PHYSICS

Academician of the Academy of Sciences of the Belorussian SSR N. N. Sirota and N. M. Olekhnovich

1961

SovietRxiv

Abstract

Full Text

PHYSICS

Academician of the Academy of Sciences of the Belorussian SSR N. N. Sirota and N. M. Olekhnovich

DISTRIBUTION OF THE ELECTRON DENSITY OF THE ELECTRONS OF THE $3d$ SHELL RESPONSIBLE FOR THE FERROMAGNETISM OF NICKEL, COBALT, AND IRON

The discovery of neutrons and of the methods of neutronography gives researchers new powerful means for studying the nature of magnetism, the arrangement of magnetic spins in the crystal lattice, and the character of the distribution of the electrons responsible for ferromagnetism or antiferromagnetism.

The study of Bragg coherent scattering of x-rays by a crystal lattice makes it possible to find atomic scattering factors (x-ray form factors) as a function of the angle of reflection or of the sum of the squares of the Miller indices. Using the values of the atomic scattering factors, by summing three-dimensional Fourier series one can find the distribution of the electron density in the crystal lattice. New information is provided by the study of neutron scattering by the crystal lattice of a ferromagnet or antiferromagnet.

Since the neutron possesses a magnetic moment, neutron scattering occurs not only by nuclei but also by electrons that have magnetic moments uncompensated by other electrons and that form the magnetic structure. The neutron form factor, determined from diffraction lines, makes it possible to calculate the distribution in the crystal lattice of the electrons responsible for ferromagnetism or antiferromagnetism, using a method of summing three-dimensional Fourier series analogous to that used in x-ray structural analysis.

In the present work the aim was to determine the distribution of the electrons responsible for ferromagnetism in the ferromagnetic elements iron, nickel, and cobalt from known neutron scattering form factors. On the other hand, the task of the present investigation was to compare, using nickel as an example, the electron-density distribution calculated from the x-ray atomic scattering factor with the density distribution of the electrons of the $3d$ electron shell responsible for ferromagnetism.

The experimentally obtained amplitude of neutron-magnetic scattering P, as is

Figure 1

Figure 1: Figure 1

known, is determined by the relation

$$P = \frac{e^2\gamma}{mc^2} fS, \tag{1}$$

where f is the unit form factor of neutron scattering, and S is the effective quantum number. The quantity S is determined experimentally from the magnetic moment of the element under investigation:

$$S = {}^1/_2\mu. \tag{2}$$

In calculating the effective quantum number the following values of the magnetic moments are adopted: Fe 2.22, Co 1.74, Ni 0.60.

We note that the value fS is determined experimentally from neutron-scattering data independently of magnetic measurements.

Fig. 1 shows the values of the unit form factors, multiplied by the effective quantum numbers, for iron and nickel according to the data of Nathan, Shull, Shirane, and Andersen ([1]), and for cobalt according to the data of Nathan and Paoletti ([2]).

Summation of three-dimensional Fourier series either directly, where this is possible, or by means of an approximation method used to eliminate the effect of truncation of the series, makes it possible to calculate the electron density ρ at each point of the unit cell, as well as the radial electron density of the electrons of the $3d$-electron shell responsible for ferromagnetism. For the calculations we used the method described by us earlier ([3]).

Fig. 1. Variation of the unit form factors, multiplied by the effective quantum numbers, of iron (1), nickel (2), and cobalt (3) as a function of

$$\sum_{i=1}^{3} h_i^2 \ ([1,2])$$

In Fig. 2, as functions of the distance from the atomic centers, curves are given for the change in the electron density ρ of the electrons of the $3d$-electron shell responsible for the ferromagnetism of nickel, cobalt, and iron (Fig. 2a), and for the radial electron density $u(r) = 4\pi r^2\rho(r)$ (Fig. 2b). The following essential circumstances are noteworthy. The calculated electron density for Ni, Co, and Fe reaches a maximum near the centers of the atoms; the probability of finding an electron at a given point of the volume of the unit cell decreases

Figure 2

Figure 2: Figure 2

Fig. 3. Radial distribution of all electrons of nickel (1) and electrons of the 3d shell (2) responsible for ferromagnetism as a function of distance from the center of the atom.

Figure 3: Fig. 3. Radial distribution of all electrons of nickel (1) and electrons of the 3d shell (2) responsible for ferromagnetism as a function of distance from the center of the atom.

rapidly with distance from the atomic center, practically according to the law of a Gaussian distribution. On the other hand, the radial electron density reaches its maximum value for nickel at 0.44 Å, for iron at 0.40 Å, and for cobalt at 0.39 Å, and then rapidly decreases practically to zero at a distance of 1.1–1.2 Å from the atomic centers, which does not exceed half the distance between nearest ions in the lattice of the indicated elements. The latter circumstance

Fig. 2. Variation of the electron density (a) and radial density (b) of the electrons of the 3*d*-shell responsible for the ferromagnetism of iron (1), nickel (2), and cobalt (3), as a function of the distance from the atomic centers.

indicates that the electron shells under consideration do not overlap.

Figure 3 gives the curve of the radial distribution of all the electrons of nickel, calculated from the values of the atomic scattering amplitude according to Brindley ([4]), and, for comparison, on the same scale, the curve of the radial distribution of the electrons responsible for ferromagnetism, discussed above. The latter curve is completely contained within the former. The area bounded by it is considerably smaller than the area bounded by the first curve. Its maximum is located at a greater distance from the center of the atom than the maximum of the first curve.

Fig. 3. Radial distribution of all electrons of nickel (1) and electrons of the 3*d*-shell (2) responsible for ferromagnetism as a function of distance from the center of the atom.

Fig. 4. Distribution of the electron density of all electrons (1) and of the density of "magnetic" electrons (2) between nickel atoms in the directions [111]

Fig. 4. Distribution of the electron density of all electrons (1) and of the density of "magnetic" electrons (2) between nickel atoms in the [111] and [110] directions.

Figure 4: Fig. 4. Distribution of the electron density of all electrons (1) and of the density of "magnetic" electrons (2) between nickel atoms in the [111] and [110] directions.

and [110].

Comparison of the distribution of the electron density between nickel atoms in the directions [111] and [110] (Fig. 4) with the distribution of the electron density of the "magnetic" electrons shows that the "magnetic" electrons make practically no appreciable contribution to the magnitude of the electron density in the middle region between nickel atoms, which apparently determines the conductivity.

Solid-State and Semiconductor Physics Division
Academy of Sciences of the BSSR

Received
8 V 1961

REFERENCES

1. R. Nathans, C. G. Shull, G. Shirane, A. Andersen, *Phys. Chem. Solids*, **10**, 138 (1959).
2. R. Nathans, A. Pooletti, *Phys. Rev. Letters*, **2**, 254 (1959).
3. N. N. Sirota, N. M. Olekhnovich, A. U. Sheleg, *DAN*, **132**, No. 1, 162 (1960).
4. G. W. Brindley, *Phil. Mag.*, **21**, 778 (1936).

Note: Figure translations are in progress. See original paper for figures.