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Hall Effect in the Ni-H System

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The Hall effect of the nickel-hydrogen system at high pressures of hydrogen at the temperature of 50 °C has been investigated. Relative values of the ordinary and extraordinary Hall coefficients as functions of the hydrogen pressure, relative electrical resistance, and the atomic ratio H/Ni up to H/Ni ~ 1.0 was observed.

I. INTRODUCTION

The Ni-H system is very similar in many respects to the well-known Pd-H system. This seems to be the result of the similarity of hybridized bands: 3*d*4*s* in the Ni and 4*d*5*s* in the Pd. Physicochemical properties and crystallographical data of Ni-H system are given in Refs. 1 and 2. Electric and magnetic properties were the subject of many experiments (electric resistivity,[3,4] saturation magnetization,[5] electron specific heat,[6] thermoelectric power,[7] and the Hall effect[8]). The authors of this article did not find any data in the literature concerning the Hall coefficient of Ni-H system as a function of the atomic ratio H/Ni.

In Schmidbauer's experiments[8] (on thermal dependence of the ordinary Hall coefficient, nonstoichiometric nickel hydride with atomic ratio H/Ni ~ 0.75 was used. In those experiments nickel foils were saturated by hydrogen by the electrochemical method. In our investigation the high-pressure method of saturation was used.

It was the aim of our experiments to observe the changes of magnitude of ordinary and extraordinary Hall coefficients in the Ni and also to observe the gradual disappearance of ferromagnetism with the increase of the atomic ratio H/Ni.

II. EXPERIMENTAL

Measurements were performed on 8-μm-thick nickel foils using the conventional dc method ($I_{max} = 1$ A, $B_{max} = 15$ kG). Values of magnetic induction in each measurement were checked by means of a ballistic galvanometer. The conventional four-probe potentiometric technique was used to measure the resistance of the foil. The temperature was kept at (50 ± 0.1) °C. The high-pressure apparatus described in Ref. 9 with the electromagnet placed inside of the pressure chamber was used.

III. RESULTS AND DISCUSSION

The Hall resistivities ρ_H as functions of magnetic induction B obtained for one of the specimens are shown in Figs. 1 and 2. The numbers of the curves signify the order of succession in the hydrogen-saturation process. Curve 1 is the curve $\rho_H(B)$ for pure nickel (before saturation). The slopes of two linear parts of the $\rho_H(B)$ curve represent the Hall coefficients: extraordinary A_1 for $B \ll I_s$, and ordi-

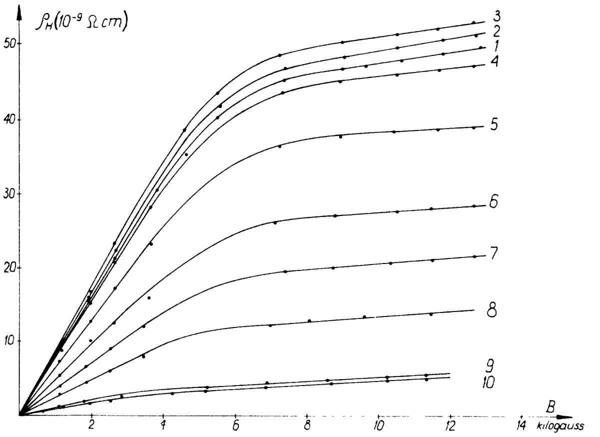

FIG. 1. Hall resistivity ρ_H vs magnetic induction B for nickel during hydrogen absorption. The curves represent the initial situation (curve 1) and process of β-phase formation.

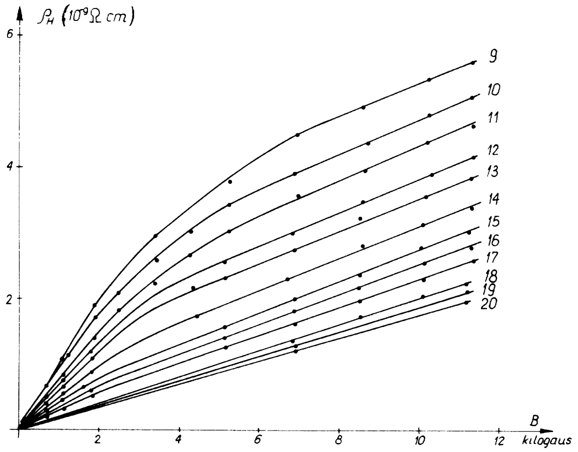

FIG. 2. Hall resistivity ρ_H vs magnetic induction B for nickel during hydrogen absorption. The curves represent the situation of α-phase diminution and disapearance of spontaneous magnetization (curve 17).

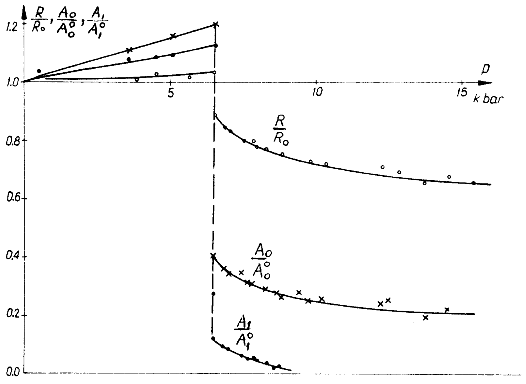

FIG. 3. Relative electrical resistance of nickel R/R_0, relative ordinary and extraordinary Hall coefficients A_0/A_0^0 and A_1/A_1^0 at 50 °C as a function of the gaseous hydrogen pressure where R, A_0, and A_1 are actual values of resistance and Hall coefficients and R_0. A_0^0 and A_1^0 are initial values of this magnitude for pure nickel.

nary A_0 for $B \gg I_s$, where I_s is a saturation of magnetization. The extraordinary Hall coefficient A_1 and the ordinary A_0 (relative values) found in this manner as functions of gaseous hydrogen pressure are shown in Fig. 3. In this figure there is also shown the relationship between relative electric resistance R/R_0 and the gaseous hydrogen pressure p, where R is the actual electric resistance of saturated specimen and R_0 is the initial value for pure nickel under pressure of 1 atm. One can see in Fig. 3 that the changes of electric resistance and Hall coefficients A_0, A_1 as functions of gaseous hydrogen pressure are similar. This suggests the existence of some simple correlation between these physical quantities.

Relative values of the Hall coefficients A_0, A_1, and A_s (the spontaneous Hall coefficient $A_s = A_1 - A_0$) as functions of the relative electric resistance are shown in Fig. 4. The bend of the curve A_1 (R/R_0), (for $R/R_0 = 0.88$ and $\text{H/Ni} \approx 0.65$) seems to be connected with the disappearance of ferromagnetism observed by Bauer and Schmidbauer[5] with the use of a ballistic method. This value of the atomic ratio H/Ni agrees with the well-known band model of nickel with 0.6 holes per atom in the $3d$ band.

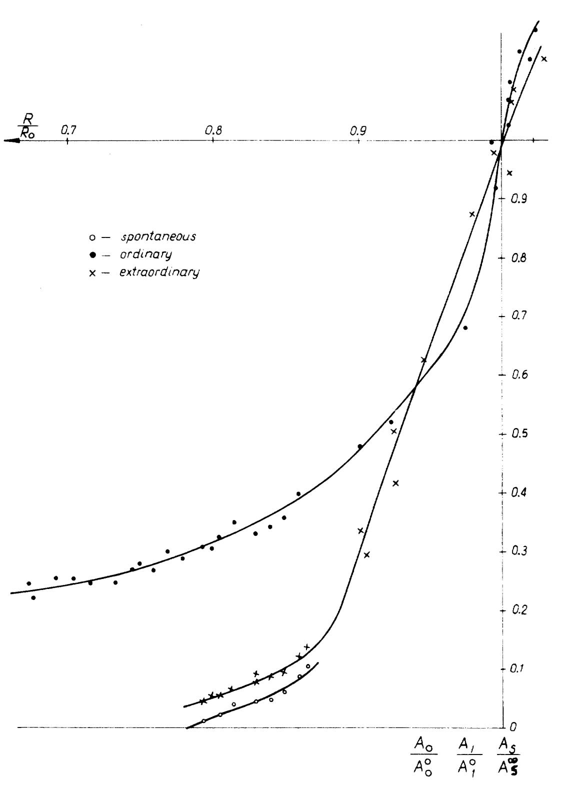

FIG. 4. Relative Hall coefficients A_0/A_0^0, A_1/A_1^0, and A_s/A_s^0 vs relative electrical resistance R/R_0 of the nickel specimens.

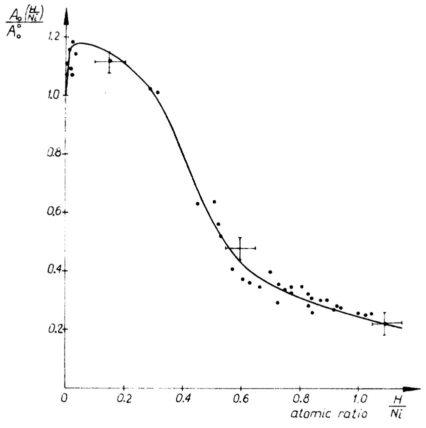

FIG. 5. Relative ordinary Hall coefficient of nickel A_0/A_0^0 vs atomic ratio H/Ni.

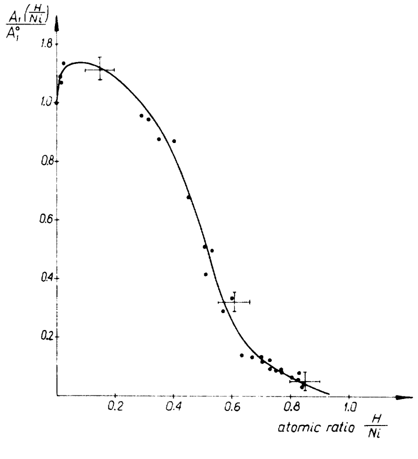

FIG. 6. Relative extraordinary Hall coefficient of nickel A_1/A_1^0 vs atomic ratio H/Ni.

However, the spontaneous Hall coefficient is different from 0 up to the point $R/R_0 = 0.78$, and H/Ni $= 0.85$. It means that in the region of the atomic ratio $0.6 < \mathrm{H/Ni} < 0.85$ weak ferromagnetism exists ($A_s > 0$). This fact corresponds to the x-ray data of Majchrzak,[10] on the basis of which the existence of the ferromagnetic α phase up to H/Ni $= 0.85$ was proven. Figures 5 and 6 show relative values of A_0 and A_1 as functions of the atomic ratios H/Ni. The atomic ratios were taken from Ref. 3. The ordinary Hall coefficient's dependence on the atomic ratio H/Ni is similar to the earlier observed dependence in the Pd-H system, but the interpretation of this situation in the present case is more complicated. In the Ni-H system the ordinary Hall coefficient rapidly decreases at the atomic ratio H/Ni ≈ 0.3, whereas this decrease is observed in the Pd-H system for H/Pd $= 0.83$.[11]

The measurements of Hall coefficients for pure Ni under high hydrostatic pressure (up to 20 kbar) using gasoline as a pressure medium have not shown changes of the ordinary Hall coefficient A_0 exceeding ± 2%; the extraordinary Hall coefficient A_1 decreases about 7%. The changes of spontaneous magnetization observed in our experiments will be discussed elsewhere.

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Plane-Wave-Gaussian Energy-Band Study of Nb

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The numerical accuracy of the plane-wave–Gaussian (PWG) mixed-basis method of calculating crystalline energy bands is displayed for Nb. Atomic studies involving the Gaussian basis and crystalline studies involving the PWG mixed basis are systematically developed to establish the dependence of the energy eigenvalues upon the number of Gaussians, the number of plane waves, and the Gaussian overlap parameter. Use of the Nb crystalline potential of Deegan and Twose allows comparison with their results.

I. INTRODUCTION

The purpose of this paper is to establish the quantitative validity of the plane-wave–Gaussian (PWG) mixed-basis set[1] for crystalline electron energy-band and wave-function calculations. To do this, the results of systematic studies are presented in order to establish the dependence of the energy eigenvalues upon the number of Gaussians, the number of plane waves, and the Gaussian overlap parameter in wave-function and potential expansions. The use of Deegan and Twose's[2] muffin-tin potential also allows comparison of PWG results with their results.

An earlier paper,[1] which introduced the PWG mixed basis, focused upon the excellent plane-wave convergence properties of this particular mixed-basis set. A future paper will present the self-consistent PWG formalism in which the crystalline PWG wave functions are used to calculate a new crystalline charge density, which, in turn, yields a new crystalline potential. This self-consistent formalism is simple, and the early computational results are very promising. How successful this particular mixed basis will be for total-energy calculations is not yet known, however.

The background of the PWG mixed-basis method is briefly as follows. Of the best-known techniques for mathematically describing crystalline electron wave functions, only the linear combination of atomic orbitals (LCAO) and the orthogonalized-plane-wave (OPW) methods are not oriented toward muffin-tin potentials. The most successful LCAO calculations[3] involve overlapping Gaussians cen-