A CLUSTER CALCULATION OF THE MUON HYPERFINE FIELD IN NICKEL

B. D. Patterson*, Physik-Institut der Universität Zürich, Switzerland
and
J. Keller†, E. T. H. Hönggerberg, Switzerland

ABSTRACT

We have performed a partially self-consistent, first-principles calculation of the hyperfine field at a μ+ at the octahedral interstitial site in ferromagnetic nickel. Using a package of programs made available by the Department of Theoretical Chemistry of the University of Mexico, various calculations were performed of the spin-dependent charge density in the central region of a spherically averaged superposition of atomic charge densities. In this way it was found that: (1) The electronic configuration of bulk Ni contains a significant amount of 4p-states, in agreement with other calculations. (2) The μ+ produces only a weak perturbation on its nearest-neighbor Ni atoms. (3) The hyperfine field at the μ+ is opposite to the bulk magnetization and has the value -590 G, in good agreement with the measured value of -641 G.

Nickel was the first ferromagnetic material in which a μSR signal was observed, and several attempts have been made to theoretically explain the observed hyperfine field. This calculation is the first attempt at a first-principles description of the electronic environment of the interstitial μ+ in a ferromagnet. We made use of an existing package of four sophisticated computer programs, the functions of which are described below.

The first step in the calculation was to generate a reliable approximation to the atomic electron configuration for a Ni atom in pure, ferromagnetic nickel. An initial guess was made of the occupation of the valence levels (i.e., 3d, 4s, 4p for both majority and minority spin directions) which was consistent with charge neutrality and the measured magnetic moment per atom in bulk Ni, and used as input to the program HEX. This program performed a relativistic, spin-polarized calculation of the atomic wave functions and the corresponding Coulomb potential. The exchange and correlation contributions to the total energy were included in the "Xαβ" approximation, where the parameters α and β had "universal" values. The calculation was repeated with new valence level occupations until an approximate energy minimum was found.

The resulting atomic wave functions and potentials were then introduced into the program CRYSDERI where a crystalline potential for pure bulk Ni was constructed. This potential, centered on a central Ni atom, consisted of the superposed atomic Coulomb potentials of seven shells of Ni neighbors plus the exchange and correlation contributions computed from the superposed atomic charge densities using the Xαβ approximation. Only the $\zeta=0$ term in the spherical
harmonic expansion of the potential was retained, and only within a radius equal to a muffin tin radius (i.e., containing a single atom).

CRYSDERI then integrated the Schrödinger equation from the center of the cell to the cell boundary at 50 different energies for each of the valence states. The resulting energy-dependent logarithmic derivatives of the wave functions at the boundary then established the positions of the various bands (the logarithmic derivative is less than zero in the interior of a band). Multi-state interference effects which would lead to structure within the bands were lacking in this single-site approximation. The logarithmic derivatives were then matched to those for plane waves external to the cell, the external potential being taken to be constant. This resulted in scattering phase shifts \( \eta_k(E) \) for the different bands and spin states. A Friedel analysis of these phase shifts yielded the single-site integrated density of states which in turn determined the resultant band occupations and Fermi level \( E_F \) for each spin orientation.

In the early attempts, either the initial and resultant band occupations were in disagreement, or \( E_F^{(maj)} \) was not equal to \( E_F^{(min)} \), requiring a return to HEX with new initial valence state occupations. After a few HEX-CRYSDERI cycles, however, consistency was achieved. The final occupations for pure bulk Ni were as follows:

<table>
<thead>
<tr>
<th></th>
<th>maj.</th>
<th>min.</th>
</tr>
</thead>
<tbody>
<tr>
<td>3d</td>
<td>4.374</td>
<td>3.894</td>
</tr>
<tr>
<td>4s</td>
<td>0.369</td>
<td>0.369</td>
</tr>
<tr>
<td>4p</td>
<td>0.537</td>
<td>0.457</td>
</tr>
</tbody>
</table>

in reasonable agreement with more detailed band structure calculations\(^1\). This configuration was subsequently taken to be the description of unperturbed Ni atoms.

HEX-CRYSDERI calculations were also performed with an interstitial muonium atom in the central cell, taking into account the potential tails of seven shells of Ni neighbors, or with the central cell occupied by a perturbed Ni atom which was a nearest neighbor of an interstitial muonium atom. Various combinations of nearest-neighbor perturbations and muonium magnetic moments were attempted, but it was found that agreement between the initial and resultant occupations and between \( E_F^{(maj)} \) and \( E_F^{(min)} \) was achieved only for an essentially non-magnetic muonium atom surrounded by very weakly perturbed Ni neighbors. In the remainder of the calculation, the neighbors of the muon were taken to be unperturbed.

Next the program MOLPOT used the resulting Mu and Ni electronic configurations to compute the spherically averaged potential (Coulomb plus X\(\alpha\) exchange and correlation) for both the muonium central cell and the outer shell (seven Ni shells) on a very fine mesh.

The program CELLULAR was then used to perform an integration of the Schrödinger equation for the central cell (now taken to be of the correct size to guarantee neutrality) and for the outer shell. Matching the wave functions at the boundary allowed a normalization of the wave function and a determination of the energy eigenvalue for each state found. The result was a series of eigenstates with increasing energy for each spin direction. One should have then proceeded to occupy these states self-consistently in such a way as to minimize the total energy of the cluster. It was found, however, that the lowest two states of each spin could easily accommodate the required electron and that the spin density which resulted at the muon was almost independent of the way in which these states were