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# The mechanism of interlayer exchange coupling in silicon/iron layered structures

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**Abstract**

We propose a new mechanism of interlayer exchange coupling in a-Si/Fe structures, based on the indirect tunneling of spin-polarized electrons across the semiconductors spacer. This tunneling is effectuated by virtual hopping process over a narrow band, laying close to the Fermi level and leading to the sharp peak in the density of electron states. We take into account the iron-silicide formation inside the spacer and estimate the parameters of an effective exchange.


*Keywords:* Interlayer exchange coupling; a-Si/Fe structures; Indirect tunneling

## 1. Introduction

During the last years the a-Si/Fe sandwiches and multilayers became a particular topic of experimental and theoretical researches, due to their unusual yet not fully explained magnetic properties (see, for example Ref. [1]). Although a number of works have been done to understand the mechanisms of an exchange coupling between Fe layers across the amorphous Si spacer, the results are still controversial. The more intriguing appear the unusual dependences of the exchange coupling integral $J(T, t)$ on the temperature ($T$) and the spacer thickness ($t$). The antiferromagnetic (AFM) character of $J(T, t)$ is well established at $t > 8$–$10$ Å for all temperatures, but the main features of the $J(T, t)$ dependence remain unexplained. A very weak AFM coupling, increasing with temperature, was found in Ref. [2]; however, unusually strong AFM coupling, decreasing with temperature, has been also observed by different groups [1,3,4]. Moreover, the strong nonlinear (biquadratic) part of this coupling has been clearly demonstrated [3,4]. Experiments have also shown the pronounced maximum of $J(T, t)$ at some characteristic thickness $t_{max}(T)$ in the wide region, from ~8–10 to ~18–20 Å [1]. The dramatic increasing of $J(T, t)$ with temperature and evident crossover from the AFM to the ferromagnetic (FM) character of a coupling at $t < 8$–$10$ Å was observed in Ref. [5].

Following the theories [6,7], the exchange coupling between FM layers through insulating (I) or semiconducting (SC) spacer results from the spin-dependent electron tunneling and is expected to be exponentially decaying as the spacer thickness $t$ increases. On the other hand, it is well known that interlayer coupling through metallic spacer is associated with the indirect RKKY-type exchange, which oscillates from FM to AFM as a function of $t$. The situation in a-Si/Fe systems is, however, far from to be explained within these simple models, due to some serious complications.

The interpretation of the coupling data in terms of a tunneling between FM layers across SC spacer is hampered by the lack of knowledge about the spontaneously formed iron-silicide interlayer, due to Fe diffusing into Si spacer through the Fe/Si interface. There were various suggestions about the composition of this interlayer, from the metallic compound in the simple cubic structure (c-FeSi) to a semiconductor or semimetal in the more complex structures. It has been established in Refs. [8,9] that an interlayer coupling is exponentially decaying in a-Si/Fe systems at large $t$, but these results were obtained on samples, where the iron diffused into the silicon in the uncontrolled way.

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Experiments similar to [8] have been performed on samples with a controlled composition of the iron-silicide [1], and the coupling through the $Fe_{1-x}Si_x$ spacer with $0.5<x<1$ was studied as a function of $T$, $t$ and $x$. It has been demonstrated within the LEED measurements, that the growth of a thin (5 Å) $Fe_{1-x}Si_x$ layer on Fe(001) substrate is pseudomorphic, even at $x\sim 1$ (i.e. for nominally pure silicon). So, a good compatibility of the Fe and $Fe_{1-x}Si_x$ lattices and an almost ideal quality of their interfaces have been guaranteed in these experiments. At the large Fe content ($x$ is close to 0.5) the AFM coupling with both exponential and oscillatory components has been found, showing a pronounced maximum at $t\sim 16$–$18$ Å. Upon increasing the Si content (when $x$ approaches to 1) the dramatic rise of a coupling strength, sharp peak at $t\sim 8$–$10$ Å and exponential decay at large $t$ have been detected.

The obtained results revealed significant difference between samples with a controlled composition and samples with an uncontrolled, probably inhomogeneous content of a spacer (i.e. structures having the nominal spacer thickness $t$ with a mixed or fluctuating composition). Both types of structures have their peculiarities, which prevent a direct use of the standard theoretical results.

From these brief remarks we conclude that mechanisms of an exchange coupling in a-Si/Fe systems are still far from being understood.

## 2. The model and results

Below, we consider an indirect tunneling of spin-polarized electrons as the main mechanism of an interlayer exchange coupling in a-Si/Fe structures. This tunneling is effectuated across the spacer by virtual hopping process over a narrow band, lying close to the Fermi level and leading to the sharp peak in the density of electron states (DOS). We suppose that such a band is formed by the 'tails' of localized sp-electron states, provided from compositional disorder inside amorphous semiconductors, and/or by the hybridized (d–sp)-electron states, existing even in regular iron-silicides.

We consider the simple model of a three layered FM/SC/FM structure with an indirect tunneling of spin-polarized itinerant d-electrons between the right and left FM layers through the narrow band with the spectrum $E_h(\vec{k})$ inside SC spacer, where $\vec{k}=(k_x,\vec{k}_\perp)$, $k_x$ is longitudinal and $\vec{k}_\perp$ is transverse part of a quasimomentum $\vec{k}$, correspondingly. Such tunneling appears from hybridization of the FM and SC one-electron states at their interfaces, since the matrix element $V$ of an interface potential over these states is non-zero. The position of the chemical potential $\mu$ of the system is fixed by the metallic layers and we assume $\mu<E_h(\vec{k})$, so all states in the narrow band are empty. The energy of coupling between metallic layers may be written in terms of the Green's functions at $T=0$ as

$$F(\vec{S}^-\vec{S}^+)=\oint\frac{d\omega}{2\pi i}\int\frac{d\vec{k}_\perp}{(2\pi)^2}G\left(-\frac{t}{2},-\frac{t}{2},\vec{k}_\perp,\omega;\vec{S}^-\right)\times Vg\left(-\frac{t}{2},\frac{t}{2},\vec{k}_\perp,\omega\right)VG\left(\frac{t}{2},\frac{t}{2},\vec{k}_\perp,\omega;\vec{S}^+\right)\times Vg\left(\frac{t}{2},\frac{t}{2},\vec{k}_\perp,\omega\right)V, \quad (1)$$

where $G$ is the electron Green's function of FM layers, $\vec{S}^-$, $\vec{S}^+$ are unit vectors of magnetization in the left $(-)$ and right $(+)$ layer, correspondingly; $g$ is the electron Green's function of SC spacer; $\vec{x}$ is the direction of a growing; integration over the frequency $\omega$ covers only the filled states of FM metal.

After integration over the frequency and transverse quasimomentum we obtain for the coupling energy

$$F_{cx}=I(t)\vec{S}^-\vec{S}^+, \quad (2)$$

where $I(t)=(F(\uparrow\uparrow)-F(\uparrow\downarrow))/2$ is an effective exchange integral; within an exponential approximation we estimate:

$$I(t)\sim[\Delta^2V^4/(W_m^4W_s)]\exp(-t/t_0). \quad (3)$$

Here, $\Delta$ is the energy of FM splitting in the metal, $W_m$ and $W_s$ are the bandwidths of FM and SC, correspondingly; $t_0$ is the characteristic length, defined as

$$t_0=\frac{1}{2}\left(\sqrt{2m^*(E_h(0)-\mu)}\right)^{-1}, \quad (4)$$

$m^*$ is the electron effective mass in the extremum of a narrow band. We see from (2) to (4) that an effective exchange in our model is antiferromagnetic (AFM) and strongly depends on the band structure parameters of FM and SC. Does the empty narrow band really exist in the iron/silicon structures and how are its parameters? To answer these questions, we have performed band structure calculations for the iron-silicide with the B2 structure (c-FeSi) in the Fe/c-FeSi/Fe system. We optimized the c-FeSi lattice parameter, supposing that ideal interfaces Fe/c-FeSi have

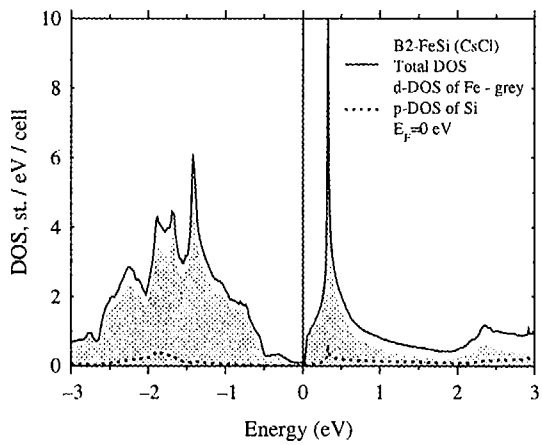


Fig. 1. Calculated DOS in c-FeSi.

been formed during the growing process. The results of calculations are presented in Fig. 1. They show that the empty narrow band appears close to the Fermi level, at distance $E_h(0)-\mu\sim 0.3$ eV, and $m^*\sim 0.5$ m, where $m$ is the free electron mass. From (4) we estimated the characteristic length as $t_0\sim 2$–$2.5$ Å, that qualitatively coincides to the experimental value in [1].

## 3. Concluding remarks

Besides the tunneling mechanism, which is presumed to exist in all systems under consideration, additional mechanisms of a coupling, provided from the interface bands, the RKKY-like exchange and exchange by spin fluctuations also appear. The last two types of coupling are purposed to play an important role in case of a spacer, enriched by the metallic iron-silicide, while the first one is suggested to be important, if the nominal content of a spacer is close to the pure silicon. Of course, there is no universal origin of the coupling in all a-Si/Fe structures, and the qualitative model is necessary to explain controversial experimental results, taking into consideration multiple particularities of the spacer composition, geometry and growing of the concrete structure. The main theoretical difficulties provide in such a way from the following circumstances. Firstly, the $Fe_{1-x}Si_x$ compound inside the spacer has to be considered as heavily doped amorphous magnetic SC. It is well established that in such systems different kinds of compositional disorder are present [10], associated with intrinsic defects (dangling bonds, vacancies, substitution and interstitial centers). As a result, very complex electron structure, composed from the wide and narrow bands formed by itinerant and localized electron states, exists in these materials. Secondly, the electron density redistribution between FM and SC close to the FM/SC interfaces can strongly modify the Fermi level position and occupation of electron states inside the spacer, at distances of order of the screening length. This signifies that nominal composition, even being strictly controlled, cannot define with confidence the metallic or insulating character of an electron spectrum inside the spacer, in distinction from the bulk materials. Thirdly, not only one-electron, but also collective excitations (spin fluctuations) and, possibly, the short range magnetic order inside the spacer, have to be taken into account due to the strong electron–electron correlations in the iron-silicides. Fourthly, reconstruction and relaxation effects at the FM/SC interface can strongly modify the electron structure of a spacer (particularly, the interface bands appear), which have to be also considered to understand the mechanisms of an exchange coupling through the thin spacers. We hope, our approach is able to take into consideration these modifications and complexities.

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