker/11 Cr/20 Fe/20 Au(001). $J_1=-0.4$ ergs/cm$^2$, $J_2=0.18$ ergs/cm$^2$. (b) Fe whisker/11 Cr/2 Cu/20 Fe/20 Au(001). $J_1=-0.86$ ergs/cm$^2$, $J_2=0.3$ ergs/cm$^2$. The integers represent the number of atomic layers. $J_1$ and $J_2$ were obtained by fitting the critical fields $H_1$ and $H_2$ using the microscopic calculations for samples grown on Fe whiskers (Refs. 2 and 21). Note that the sample reached full saturation for $H>H_1$.

magnetic layers. The situation for Fe/Cr/Cu/Fe(001) is definitely different. During the recent Fe/Cr workshop, held in Strasbourg, Sussanne Mirbt presented calculations[19] that are in accord with the measured exchange coupling for our heterogeneous Cr spacers. In fact, by complete coincidence, the calculations were carried out for the same structures that we used. The enhanced coupling strength is due to a change in the spin dependent reflectivity of the Cr spacer electrons at the Cr/Cu/Fe interface. The presence of the Cu atoms changes the spin dependent interface potential. The Cu electrons will hybridize with both Fe and Cr. Since the majority spin Fe band (which participates in the exchange coupling) lies closest to the Cu conduction band the effect of hybridization will be most pronounced for the majority spin Fe band. The hybridization with Cu results in a downward energy shift that moves the Fe majority spin band below the Fermi level.[20] An energy gap is created at the Cu/Fe interface, and consequently the majority spin electrons in Cr undergo a nearly perfect reflection. The states for minority spin electrons are very little affected by the Cu, and therefore their reflectivity is left unchanged. It follows that the spin reflectivity asymmetry is increased leading to an increased coupling. The situation with Cr/Ag(001) heterogeneous spacers is less dramatic. The exchange coupling is somewhat decreased by the presence of Ag, $J_1=1.3$ and 1.0 ergs/cm$^2$ in {11 Cr(001)} and {11 Cr,2 Ag(001)} spacers, respectively. Calculations show that the spin reflectivities for minority and majority spin electrons are somewhat decreased leading to an overall decrease in the exchange coupling. The theoretical calculations by Mirbt can explain our results very well. This implies that the coupling through Cr(001) is affected by the spin dependent reflectivities at the interfaces. The spin reflectivities are typical parameters closely associated with the paramagnetic behavior and this therefore raises an important question: ''Is the origin of the spin density wave in Cr(001) intrinsic, or is it extrinsic even in samples having a low density of atomic steps?''

## ACKNOWLEDGMENT

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