Magnetic 4f-systems and their applications in spintronics

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Abstract. Magnetic semiconductors are materials that exhibit magnetic behaviour as well as typical semiconductor properties that are useful in the processing of information in conventional electronic devices. However, whereas traditional devices only control the charge carriers, magnetic semiconductors also give access to the electron spin and thus the storage of information. It is shown that a thin layer of Fe grown on top of (GaMn)As induces ferromagnetic ordering of the Mn magnetic ions several layers across the interface. Furthermore, the magnetization persists at temperatures close to room temperature which makes hybrid ferromagnetic metal/semiconductor structures promising applications in spintronics. Spintronics or spin electronics is a new area of research where the results of conventional magnetism and semiconductor physics are correlated. Hybrid structures of the above type have the potential to optimize information storage and processing in the design of enhanced electronic devices.

1.Introduction

In conventional electronic devices the processing of information is done in semiconductors based on the charge of the electron. On the other hand, information storage is done in metal based magnetic devices using the electron spin. Much energy and time could be saved if storage and processing of information could be brought together on a single chip. To achieve this spin dependent electron transport phenomena would be desirable that are typically observed in ferromagnetic metals due to a spin dependent energy splitting between the ↑ and ↓ density of states, or alternatively in magnetic 4f-systems where magnetism and the electric current are carried by two different electron groups. The magnetic moment stems from the only partially filled 4f-shell of the rare earth atom while the outer 6s-electrons become the quasi free conduction electrons that can move through the entire system.
Prototypes of these materials are the EuX, X=O, S, Se, Te or the metallic Gd; the europium chalcogenides have the additional advantage that they are semiconductors with all the above mentioned useful properties.

Magnetic semiconductors are theoretically described by the sf-model [1] that is introduced in the following section. In Section 3 it is then shown that the sf-model describes magnetism in magnetic semiconductors reasonably well. However, their disadvantages are their low critical temperatures. In Section 4 hybrid metal/semiconductor structures are shown to overcome these difficulties with promising applications to electronic devices and components.

2.The sf-Model

The sf-model describes the mutual effects between the two different electron groups in magnetic semiconductors and is defined by the Hamiltonian

$$H = H_s + H_f + H_{sf}$$

$$H_s = \sum_{ij\sigma} T_{ij}\, c_{i\sigma}^{+} c_{j\sigma} + \frac{1}{2}\, U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \qquad (1)$$

Here $c_{i\sigma}^{+}$ denotes the creation operator for a σ-electron at lattice site R_i, $c_{i\sigma}$ is the corresponding annihilation operator and

$n_{i\sigma} = c_{i\sigma}^{+} c_{i\sigma}$

H_s describes the system of itinerant conduction electrons that are treated as s-electrons and has the well known form of the Hubbard model. Note that the Coulomb interaction is only considered in its simplified intraatomic version. U is the corresponding Coulomb matrix element: T_{ij} are the hopping integrals. The subsystem of localized magnetic moments is described in a realistic manner by the Heisenberg model

$$H_f = -\sum_{ij} J_{ij}\, S_i \cdot S_j \qquad (2)$$

The spins at R_i and R_j interact via the exchange integrals J_{ij}. The two subsystems are coupled by an sf-exchange, i.e. a local interaction between the 4f-spin S_i and the conduction electron spin σ_i

$$H_{sf} = -g \sum_i \sigma_i \cdot S_i = -\frac{1}{2}\, g \sum_{i\sigma} (z_\sigma S_i^z n_{i\sigma} + S_i^\sigma c_{i-\sigma}^{+} c_{i\sigma}) \qquad (3)$$

g is the intraatomic sf-exchange constant. The Hamiltonian of Eq (1) describes a non-trivial many body problem that is generally not exactly solvable. However, there are a couple of exactly solvable limiting cases that are discussed in Section 3.

3.Results

The sf-model of the previous section is rigidly solved in the zero bandwidth limit [2] and the case ($T = 0, n = 0$) describing one electron in an otherwise empty conduction band [3]. It follows already from the molecular field approximation of the model that the magnetization as a function of temperature has the typical form of a Brillouin function

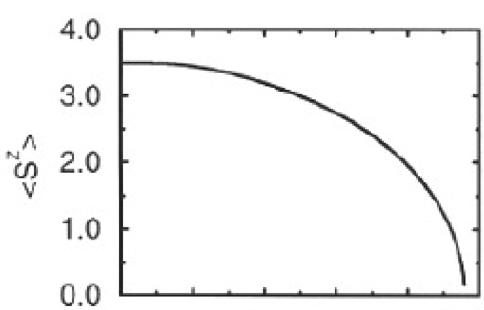


Fig 1: magnetization $\langle S^z \rangle (T)$ as a function of temperature in the case $n = 0$, i.e. empty conduction band.

with the saturation magnetization

$$\langle S^z \rangle \,(T = 0, n = 0) \; = S = \, ^7/_2$$

The Curie temperature is the temperature where

$$\langle S^z \rangle \,(T = T_c) = 0$$

On the other hand, at finite band occupations n the saturation magnetization

$$\langle S^z \rangle \,(T = 0 \;, n \;\neq 0) \leq S \tag{4}$$

is reduced while the Curie temperature T_C is enhanced. This is due to the fact that according to the RKKY-interaction [4] the effective coupling between the localized magnetic moments is caused by the quasi-free conduction electrons of the semiconductor, so one may expect

$$k_B \, T_C \, \propto J_{ij}^{RKKY} \, \propto n_e^{4/3} \tag{5}$$

A similar increase of T_C as a function of n is also observed by the authors of reference [5]. W Nolting et al [6.7] combine the many body problem of the sf-model with a selfconsistent band structure calculation based on DFT to obtain highly realistic results for the Curie temperature T_C of ferromagnetic 4f-systems.

Obviously, the sf-model describes magnetism in magnetic semiconductors reasonably well. Furthermore, magnetic semiconductors combine all properties needed for both the storage and processing of information in one material. However, their $(n = 0)$ critical temperatures are generally too low. In that case the sf-model reduces to the Heisenberg Hamiltonian of Eq (2) and one obtains from a mean field approximation the following results

$$\rho_\sigma \,(E) = \; \rho_0 \,(\, E - U \,\langle n_{-\sigma} \rangle + \frac{1}{2} \, g z_\sigma \,\langle S^z \rangle \,)$$

The quasiparticle densities of state $\rho_\sigma \,(E)$ are rigidly shifted with respect to the free Bloch density $\rho_0 \,(E)$. At $T = T_C$ the two densities coincide, i.e.

$$\rho_\uparrow \,(E) = \; \rho_\downarrow \,(E) = \; \rho_0 \,(\, E - \frac{1}{2} \, U \, n)$$

and a paramagnetic state is obtained. This happens at the Curie temperature

$$k_B \, T_C = \frac{2}{3} \, S \,(S + 1) \,(\, z_1 J_1 \, + \, z_2 J_2 \,) \tag{6}$$

Here z_1, z_2 are the number of nearest and next nearest neighbors; J_1, J_2 are the corresponding exchange integrals. Eq (6) also qualitatively explains why a sufficient number of interactions are important regarding a ferromagnetic order of the magnetic moments and why in some systems of lower dimensions ferromagnetic solutions are according to the Mermin-Wagner theorem not possible (see reference [1]).

Experimental and theoretical values for the critical temperatures of EuX are listed in the table below.

Table 1: experimental and theoretical values for the critical temperatures of EuX.

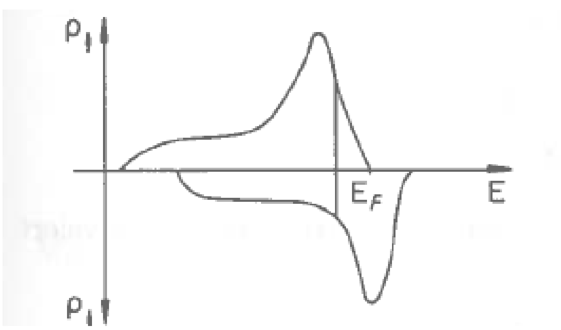
X	Exp value for critical temperature	Theoretical value for critical temperature	Type of magnetism
O	66.8 K	86.6 K	ferromagnetic
S	16.6 K	21.5 K	ferromagnetic
Se	4.6 K	-4.0K	metamagnetic
Te	9.6 K	8.5 K	antiferromagnetic

While the experimental values are taken from ref [8] the theoretical calculations are based on a mean field approximation MFA of the Heisenberg model. Generally one observes the typically enhanced values in the MFA. Especially for $X = O, S$ very similar values for the critical temperature are cited in

ref [9]. For the antiferromagnet $EuTe$ Eq (6) yields the paramagnetic Curie temperature Θ which is negative and unequal to T_N. Again, very similar values for both T_N and Θ are also cited in ref [10].
Note that in EuSe the exchange integrals from nearest and next nearest neighbors compensate each other resulting in an antiferromagnetic state. However, ferromagnetic order may be induced by applying a moderate pressure of $0.5\ GPa$.

4.Applications

The EuX have become objects of interest regarding spintronics as the critical temperature T_C can generally be enhanced by applying pressure. The effect of pressure is a hybridization between the itinerant conduction band states and the localized 4f-states and this phenomenon is often described by the Anderson model [11]. As pressure also changes the lattice parameters of the solid, the authors of ref [12] use a density functional theory method with the LDA+U functional to calculate the critical temperature as a function of the lattice constant; values close to $200K$ are obtained.
On the other hand, in ferromagnetic metals spin dependent electron conduction can be explained from the band structure or density of states of the metal.



Both $\uparrow$ and $\downarrow$-bands are filled up to the Fermi energy ε_F. However, as the two bands are shifted against each other $n_\uparrow > n_\downarrow$ and therefore the spin polarization

$$P = \frac{n_\uparrow - n_\downarrow}{n_\uparrow + n_\downarrow} \leq 1$$

resulting in spin dependent currents. Spin polarizations close to 1 have indeed been calculated with the sf-model for small band occupations n and $T \leq T_c$ [13].
For the propagation of a spin polarized current through the interface between a ferromagnetic metal and a non-magnetic material the current must be injected through a magnetic tunnel junction MTJ. The MTJ consists of two layers of magnetic metals separated by a very thin insulating layer so that the electrons tunnel through the barrier. The tunneling current depends on the magnetization of the ferromagnetic layers and the tunnel resistance [14].
In hybrid metal/semiconductor structures a ferromagnetic metal with its high Curie temperature is combined with a non-magnetic semiconductor to enhance its magnetic properties. A thin layer of Fe is grown over GaAs doped with magnetic Mn-ions so that only a few percent of the Ga-atoms are replaced. The Fe lattice structure is nearly lattice matched to GaAs with a small lattice misfit

$$a_{Fe} \cong \frac{1}{2}\ a_{GaAs}$$

$$\eta = 0.014$$

allowing for epitaxial growth.

The magnetic properties of the Fe/GaAs hybrid structure have been studied extensively [15.16]. Both ab initio and Monte Carlo calculations show that the exchange interaction in Fe stabilizes ferromagnetism in a region of about four atomic layers across the interface. An RKKY type of interaction leads to an effective coupling between the Mn-ions which is ferromagnetic in nature. The induced magnetization in the semiconductor is opposite in direction to that of the iron. Furthermore, the Curie temperature depends on the carrier concentration. If n_e is low, then the coupling between the magnetic moments is weak and paramagnetism is observed. However, for carrier concentrations

$$n_e \cong 10^{20}\ cm^{-3} = \frac{1}{100}\ n_{metal} \rightarrow T_C \cong 200K$$

Curie temperatures close to room temperature are obtained. Similar results of high Curie temperatures in ferromagnetic semiconductors are reported in Co doped ZnO [17] and Mn doped $Pb_{1-x}Sn_xTe$ [18].

5 Summary and Conclusions

It has been shown in the previous sections that hybrid metal/semiconductor structures are interesting examples for spintronic devices and could result in significant gains regarding energy and time consumption as far as the exchange of information in electronic components is concerned. Then it is important to find ways to increase the critical temperature up to room temperature and the numerical results mentioned in the previous section are encouraging in this respect. Furthermore, the near perfect lattice match of Fe and $GaAs$ makes them promising applications for the development of multilayer functional devices. Note that for the devices to function very thin layers of only a few nm are required as the layer thickness must be smaller than the electron's mean free path $l \cong 10\,nm$ at room temperature.

Recent developments in spintronics have increased the capacity of computer hard disks and have extended the technology to mobile appliances. New concepts and ideas include magnetic memory MRAM, spin LED, and the giant magnetoresistance GMR devices [14].

References

[1] W. Nolting: Quantum Theory of Magnetism, Teubner (1986)
[2] W. Nolting and M. Matlak, phys stat sol (b) 123, 155 (1984)
[3] W. Nolting, U. Dubil, and M. Matlak, J. Phys. C 18, 3687 (1985)
[4] A.A. Rudermann and C. Kittel, Phys Rev 96, 99 (1954)
[5] V. Nolting and W. Nolting, phys stat sol (b) 149, 313 (1988)
[6] W. Nolting et al, Phys Rev B35, 7015 (1987)
[7] W. Nolting et al, Phys Rev B35, 7025 (1987)
[8] P. Larson and W.R.L. Lambrecht, J. Phys. Cond. Matter 18, 11333 (2006)
[9] X. Wan et al, arXiv:1003.2039v1, 10 March 2010
[10] A. Radomska and T. Balcerzak, Acta Physica Polonica 98, 83 (2000)
[11] P.W. Anderson, Phys Rev 124, 41 (1961)
[12] J. Kunes, W. Ku, and W.E. Pickett, J. Phys. Soc. Japan 74, 1408 (2005)
[13] W. Borgiel, W. Nolting, and G. Borstel, phys. Stat. sol (b) 136, 131 (1986)
[14] A. Fert, Rev. Mod. Phys. 80, 1517 (2008)
[15] C. Gould and L.W. Molenkamp, Physics 1, 43 (2008)
[16] F. Maccherozzi et al, Phys Rev Lett 101, 267201 (2008)
[17] K. Kittilstved et al, Phys Rev Lett 97, 37203 (2006)
[18] T. Story et al, Phys Rev Lett 56, 777 (1986)