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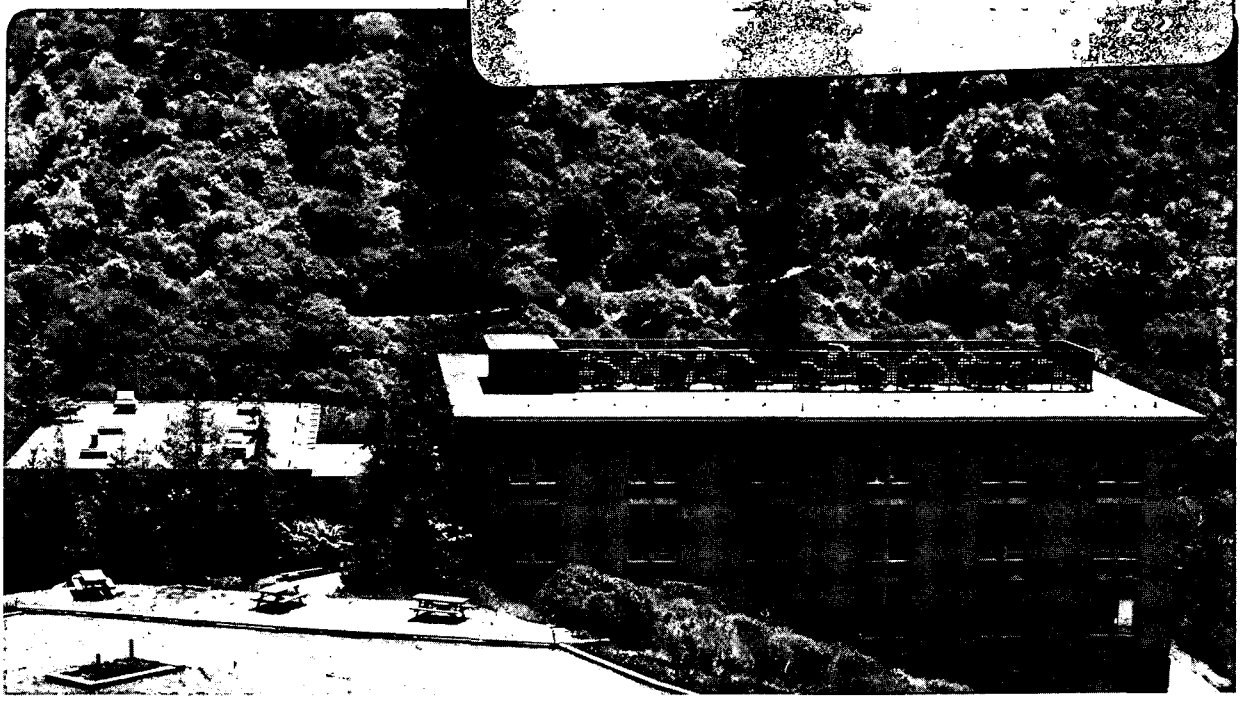

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ELECTRONIC AND MAGNETIC PROPERTIES OF NOBLE-METAL AND TRANSITION-METAL ALLOYS, INTERFACES AND OVERLAYERS

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Summary

The electronic and magnetic properties of noble-metal and transition-metal alloys, interfaces and overlayers are examined theoretically. In particular, results are reported on the electronic and magnetic structure of: 1) nickel-copper alloys; 2) cobalt-iron alloys; 3) nickel-copper interfaces; 4) chromium, cobalt, nickel and copper overlayers on a variety of substrates. General trends are examined and qualitative rules derived.

Itinerant Magnetism in Heterogeneous Systems

In recent years, there has been considerable technological interest in the electronic and magnetic properties of transition-metal and noble-metal alloys, surfaces, and overlayers. This interest stems from the importance of such processes as thin-film magnetic recording and surface passivation, in which a reactive substrate is covered by a non-reactive overlayer. Catalysis is another process of ever increasing relevance, in which the catalyst often consists of small clusters of a reactive transition metal or transition-metal alloy atop an inert substrate. Alloying is of obvious use in producing materials with the most desired properties of several constituent elements. New techniques such as molecular beam epitaxy promise the creation of whole new classes of materials with properties tailored to particular uses.

The study of heterogeneous systems is also useful for providing information about basic properties of magnetism. Alloys, for example, may be viewed as "elements" intermediate between the actual elements, and thus may yield additional data points for discussions of trends in the periodic table. Thin magnetic overlayers provide representations of two-dimensional magnetic systems, a topic of great fundamental interest, particularly in statistical mechanics. The sensitivity of the d electrons to local environment may be probed by the absence of neighboring atoms at a surface or the presence of dissimilar neighbors as found in an alloy. This environmental effect provides information on magnetic healing lengths and the importance of the d-electron itineracy to the magnetic moment.

In moving down the periodic table from Cu, there is a decrease in the number of d electrons (an increase in the number of d holes), and a consequent increase in the bulk elemental magnetization (1) from 0.616 Bohr magnetons in Ni, to 1.72 in Co, and 2.22 in Fe. Beyond Fe lie the more complicated magnetic structures of Mn and Cr. In particular Cr has an antiferromagnetic ground state (2) in which, at the maximum of an incommensurable spin-density wave, there is a magnetization of 0.59 Bohr magnetons. In all these elements, the itinerant nature of the d electrons makes the magnetic properties a sensitive function of local environment. Consequently the presence of a dissimilar neighbor, as found in an alloy or an interface, or the absence of some neighbors, as found at a surface, may cause considerable changes in the local magnetic properties.

With the invaluable help of several collaborators I have calculated the electronic and magnetic properties for several alloys (3,4), and for many surface and overlayer systems (5-10). We use a Slater-Koster parametrized tight-binding scheme in which the one- and two-center integrals are fitted to the bulk band structures of the elements; 4s, 4p and 3d electrons are included. The electron-electron interaction consists of single-site contributions and is sufficiently general to allow for realistic effects such as non-rigid exchange splitting. The interaction is treated self-consistently in the Hartree-Fock approximation. Our scheme has been tested against experimental data (11,12) and against state-of-the-art first-principles calculations (13,14) on several occasions, and has produced consistently excellent agreement (7-9,15). The method has also produced results of interest in catalysis (16).

In this review several of the issues concerning the electronic and magnetic properties of heterogeneous systems are examined. The various specific cases discussed here are clearly susceptible to generalizations--qualitative rules--which are presented in the final section (17).

Magnetization of the (Artificially) Ordered Ni-Cu Alloys

For almost half a century the magnetic behavior of Ni-Cu alloys has been a model problem in itinerant ferromagnetism. The magnetic and electronic properties of these alloys have been extensively studied both experimentally (18,19) and theoretically (20-23). The most striking feature is that the magnetic moment per Ni atom of the alloys decreases approximately linearly with Cu concentration, from 0.616 μ_B for pure Ni to zero at about 60 at. % Cu.

Mott (24) proposed a rigid-band model in which conduction electrons are shared equally among Cu and Ni sites. It results in charge transfer from Cu to Ni, with filling of the Ni minority-spin band, and consequent reduction of magnetization. The theory gives excellent results for the magnetic moment as a function of concentration. However, the very different behavior of alloys of Fe and Co with nonmagnetic metals (25) suggests that the success of the rigid-band model for Ni is fortuitous. More recent experiments (18, 26) moreover suggest that d-band filling is less important than local environment effects in reducing the alloy magnetization.

Unfortunately, the fully self-consistent calculation of electronic properties of random transition-metal alloys is not yet feasible, despite recent progress (27). Some magnetic coherent potential approximation (CPA) calculations have been performed for simple model Hamiltonians (20-22), but these have not included hybridization between the sp and d bands. Such hybridization is crucial for a realistic physical description, as we see below.

In order to examine the basic physical mechanisms responsible for the extinction of ferromagnetism in the Ni-Cu alloys, and to gain some idea of their relative importance, we have therefore calculated the electronic and magnetic properties of some ordered Ni-Cu alloys (3). Specifically, we consider those geometries which can be represented with a four-atom supercell, the conventional cubic cell for the fcc lattice. These structures are entirely artificial for the Ni-Cu alloy, and in interpreting our results we try to distinguish between those effects which are sensitive to the precise geometry, and those which are not.

We find three distinct effects which are important: The effective exchange interaction is reduced in the alloy, relative to pure Ni, by hybridization of the Ni d band with the conduction band, which increases the partial sp character of the d-like states at E_F, the Fermi level, by changes in the shape of the density of states (DOS) projected at the Ni sites, and there is some d-band filling, though it cannot be described in a rigid-band model such as Mott's. Our results are summarized in Table I where, for the sake of uniformity, I display the spin imbalance S rather than the magnetization μ--they differ by a factor equal to one-half of the g-factor, 1.1 in Ni. For the geometries considered, all Ni sites are equivalent. In all cases the spin imbalance at a Cu site is negligible, in agreement with experimental results of Medina and Cable (18). All sites are essentially charge neutral.

Some simple trends are immediately evident from Table I. The magnetization of course decreases with increasing Cu concentration. Our results for the Ni spin polarizations of the two ferromagnetic alloys are in excellent agreement (within 0.04 electron per Ni atom) with experimental results of Medina and Cable (18), interpolated to 25 and 50 at. % Cu. This agreement may be regarded in part as fortuitous, though, in view of the artificial geometries used here.

There is a significant filling of Ni d orbitals in the alloy, relative

Table I. Spin Imbalance S of the Magnetic Transition Metals in Various Configurations

Configuration	Z(Ni)	Z(Cu)	Z(Fe)	Z(Co)	Z(Cr)	S
Ferromagnetic bulk fcc nickel	12					0.56
Nickel in Ni_3Cu quenched alloy	8	4				0.42
Nickel in NiCu quenched alloy	4	8				0.08
Nickel in $NiCu_3$ quenched alloy	0	12				0
Nickel at the (100) free surface	8					0.74
Nickel at the (111) free surface	9					0.65
Nickel under a (100) Cu monolayer	8	4				0.37
Nickel under a (111) Cu monolayer	9	3				0.38
Nickel monolayer on top of Cu (100)	4	4				0.48
Nickel monolayer on top of Cu (111)	6	3				0.08
Ferromagnetic bulk hcp cobalt				12		1.56
Cobalt in the FeCo ordered alloy			8	0		1.78
Cobalt at the (100) surface of the FeCo alloy			4	0		2.03
Cobalt at the (110) surface of the FeCo alloy			6	0		1.86
Cobalt monolayer on top of Cu (111)		3		6		1.63
Ferromagnetic bulk bcc iron			8			2.12
Iron in the FeCo ordered alloy			0	8		2.66
Iron at the (100) free surface			4			2.90
Iron at the (110) free surface			6			2.55
Iron at the (100) free surface of the FeCo alloy			0	4		2.95
Iron at the (110) free surface of the FeCo alloy			0	6		2.75
Iron under a (100) Cr monolayer			4		4	1.95
Antiferromagnetic bulk chromium (incommensurable phase)					8	0.59
Antiferromagnetic bulk chromium (commensurable phase)					8	0.67
Chromium at the (100) free surface					4	3.00
Chromium at the (110) free surface					6	2.31
Chromium monolayer on top of Fe (100)			4		0	3.63
Chromium monolayer on top of Fe (110)			2		4	2.25

Z(A) is the number of nearest neighbors of element A.

to pure Ni. This filling is approximately linear in the number of Cu neighbors. The d-band filling is due to narrowing of the projected Ni d-band with reduced Ni-Ni coordination. The d band is centered well below E_F, so as it narrows, it pulls below E_F and becomes fuller. This is possible because charge neutrality can be maintained at only moderate cost in energy by transferring electrons from the sp band to the d band at the Ni site. This mechanism for d-band filling is suggested by results of calculations for the random paramagnetic Ni-Cu alloy (23) using a non-self-consistent potential. We find that this effect is modified by self-consistency but not eliminated, as it would be in a calculation which omitted the sp band. Note that this is completely unrelated to the Mott rigid-band picture. Also, the driving force for charge transfer is band narrowing, which is absent in a rigid-band model. Most important, the d-band filling accounts for only a fraction of the change in magnetization.

A major cause of the reduced magnetization is the following: In the alloy, the upper edge of the d band becomes rounded. This reduces the DOS at E_F, and hence the magnetization. We believe this DOS "shape" effect to be a crucial factor for magnetism in Ni alloys.

Magnetization of Iron-Cobalt Ordered and Disordered Alloys

One of the most famous plots in the solid-state literature is the Slater-Pauling curve (29). This plot displays magnetization versus the electron-to-atom ratio for a large variety of chemically disordered transition-metal alloys. One of the most interesting features of the curve is the abrupt change in its slope as it passes through its maximum at approximately 26.3 electrons per atom. Several explanations have been proposed for this feature. Pauling (30) argued that the number of unbalanced d holes could not exceed approximately 2.4 because the other 2.6 d electrons of each spin belong to a lower band which cannot lose electrons until the upper one is completely emptied. A somewhat different point of view is provided by Williams et al. (31) who argued that the only two relevant features are magnetic saturation, which occurs on the Co side of the maximum, and ferromagnetic weakness, which occurs on the Fe side of the maximum. It is noted (32) that this ferromagnetic weakness coincides with the pinning of the Fermi level at a valley in the minority-spin density of states. Finally, one might expect that band narrowing and other complicated band-structure effects, such as those which occur in Ni-Cu alloys, may be causing the maximum.

The uppermost and sharpest maximum on the Slater-Pauling curves is formed by the Fe-Co alloy system. Consequently, one expects that a complete understanding of this alloy would lead to the correct explanation for the Slater-Pauling maxima. Several experimental and theoretical studies have been performed for Fe-Co. Early experimental measurements of the saturation magnetization were made by Weiss and Forrer (33). Later, after the discovery of an ordered structure near the equiatomic alloy, Bardos (34) remeasured the disordered substance. It is also known (35) that Fe-Co undergoes structural phase transitions with a change in concentration: Iron-cobalt is bcc for 25% or more iron; it is fcc or hcp for less than 10% iron, and there is a mixed phase in between. Meyer and Asch (36) determined the g factors for the Fe-Co alloys, thus allowing a comparison of the experimentally measured magnetization with the theoretically predicted spin polarization. Neutron-diffraction (37) studies indicate that the vast majority of the anomalous increase in the magnetic moment is due to an increase in the Fe magnetic moment from 2.2 μ_B to approximately 3.0 μ_B, while the Co magnetic moment remains approximately constant at 1.8 μ_B.

We have calculated the magnetic properties of the ordered equiatomic

FeCo alloy (9), and the disordered Fe-Co system over the whole concentration range (4). Disorder was introduced by the use of the virtual crystal approximation, which in this particular case is excellent because of the great similarity of the iron and cobalt band structures. Results are shown in Table I and Figure 1. Agreement with experiment is excellent and the anomalous behavior is fully reproduced. In the Co-rich region, the Fermi level lies above the majority DOS and the magnetization essentially depends on the number of available d holes. In the Fe-rich region, a relatively weak electron-electron interaction allows the Fermi level to lie in a valley separating the minority bcc DOS into an upper and lower band. The intersection of this weakly ferromagnetic region with the saturated region of the Co-rich alloys produces a maximum in the magnetization at approximately 30 at. % Co.

Figure 2 provides an explanation for the curve by plotting the Fe-Co results versus an imaginary "element" described by the Co Hamiltonian, but with a decreasing number of electrons as one approaches the Fe side of the plot. This imaginary element differs from the Fe-Co alloy in that it possesses a much stronger electron-electron interaction than that associated with iron. (Iron has an electron-electron interaction to bandwidth ratio that is only two-thirds as large as that of cobalt or nickel.) The plot demonstrates that the effect of this strong interaction is to raise drastically the Fe magnetization and remove the intermediate maximum. On the other hand, it causes little change on the Co side of the curve, suggesting that in this range saturation has been reached, i.e., all possible d holes are already magnetized. A reasonable conclusion is that the anomalous Fe-Co curve is dominated by magnetic saturation except in those regions of low Co content where an electron-electron interaction insufficient to cause saturation is more important.

Figure 2 also demonstrates that Pauling's explanation of the Fe-Co curve is not to be taken literally. Although we do find that for concentrations

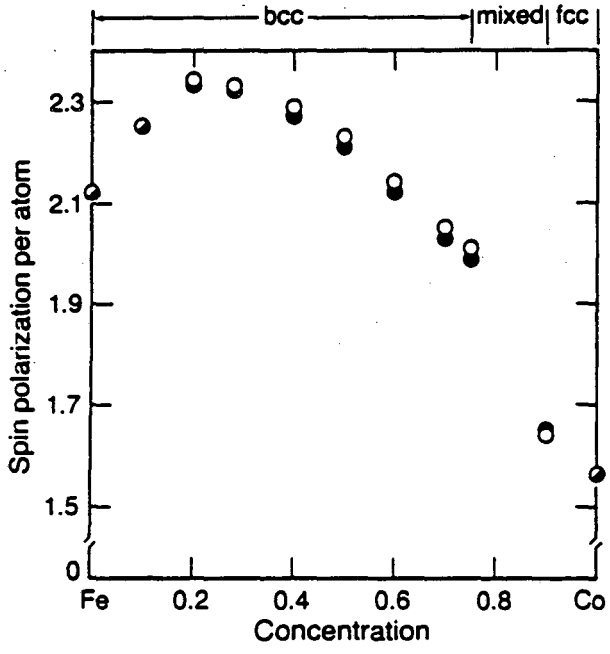

Figure 1 - Spin polarization as a function of Co concentration x in $Fe_{1-x}Co_x$. Open circles are theoretical results; closed circles are experimental results taken from Refs. 33 and 34 with g factors from Ref. 36.

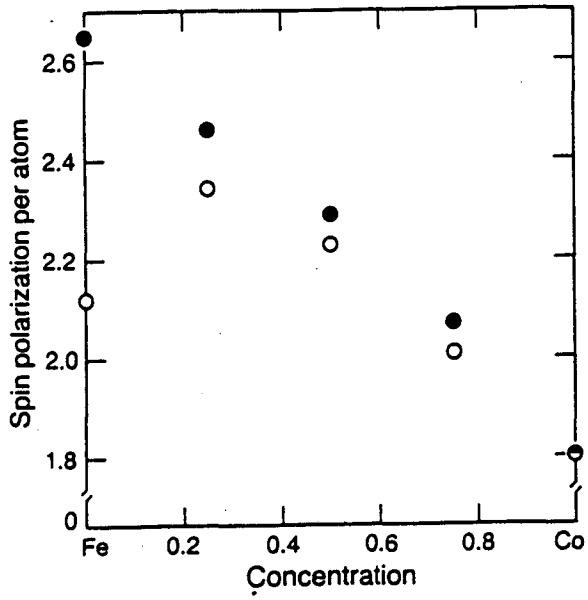

Figure 2 - Spin polarization as a function of electron concentration using a virtual-crystal Hamiltonian (open circles) and a pure Cc Hamiltonian (closed circles).

of Fe greater than 80%, the Fermi level lies in a minority-spin DOS valley as Pauling's argument predicts, it is clear from Fig. 2 that if the electron-electron interaction to bandwidth ratio had not decreased as the Fe concentration increased, then the Fermi level would have been at its normal strong ferromagnetic position above all of the majority states and hence would have arbitrarily cut the minority density of states. This can be restated in the language of Pauling by noting that the spin polarization at the Fe end of the curve, 2.65, requires an emptying of 2.4 "upper-band" states and 0.25 "lower-band" states. In conclusion, it is clear that a decreasing electron-electron interaction to bandwidth ratio is at least as important as any band-splitting effects.

It is likely that our conclusions for the Fe-Co system have application to many other transition-metal alloys. For example, Fe-Ni demonstrates the same sort of maximum at approximately 10 at. % Ni. Other alloys such as Ni-Cr, Ni-V, Co-Cr, and Co-Mn display magnetization curves at right angles to the saturation line. It is possible that this too is the result of a weak electron-electron interaction. However, the testing of these suggestions may need to be performed within an approximation more accurate than the virtual crystal, because of the increasing dissimilarity of the band structures.

Interfaces

In order to understand the magnetic properties of overlayers we have first calculated the electronic and magnetic properties of some interfaces (5,7). In particular we have examined (7) the nickel-copper (100) and (111) interfaces. We found that the sp electrons of Cu hybridize considerably with the Ni d electrons. This effect reduces the interface-projected DOS near the Fermi level and makes it difficult for the interface Ni atoms to achieve saturation. As a consequence the spin polarization of Ni at both the (100) and the (111) interfaces is found to be 0.38, a considerable reduction from the 0.56 bulk value. We also found that if the Ni-substrate coupling is increased above its Ni-Cu value, as should be the case for simple metals like lead and aluminum, then the interface layer is unmagnetized for the

(100) case. These results point out that the effect of a nonmagnetic substrate such as Cu is to reduce the magnetic moment of the transition metal in direct contact with it to a value below that of the bulk.

Overlayers

Overlayers of magnetic transition-metals are subject to two independent influences: (a) the magnetization enhancement caused by the free surface (see Table I), and (b) the independent effect--either enhancement or quenching--of the substrate.

Monoatomic overlayers of Ni on Cu (100) and on Cu (111) surfaces provide a clear example of this point. As discussed previously, the effect of the Cu interface is to decrease the Ni magnetization. On the other hand the effect of the free surface is to enhance it. Our calculations (7) show that the magnetization of the (111) Ni monolayer is nearly zero, whereas the (100) monolayer has essentially the bulk magnetization. These results correspond well with calculations that show (7) that face-centered-cubic (100) surfaces have higher magnetization than (111) surfaces (see Table I).

Comparison with the interface results is, however, not so straightforward. As previously noted, the spin polarization of both interfaces is 0.38, a decrease by a factor of 1.47 from the bulk value. Clearly the exchange splitting of the bulk atoms helps to maintain a sizeable magnetization at the interface. On the other hand, the presence of a surface ("the other side" of a monolayer) also tends to enhance the magnetization. Which effect is more important--hybridization with the strongly magnetized bulk atoms or the enhancement caused by the free surface--is clearly a sensitive function of environmental variables such as surface orientation and chemical composition, and not susceptible to simple qualitative arguments.

The extent of this sensitivity is demonstrated by our calculations (8) for Co overlayers on the Cu (111) surface. Here the monolayer has a spin polarization of 1.63, greater than the values for the inner atoms of the dilayer: 1.58. In other words, the surface enhancement of the magnetization is more important in this case than the enhancement caused by the nearest neighbor exchange splitting. It is probably the result of Co having more holes than Ni, and a monolayer moment close to the bulk value, a case similar to the monolayer of Ni on Cu (100).

A more predictable system is that consisting of an Fe monolayer on the (110) surface of the ordered FeCo alloy. Here the Fe magnetization is expected to be higher than its ordinary value at the (110) surface of body-centered-cubic Fe: the substrate has a larger exchange splitting in the alloy than in pure Fe. Our calculation (9) finds the additional enhancement to be 0.08 and 0.12, depending on the Fe atom position, relative to the spin polarization of 2.55 found at the Fe (110) free surface.

Another result of considerable interest (7) is the fact that in the extreme strong coupling limit, when the magnetic transition metal hybridizes infinitely strongly to the conduction states of the substrate, both a monolayer and a dilayer of Ni (100) show no magnetization whatsoever--two "dead" magnetic layers--whereas a triatomic layer shows considerable spin polarization (0.61 at the surface, 0.45 for the intermediate atoms) even though the interface Ni atoms are magnetically dead.

Finally, Cr monolayers on Fe are found to be ferromagnetic, with the Cr spins aligned in the opposite direction to the Fe spins (10). At the (110) surface this arrangement forces Cr nearest neighbors to have the same spin

direction, a result which indicates the considerable strength of the Fe-Cr interaction. The (100) Cr monolayer possesses the largest spin polarization for a transition-metal system known to the author. This polarization, 3.63 electrons, is caused by the combination of (100) surface band narrowing and the strong antiferromagnetic Fe-Cr interaction.

General Trends and Qualitative Rules

The results reported here--see especially Table I--lead directly to the following observations (17) which I would call qualitative rules.

1. The removal of nearest neighbors of its own kind reduces the projected bandwidth of a magnetic transition metal atom and thus increases the electron-electron interaction to bandwidth ratio. This effect, most evident at surfaces, tends to enhance magnetism.

2. Magnetization enhancement is sizeable only in those elements where the bulk magnetization is not close to saturation, i.e. where there exist holes in the d-band which can still be polarized. Considerable enhancement is therefore expected for Cr and Fe; the effect is small for Co and Ni. It is also small for the surface enhancement of Fe in the FeCo alloy, where the alloying effect has already produced "saturation" of the Fe magnetization.

3. The presence of a strongly magnetized atom with a large exchange splitting near a weakly magnetic but polarizable atom with a smaller splitting considerably enhances the magnetization of the latter.

4. The presence of a nonmagnetic unpolarizable atom next to--and coupled to--a magnetic transition-element atom tends to decrease or fully destroy the magnetization of the latter.

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