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LETTER TO THE EDITOR

A double-quantum-well model of the exchange coupling in Fe/ZnSe/Fe

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Abstract

In this letter, we investigate the interlayer exchange coupling between two finitely thick ferromagnets (FM), separated by a non-metallic spacer, taking into account the contributions from double-well states. It is found that the negative temperature coefficient of the exchange coupling can be explained by the resonant tunnelling between two FM wells, whereas the positive temperature coefficient for the antiferromagnetic coupling can be attributed to non-resonant tunnelling. Our calculation of the electronic structure indicates that this temperature dependence is related to the relative magnitudes of the densities of states close to the Fermi surface for the cases of parallel and antiparallel alignments of the FMs. Also, the present model provides us with a new physical explanation for recent experimental observations.

The discoveries of the weak antiferromagnetic (AF) interlayer exchange coupling across amorphous (α-) Si in Fe/α-Si/Fe sandwiches [1] and the strong AF coupling in Fe/Si multilayers [2] have given rise to considerable interest in magnetic multilayers with non-metallic spacers. In particular, recently, attention has been given to the temperature dependence of the exchange coupling in Fe/Si(FeSi, Ge) heterostructures. It was observed that, in Fe/α-Si(Ge)/Fe trilayers prepared at low temperature, the AF coupling strength has a positive temperature coefficient (heat-induced coupling) [1, 3, 4]. In striking contrast, multilayers of Fe and Si or Ge that are prepared at room temperature (RT) exhibit a stronger AF coupling with a negative temperature coefficient [2, 6–12]. Moreover, a non-monotonic temperature dependence of the exchange coupling has recently been found in Fe/ZnSe/Fe sandwiches, where a reversible transition from FM coupling to AF coupling upon heating takes place [5]. It was argued that the positive temperature coefficient of exchange coupling is due to the localized defect states in the gaps of spacers [3–5], while the negative one arises because the spacers of multilayers prepared at RT are not amorphous semiconductors, but crystalline metallic Fe–Si compounds

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[2, 7], which have the same origin as the coupling in metallic multilayers. Furthermore, on the basis of analyses of hysteresis loops, it was suggested that a strongly temperature-dependent biquadratic coupling is responsible for the observed appearance of a remanent magnetization at low temperature [10, 13, 14]. However, it was also argued that the vertical and lateral variations in bilinear AF and FM coupling are able to mimic strong biquadratic coupling [15, 16]. Therefore, the nature of the exchange couplings as well as their temperature dependences in Fe/Si(FeSi, Ge) heterostructures are still unclear and remain matters of debate. This interaction between magnetic layers has become an important issue in semiconductor physics as a result of the recent developments in GaMnAs/GaAlAs heterostructures [17].

Several theoretical models have been proposed to account for the interlayer exchange coupling across non-metallic spacers. The first was the spin-current model of Slonczewski for $T = 0$ [18]. The second was the quantum interference model of Bruno [19], which may be used to describe the exchange couplings across metallic and non-metallic spacers. Furthermore, a positive temperature coefficient for the AF coupling strength across an insulating spacer is derived. The indirect exchange between localized moments in a symmetric double quantum well with the presence of a longitudinal electric field can be factored into a two-dimensional Ruderman–Kittel–Kasuya–Yosida interaction, where the form factor contains all of the information of the structure parameters [17]. In each magnetic layer, as the high-density system of magnetically ordered moments exists in the plane, the exchange becomes more complex due to the planar lattice bounds of a state [17, 20]. This is also an interesting problem for further study in multilayer physics. In addition, there is the Kondo lattice model of Shi *et al* [21], which treats FeSi as a Kondo insulator in order to explain the photo-induced AF coupling. It can be seen that the negative temperature coefficients of exchange coupling and the non-monotonic thermal dependence of the exchange coupling J cannot be derived from the above mechanisms. As far as the models themselves are concerned, all of them treat the FM thickness as semi-infinite. In this letter, we consider FM thickness of the order of nanometres, where the quantum-size effect is remarkable and dominant in the exchange interaction.

In the present work, with emphasis on the quantum-size effect arising from FM thickness, we set up a model of a double quantum well, which is an extension of the quantum well theories of metallic multilayers [22, 23]. Owing to the tunnelling effect and the reflections of electron waves at the film surfaces, the electrons would interfere in the wells and give rise to resonant tunnelling, which is responsible for the negative temperature coefficients of the strength of the exchange coupling. For the non-resonant tunnelling, the coupling increases with increasing temperature. Furthermore, the non-monotonic temperature dependence of J can be derived also. Therefore, all of the phenomena related to the thermal dependences of the exchange coupling can be derived from our model.

Consider a sandwiched structure $FM_1/ZnSe/FM_2$, where ZnSe denotes the barrier layer with thickness d_b. For simplicity, it is assumed that FM_1 and FM_2 have the same thickness d_{FM} and the same magnitude of molecular field h, but different magnetization directions, which make angles of $\pm\theta/2$ with the z-axis respectively (the film plane is parallel to the y–z plane, and perpendicular to the x-axis). Within the spin-polarized free-electron approximation, the conduction electrons move freely in the film plane, but are subject to a rectangular barrier U_0 and two infinitely high barriers in the x-direction. Owing to the s–d exchange interaction with the localized spins in the FMs, the effective potential for conduction electrons is spin dependent as shown in figure 1. The relevant eigen-energies can be determined from the Schrödinger equation with the single-electron Hamiltonian

$$H = -\nabla^2 + U(x) + \boldsymbol{h}(x) \cdot \boldsymbol{\sigma} \tag{1}$$

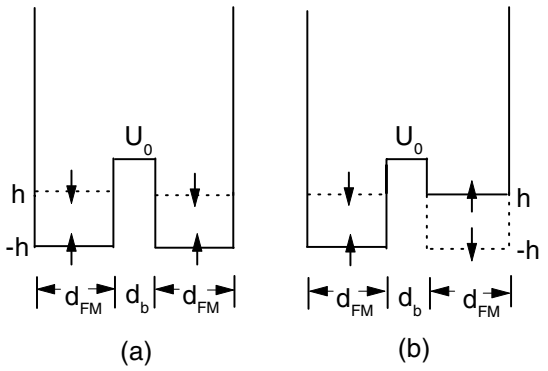


Figure 1. A schematic illustration of the spin-dependent effective potential for the parallel (a) and antiparallel (b) configurations of the two FMs. The solid and dotted lines correspond to the electrons with majority spin and minority spin, respectively.

where $\boldsymbol{\sigma}$ is the Pauli spin operator, $U(x)$ represents the potential profile and

$$U(x) + \boldsymbol{h}(x) \cdot \boldsymbol{\sigma} = \begin{cases} h[\cos(\theta/2)\sigma_z - \sin(\theta/2)\sigma_y] & \text{FM}_1 \\ U_0 & \text{I (S)} \\ h[\cos(\theta/2)\sigma_z + \sin(\theta/2)\sigma_y] & \text{FM}_2. \end{cases} \tag{2}$$

As the structure has π-angle rotational symmetry round the z-axis, we can use the parity operator $T = I\sigma_z$ to simplify the calculation. By means of the boundary conditions on the wave functions and their first derivatives, we can strictly derive the eigen-energy spectrum E_{xj} from [24]:

$$\frac{AD + BC}{AD - BC} = \pm\cos(\theta/2) \tag{3}$$

where $\theta = 0$, π, and $\pi/2$ correspond to the parallel, antiparallel, and 90° configurations of two FMs, $\pm$ the eigenvalues of the parity operator T, and

$$\begin{aligned} A &= p\cos(\alpha)\sinh(\gamma) + r\sinh(\alpha)\cosh(\gamma) \\ B &= p\cos(\alpha)\cosh(\gamma) + r\sinh(\alpha)\sinh(\gamma) \\ C &= q\cos(\beta)\sinh(\gamma) + r\sin(\beta)\cosh(\gamma) \\ D &= q\cos(\beta)\cosh(\gamma) + r\sin(\beta)\sinh(\gamma) \end{aligned} \tag{4}$$

with $\alpha = pd_{\text{FM}}$, $\beta = qd_{\text{FM}}$, $\gamma = rd_{\text{b}}/2$; $p = (E_x - h)^{1/2}$, $q = (E_x + h)^{1/2}$, $r = (U_0 - E_x)^{1/2}$.

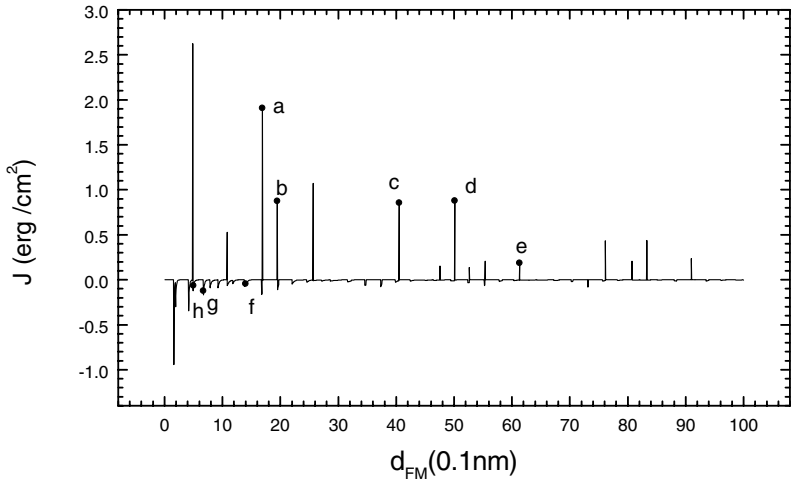
At $T \neq 0$, on the basis of the eigen-energies derived, we can calculate the total energy $E(\theta, T)$ for the system. The exchange coupling J is defined as

$$J(T) = \frac{1}{2S}[E(0, T) - E(\pi, T)] \tag{5}$$

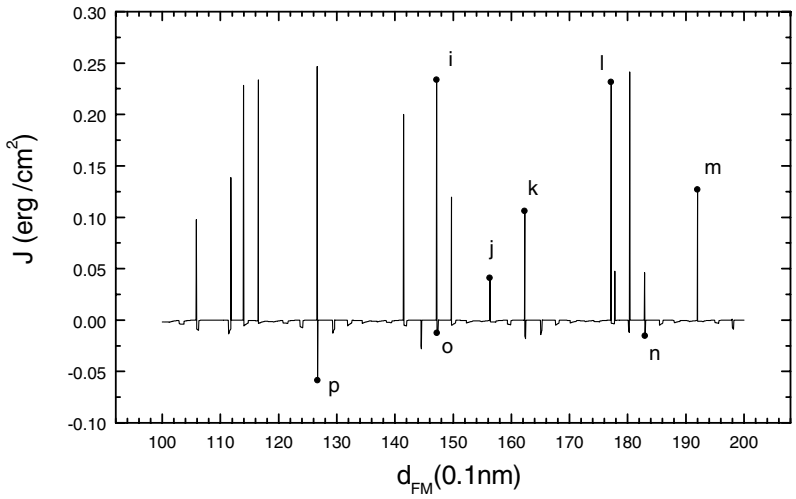
where S denotes the film area. When $J > 0$, the exchange coupling favours AF coupling. The total energy of the system is

$$E(\theta, T) = \frac{S}{4\pi^2}\sum_{j=0}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{E_{xj}(\theta) + k_y^2 + k_z^2}{\exp[(E_{xj}(\theta) + k_y^2 + k_z^2 - E_{\text{F}})/k_B T] + 1}\,\mathrm{d}k_y\,\mathrm{d}k_z. \tag{6}$$

First of all, let us investigate the dependence of the exchange coupling on the FM thickness at $T = 0$, which is shown in figures 2(a) and 2(b). The barrier height is $U - E_{\text{F}} = 0.85$ eV



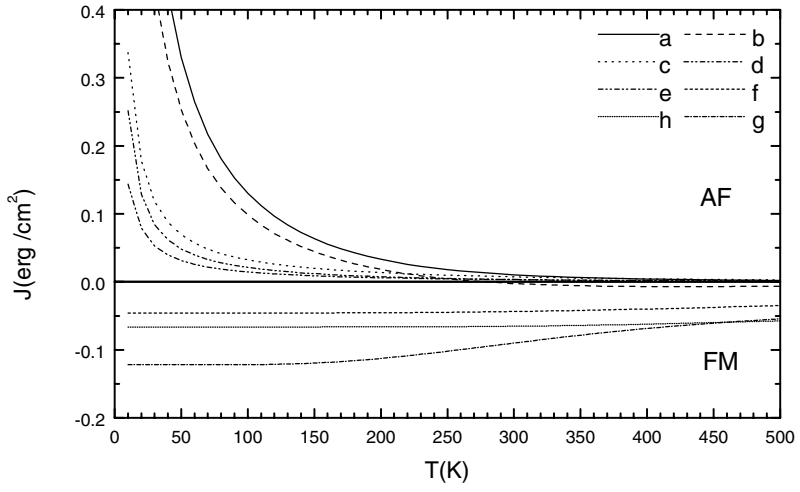
(a)



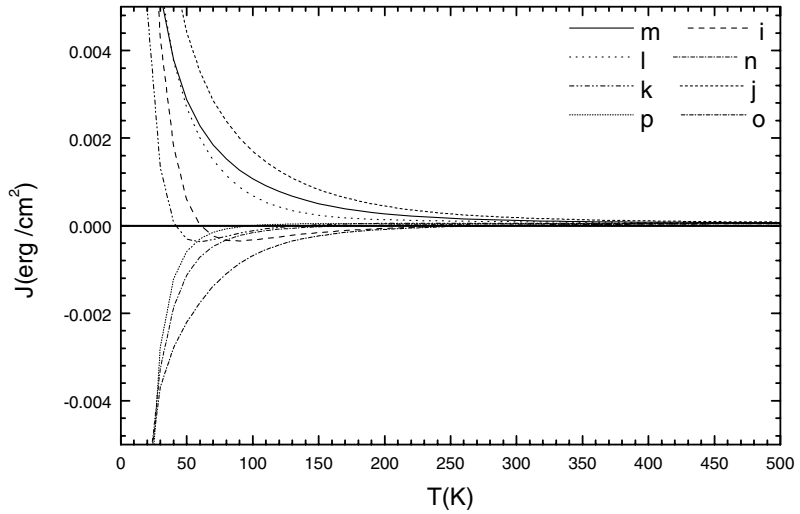
(b)

Figure 2. Exchange coupling J versus FM thickness at $T = 0$, where the relative barrier height $U - E_F = 0.85$ eV, $h = 0.75$ eV, $E_F = 5.0$ eV, and $d_b = 10$ Å; (a) the FM thickness is less than 100 Å; (b) the FM thickness is between 100 Å and 200 Å.

for ZnSe [25]. The molecular field is $h = 0.75$ eV [26] and the Fermi energy is $E_F = 5.0$ eV [27]. It is found that J is a decreasing oscillatory function of the FM thickness. During the oscillation, it exhibits many sharp peaks. These peak amplitudes are much stronger than in the ordinary situation for the coupling, which we called non-resonant coupling in this case. That is to say, the exchange couplings can be classified into two kinds: one is resonant coupling with a large magnitude but a narrow width; and the other is the non-resonant coupling with a very small magnitude but a large width. It is easier to measure the latter weak type due to its large width. We can understand the physics of the resonant exchange coupling as follows. It arises from the quantum-size effect and the interference of the tunnelling electrons in the FM well. Here the film thickness is of the order of nm and it is less than the mean free path of the



(a)



(b)

Figure 3. (a), (b) Resonant exchange coupling J versus temperature for a variety of FM thicknesses. Curves a, b, c, d, e, f, g, h, i, j, k, l, m, n, o, and p correspond to the FM thicknesses in figures 2(a) and 2(b). $U - E_F$, E_F, h, and d_b are the same as in figure 2.

electrons. The quantum-size effect is remarkable. Due to the confinement of the FM surfaces with an infinite barrier height, the tunnelling electrons are subject to spin-dependent reflection from surfaces and interfaces. Thus they can interfere in the FM wells, setting up spin-dependent quantum well states. This kind of interference may become maximal under certain conditions; then the resonant exchange coupling appears. This kind of resonant exchange coupling can be mediated by the width of the quantum well.

Now we turn to the temperature dependences of the exchange coupling for the resonant and non-resonant tunnelling, which are shown in figure 3 and figure 4 respectively. It can be seen from figure 3 that the strengths of resonant J decrease exponentially with the increasing

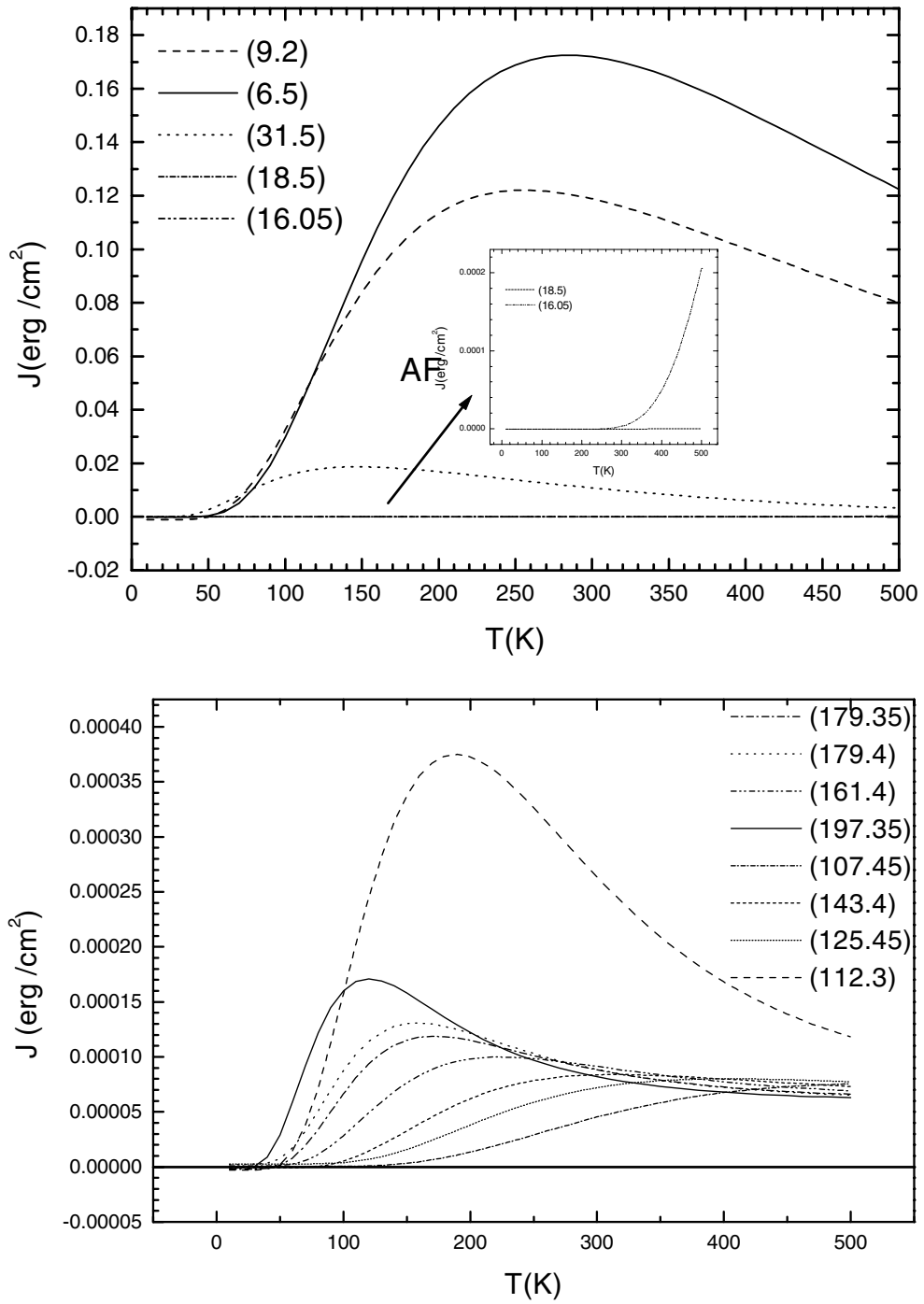


Figure 4. Non-resonant exchange coupling J versus temperature for a variety of FM thicknesses. The values 9.2, 6.5, 31.5, 18.5, 16.05, 179.35, 179.4, 161.4, ..., 125.45, 112.3 in the figures are the FM thicknesses in Å. $U - E_F$, E_F, h, and d_b are the same as in figure 2.

temperature, whether it is positive or negative. However, special cases can be found also: where the curve 'b, i, k' can change sign from '+' to '−' and the curve 'p' can change sign from '−' to '+' during variation. These results are in agreement with the observed thermal dependences of the exchange coupling in Fe/Si multilayers [6–12].

In order to explore the microscopic origin of the above phenomenon, we have calculated the densities of states (DOS) close to the Fermi surface for the parallel and antiparallel configurations of FMs, represented by DOS(0) and DOS(π) respectively. For positive J, as DOS(0) is smaller than DOS(π), the positive $E(0, T) - E(\pi, T)$ decreases with increasing temperature, so the strength of J decreases correspondingly; for negative J, as DOS(0) is larger than DOS(π), the negative $E(0, T) - E(\pi, T)$ keeps increasing until it reaches zero. So the strength of negative J keeps decreasing with increasing temperature.

As for the non-resonant tunnelling, it can be seen from figure 4 that J increases at lower temperature with increasing temperature. In other words, the thermal excitation of the conduction electrons tends to promote the exchange coupling J at lower temperature. On the same principle, this temperature dependence can also be traced to the behaviours of the DOS near the Fermi surface. It is calculated that DOS(0) is larger than DOS(π) at low temperature. So positive J increases. But the interesting feature is that, at higher temperature, the exchange coupling decreases with increasing temperature, which is similar to the behaviour of the resonant case. Generally speaking, with increasing temperature, J varies non-monotonically from increasing to decreasing. The DOS calculation indicates that: for non-monotonic temperature dependence of J, DOS(0) − DOS(π) changes from positive to negative, and hence $E(0, T) - E(\pi, T)$ has a transition point, before which J exhibits a

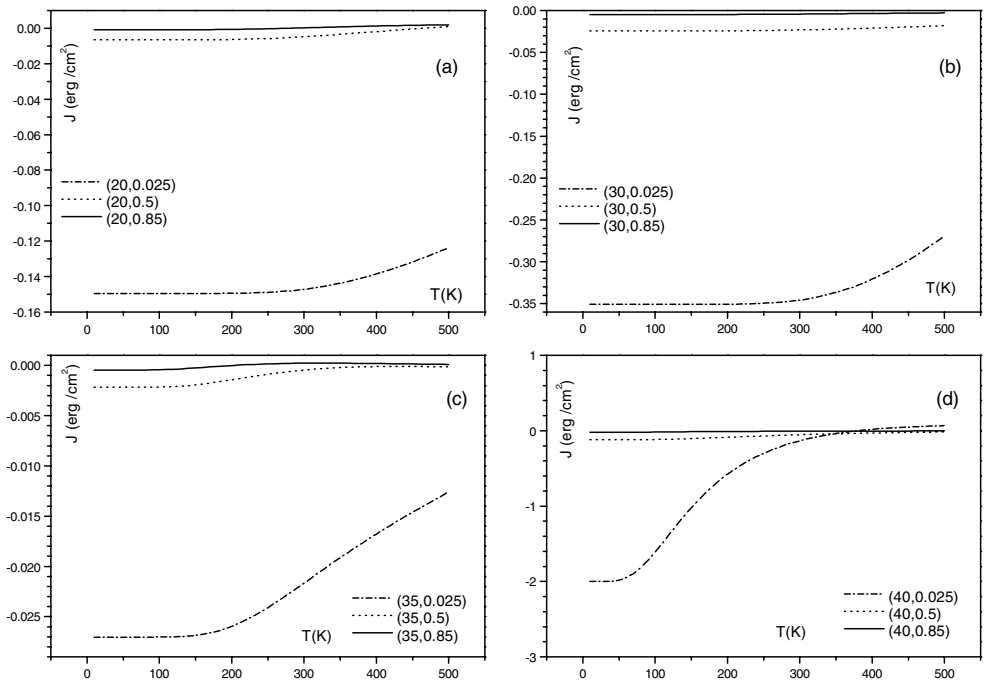


Figure 5. The influence of the barrier height on the temperature dependence of non-resonant J, where $d_{FM} = 20, 30, 35, 40$ Å, $U - E_F = 0.025, 0.5, 0.85$ eV. E_F, h, and d_b are the same as in figure 2.

positive temperature coefficient, and after which it has a negative one. The special case is for the FM thickness of 1.605 nm, where the exchange coupling is always increasing even at high temperature. In addition, we have investigated the influence of the barrier height on the temperature dependences of non-resonant couplings, which is displayed in figure 5. This shows us that the influence of barrier height becomes small when the FM thickness increases.

Although the situation of finite thickness of the metallic ferromagnetic layers at finite temperatures is discussed in this letter, the work on amorphous semiconductors [1, 3–5] has been performed on metallic substrates with infinite thickness. And the intermetallic barriers between Cu, Co, Fe are presumably not strong enough to provoke quantum-size effects. Therefore it would be interesting to compute the temperature dependences for an asymmetric situation where one of the FM layers is infinite.

In conclusion, the present model of double quantum wells leads to resonant tunnelling, which is mediated by the FM thickness and the molecular field. For the resonant coupling, due to the fact that $\mathrm{DOS}(0) - \mathrm{DOS}(\pi)$ near the Fermi surface changes sign when J changes sign from '+' to '−', the strength of J has a negative temperature coefficient. For the non-resonant coupling, as the sign of $\mathrm{DOS}(0) - \mathrm{DOS}(\pi)$ near the Fermi surface remains constant at low temperature, the exchange coupling J increases with increasing temperature. Moreover, there is a non-monotonic temperature dependence of J. These findings provide a qualitative explanation for the recent experimental observations. However, the present model, being a spin-polarized free-electron-like one, does not involve the electron–electron correlation and the scattering process. It is therefore not possible to make more detailed comparisons between the experimental observation and our calculation results, but it does provide the basis for an initial appraisal of the temperature dependences of the exchange coupling in the Fe/Si(Ge) system—particularly, for the resonant tunnelling and the quantum-size effect arising as a result of the FM thickness.

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