Electronic structure and magnetic properties of 3*d* impurities in antiferromagnetic metals

V. P. Antropov and V. I. Anisimov
Institute of Metal Physics, Sverdlovsk GSP-170, Union of Soviet Socialist Republics

A. I. Liechtenstein
Institute of Chemistry, Sverdlovsk GSP-145, Union of Soviet Socialist Republics

A. V. Postnikov*
Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-7000 Stuttgart 80, Federal Republic of Germany

(Received 5 August 1987)

The electronic structure of substitutional 3*d* impurities (from V to Ni) in *B*2 phases of antiferromagnetic Cr and Mn has been calculated by the linear-muffin-tin-orbital Green's-function method. Self-consistent values of local magnetic moments and corresponding effective exchange parameters are found. The magnetic moment of the Fe impurity is parallel to that of the substituted atom in the case of a Cr host and antiparallel in the case of a Mn host. For pure Mn, both simple antiferromagnetic and "reversed-spin" configurations are found unstable with respect to small spin deviations.

I. INTRODUCTION

Antiferromagnetism of chromium- and manganese-based diluted alloys presents one of the most complex problems of itinerant magnetism theory.[1] As is well known, the antiferromagnetic structure of pure Cr is incommensurate with the crystal lattice and has the form of a spin-density wave (see Ref. 2 for a review), specific topology of the Fermi surface being a reason for the unstability of the commensurate antiferromagnetic state.[3] Small amounts of 3*d* metal [2.5% of Fe (Ref. 4) or 1.1% of Mn (Ref. 5)], however, makes the spin-density wave commensurate, resulting in simple antiferromagnetic ordering of *B*2 type in dilute alloys.

The antiferromagnetic ground state of manganese is also rather complex, with 58 atoms of four nonequivalent positions in the unit cell (see Ref. 6). It makes the experimental determination of magnetic properties of Mn-based alloys a troublesome task.

Actually, only a few magnetic measurements for impurities in Cr and Mn have been done so far. Most of the data concern the *Cr*Fe system, for which as different values of the Fe magnetic moment as $0.08\pm0.08\mu_B$ (Ref. 7) and $2.0\pm0.2\mu_B$ (Ref. 8) have been reported obtained from polarized-neutron diffuse scattering experiments on samples containing several percent iron. In Ref. 9, magnetization measurements gave estimates of $2.7\mu_B$ for an effective magnetic moment of an Fe impurity in Cr and $2.9\mu_B$ for Co in Cr. A brief discussion concerning the experimental data for Cr-based alloys can be found in Ref. 10. In regard to impurities in Mn, we are not aware of any experiments done after that of Williams *et al.*,[6] who studied the effect of transition metal impurities on the Neél temperature of the host metal.

As far as we know, no direct study of electronic structure or theoretical *ab initio* calculations have been performed so far for impurities in antiferromagnetic metals. The aim of this paper is to present quantitative results for local magnetic moments and effective exchange parameters obtained in a self-consistent linear-muffin-tin-orbital (LMTO)–Green's function calculation for Cr- and Mn-based impurity systems.

II. CALCULATION

The method of calculation, which is similar to the formalism given in Ref. 11, has been described in some detail in our previous work concerning impurities in ferromagnets (Ref. 12, denoted as I hereafter). As we take into account the change of potential only on one site, no additional difficulties arise from the fact that the host metal now consists of two sublattices.

As a starting point to study the impurity problem, self-consistent LMTO atomic-sphere-approximation (ASA) calculations for pure host metals have been performed. In both cases, a simple antiferromagnetic *B*2 phase has been considered that corresponds to the structure of an actual impurity-doped alloy (in the case of Cr) or the high-temperature δ phase (in the case of Mn). Similar calculations for pure Cr (Refs. 13 and 14) and Mn (Ref. 15) have been performed before, giving the antiferromagnetic spin ordering and good agreement with experimental estimates of the local magnetic moment.

Starting from different initial spin configurations, in order to find all possible self-consistent solutions, impurity calculations were then performed with the impurity atomic sphere radii being constantly adjusted to retain their charge neutrality.

III. RESULTS AND DISCUSSION

Calculated densities of states of 3*d* impurities in Cr and Mn are shown in Figs. 1 and 2, respectively. The values

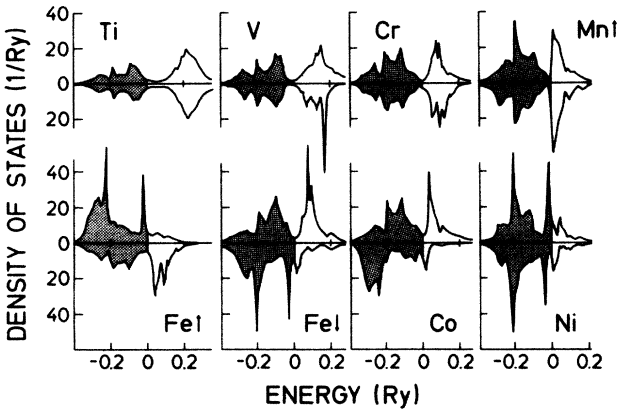

FIG. 1. Local densities of states for 3*d* impurities in Cr.

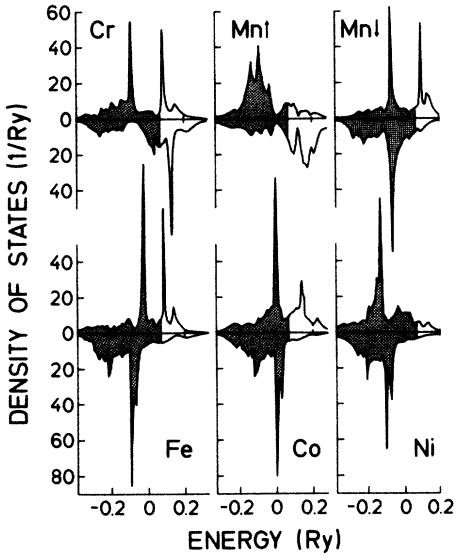

FIG. 2. Local densities of states for 3*d* impurities in Mn.

of the local magnetic moments and effective exchange parameters [calculated with Eq. (8) of I] are listed in Table I. Magnetic moments of impurities, which are directed in the same way as those of atoms they substitute, are listed as positive. Magnetic moments of several first 3*d* impurities have a tendency to antiparallel orientation with respect to moments of their nearest neighbors. The inversion of impurity spin occurs somewhere near Mn or Fe.

The said tendency is well known for impurities in ferromagnets, and we briefly discuss the reason for it in I. In contrast to impurities in ferromagnets where pronounced Lorentzian-shaped virtual bound states of light impurities, initially empty, gradually lower and dissolve in the host *d* band as we approach the end of the 3*d* row, Ti and V impurities in Cr exhibit a local density of states rather similar to that of the pure host. Electronic properties of even more concentrated alloys of these metals can probably be described in the framework of some simple approximation, say, the virtual crystal approximation.

Starting from Fe (and for Cr in Mn as well), sharp narrow peaks appear in the impurity densities of states near the Fermi level in Cr and Mn. These peaks correspond to the nonbonding impurity states which are formed in an "antiferromagnetic gap" in the middle of the host conduction band. A similar effect has been pointed out in the calculation performed for substitution impurities in the FeCo alloy,[16] where heavy 3*d* impurities (Co to Cu) at an Fe site form almost discrete levels in the region of reduced host density of states.

A spin configuration of impurities with a negative effective exchange parameter J_0 is unstable with respect to small deviations of spin (see the discussion in I). Therefore, the only solution to be retained for an Fe impurity in Cr corresponds to the same spin direction as that of the substituted atom. However, the exchange bonding between impurity and host is rather weak even compared to that in pure chromium. For a Co impurity, the value of the exchange parameter is considerably greater, in agreement with the experimental evidence of stronger exchange coupling in *Cr*Fe than in *Cr*Co alloys.[9]

The fact that both solutions for a Mn "impurity" in Mn (i.e., cases of pure antiferromagnetic metal and one with reversed spin on one site) correspond to negative values of J_0 reveals the fact that neither of these configurations occurs in reality. Formal existence of two self-consistent solutions means, however, that a magnetic moment at a Mn site is of a localized rather than an itinerant character.

TABLE I. Calculated values of local magnetic moments and effective exchange parameters for 3*d* impurities in antiferromagnetic metals.

Impurities:	V	Cr	$Mn_\uparrow$	$Mn_\downarrow$	$Fe_\uparrow$	$Fe_\downarrow$	Co	Ni
				in Cr				
M (μ_B)	0.36	0.59	0.48		2.17	−1.83	−1.63	−0.13
J_0 (mRy)	1.0	2.5	1.4		1.7	−2.8	6.2	0.4
				in Mn				
M (μ_B)	1.10	2.18	2.98	−1.12		−1.86	−1.34	−0.37
J_0 (mRy)	5.6	11.8	−8.8	−4.1		2.4	8.5	1.8

IV. CONCLUSION

In this paper, we gave new computational results concerning the electronic structure of 3*d* impurities in Cr and Mn. As soon as no experimental data are available on many of these systems, given results will be mainly of prognostic character. Certain known magnetic properties of Cr- and Mn-based diluted alloys are in agreement with our calculation.

ACKNOWLEDGMENT

One of us (A.V.P.) would like to thank the Alexander von Humboldt Stiftung for financial support.

---

*Permanent address: Institute of Metal Physics, Sverdlovsk, USSR.

[1]S. V. Vonsovskii, *Magnetism* (Wiley, New York, 1974).
[2]N. I. Kulikov and V. V. Tugushev, Usp. Fiz. Nauk **144**, 643 (1984) [Sov. Phys. Usp. **27**, 954 (1984)].
[3]W. M. Lomer, Proc. Phys. Soc. London **80**, 489 (1962).
[4]Y. Ishikawa, R. Tournier, and J. Filippi, J. Phys. Chem. Solids **26**, 1727 (1965).
[5]B. M. Geerken, R. Griessen, G. Benediktsson, H. U. Åström, and C. van Dijk, J. Phys. F **12**, 1603 (1982).
[6]W. Williams, Jr. and J. L. Stanword, Phys. Rev. B **7**, 3244 (1973).
[7]R. Cywinski and T. J. Hicks, J. Phys. F **10**, 693 (1980).
[8]F. Kajzar, G. Parette, and B. Babic, J. Phys. Chem. Solids **42**, 501 (1981).
[9]F. J. Hedgcock, J. O. Strom-Olsen, and D. F. Wilford, J. Phys. F **7**, 855 (1977).
[10]N. H. March, Ph. Lambin, and F. Herman, J. Magn. Magn. Mater. **44**, 1 (1984).
[11]C. Koenig, N. Stefanou, and J. M. Koch, Phys. Rev. B **33**, 5307 (1986).
[12]V. I. Anisimov, V. P. Antropov, A. I. Liechtenstein, V. A. Gubanov, and A. V. Postnikov, Phys. Rev. B **37**, 5598 (1988).
[13]J. Kübler, J. Magn. Magn. Mater. **20**, 277 (1980).
[14]H. L. Skriver, J. Phys. F **11**, 97 (1981).
[15]J. Kübler, J. Magn. Magn. Mater. **20**, 107 (1980).
[16]A. V. Postnikov and V. I. Anisimov, Phys. Met. Metall. (to be published).

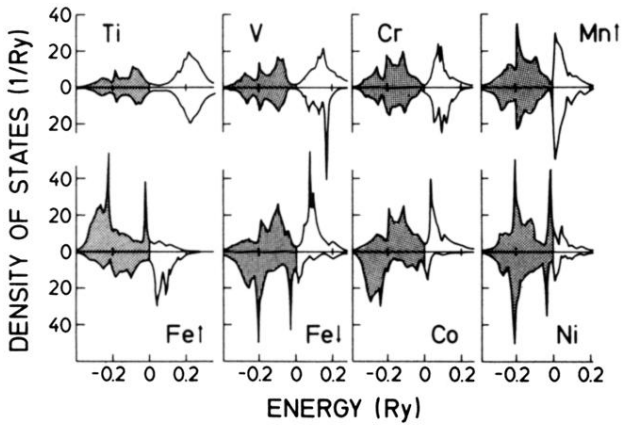

FIG. 1. Local densities of states for 3*d* impurities in Cr.

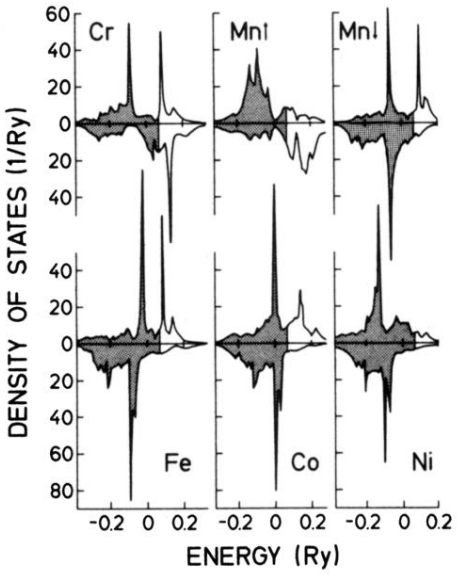

FIG. 2. Local densities of states for $3d$ impurities in Mn.