scopic probe of the host-lattice electronic system. Experiments are now under way to study the temperature and pressure dependence of the Eu^{2+} and Gd^{3+} resonances in SmS, hopefully through the semiconductor-metal transition in order to obtain information about the nature of the metallic state.

ACKNOWLEDGMENTS

We should like to thank W. F. Brinkman for a number of stimulating conversations on this work. We should also like to thank L. D. Longinotti for assistance in preparing the samples.

[1]B. T. Matthias, R. M. Bozorth, and J. H. Van Vleck, Phys. Rev. Letters 7, 160 (1961).

[2]For a review, see S. Methfessel and D. C. Mattis, in *Handbuch der Physik*, edited by S. Flügge (Springer, New York, 1968), Vol. XVIII, p. 359.

[3]T. Kasuya, IBM J. Res. Develop. 14, 214 (1970).

[4]E. Bucher, V. Narayanamurti, and A. Jayaraman, J. Appl. Phys. 42, 1741 (1971) and references therein.

[5]Initial band-structure calculations have been performed by H. L. Davis, in Proceedings of the Ninth Rare Earth Research Conference, Blaksburg, Virginia, 1971 (unpublished).

[6]G. Güntherodt, P. Wachter, and D. M. Imbuden, Physik Kondensierten Materie 12, 292 (1971).

[7]A. Jayaraman, V. Narayanamurti, E. Bucher, and R. G. Maines, Phys. Rev. Letters 25, 1730 (1970).

[8]M. T. Hutchings and W. P. Wolf, Phys. Rev. Letters 11, 187 (1963).

[9]F. Mehran, K. W. H. Stevens, R. S. Title, and F. Holtzberg, Phys. Rev. Letters 27, 1368 (1971).

[10]M. T. Hutchings, C. G. Windsor, and W. P. Wolf, Phys. Rev. 148, 444 (1966).

[11]V. V. Tien and P. Khodadad, Bull. Soc. Chim. France 2888 (1970).

[12]A. Abragam and B. Bleaney, *Electron Paramagnetic Resonance of Transition Ions* (Clarendon, Oxford, 1970).

[13]A. Dupont, J. Opt. Soc. Am. 57, 867 (1967).

[14]W. E. Bron and W. R. Heller, Phys. Rev. 136, A1433 (1964).

[15]M. B. Maple and D. Wohlleben, Phys. Rev. Letters 27, 511 (1971).

[16]A. K. Singh, A. Jayaraman, and A. Chatterjee, Solid State Commun. 9, 1459 (1971); A. Jayaraman (private communication).

[17]T. R. McGuire, M. J. Gambino, S. J. Pickart, and H. A. Alperin, J. Appl. Phys. 40, 1009 (1969).

[18]M. Peter, J. Dupraz, and H. Cottet, Helv. Phys. Acta 40, 301 (1967).

[19]H. C. Praddoude and H. Gärtner, Phys. Letters 34A, 217 (1971).

[20]M. E. Lines and E. D. Jones, Phys. Rev. 139, A1313 (1965); 141, 525 (1966); E. D. Jones, Phys. Letters 18, 98 (1965).

[21]The more general problem is discussed in some detail by J. H. Van Vleck and N. L. Huang, in *Polarisation Matière et Rayonnement*, edited by the French Physical Society (Presses Universitaires de France, Paris, 1969), p. 507, and by N. L. Huang and J. H. Van Vleck, Solid State Commun. 6, 557 (1968). For cubic symmetry anisotropic-exchange contributions to the g shifts for an S-state ion average to zero so that the isotropic Hamiltonian Eq. (1d) is adequate. However, for the Sm host-lattice susceptibility, no such simplification occurs in the theory and instead important contributions are expected from the higher-order orbital anisotropy terms even in cubic symmetry. The close agreement between the Sm^{2+}-Sm^{2+} and the Sm^{2+}-Eu^{2+} exchange sums deduced from the isotropic-exchange theory, however, would seem to indicate that in this case the net effect of these additional terms is small.

[22]R. J. Birgeneau, M. T. Hutchings, and W. P. Wolf, Phys. Rev. 179, 275 (1969).

PHYSICAL REVIEW B VOLUME 5, NUMBER 9 1 MAY 1972

Quantum-Mechanical Treatment of the Abnormal Stopping Power for Channeling

M. Kitagawa and Y. H. Ohtsuki
Department of Physics, Waseda University, 4-Nishi-Ohkubo, Shinjuku, Tokyo, Japan
(Received 18 October 1971)

A quantum-mechanical method for the calculation of the abnormal stopping power of ion channeling is proposed. It is concluded that the abnormal stopping power is not proportional to the local electron density. Numerical calculations are performed for 3-MeV He ions in the Au crystal.

I. INTRODUCTION

The trajectory of ions channeled between crystal planes is governed by their interaction with the interatomic potentials of the atoms making up the plane, and the energy loss of channeled ions depends upon the detailed stopping power (local stopping power) it has encountered along its path. The energy-loss spectra produced in beams of energetic He and I ions transmitted through thin gold monocrystals in directions lying very nearly in low-index crystallographic planes have been reported recently.[1-3] Robinson[4] made a quantitative comparison of his anharmonic-oscillation model with the experiment of Datz *et al.*[3] and concluded that the channeling stopping power $S^{pl}(\xi)$ is rep-

resented as

$$S^{pl}(\xi) = s_1 \cosh \tfrac{1}{2} b\xi \ . \tag{1}$$

Here ξ is the position of the ions under consideration measured from the midpoint of two planes of separation $2l$ and s_1 is an arbitrary constant.

This conclusion could not be interpreted by the usual assumption that the stopping power is proportional to the local density of the atomic electrons and the ionization probability, which is represented as

$$S^{pl}(\xi) = s_1 \cosh b\xi \ . \tag{2}$$

In a previous paper,[5,6] we presented a semiclassical theory of channeling stopping power and concluded that the stopping-power function $S^{pl}(\xi)$ is written approximately as Eq. (2) at the small ξ but not at the large ξ. In this paper, by considering the detailed transition probability of ionizations, we give a quantum-mechanical treatment accounting for the transition probabilities of bound electrons in the crystal.

II. WAVE FUNCTION

We take the position of the beam as $(x_0, 0, z)$, where z is the direction of moving ions. Here we assume the wave function of the beam is a wave packet localized at $(x_0, 0)$ and moving with the velocity V in the direction z; $z = Vt$.

Thus we obtain

$$\psi_K = \frac{1}{\sqrt{L}} \varphi(x,y)\, e^{iKz} \ , \tag{3}$$

where L is the normalization constant in the direction z and $\varphi(x,y)$ is the normalized minimum wave packet described as

$$\varphi(x,y) = (2\pi \Delta x\, \Delta y)^{-1/2} \times \exp\left(- \frac{y^2}{4(\Delta y)^2} - \frac{(x-x_0)^2}{4(\Delta x)^2} + i \frac{\langle p_x \rangle x + \langle p_y \rangle y}{\hbar} \right) . \tag{4}$$

We note that the probability density $|\varphi(x,y)|^2$ may be approximated by δ functions when the wave function $\varphi(x,y)$ is well localized at $(x_0, 0)$:

$$|\varphi(x,y)|^2 = \delta(x-x_0)\, \delta(y) \ . \tag{5}$$

If we consider the matrix element of an interaction Hamiltonian H', we obtain

$$\langle f | H' | i \rangle = \frac{1}{L} \int \varphi^*(x,y)\, e^{-iKz} H'_{n0}\, e^{iK_0 z} \varphi(x,y)\, dx\, dy\, dz = \frac{1}{L} \int H'_{n0}\, e^{iqz}\, \delta(x-x_0)\, \delta(y)\, dx\, dy\, dz \ , \tag{6}$$

where H'_{n0} is the matrix element between the nth excited state and the ground state of the crystal and $q = K_0 - K$. K_0 and K are wave vectors of ion beams in the initial and the final states, respectively.

III. STOPPING POWER

When we consider the ionization energy loss, the interaction Hamiltonian H' is described as

$$H' = \sum_j \frac{Z_1 e^2}{[(x-x_j)^2 + (y-y_j)^2 + (z-z_j)^2]^{1/2}} \ , \tag{7}$$

where (x_j, y_j, z_j) is the position of the atomic electron and $Z_1 e$ is the charge of the incident ion. Inserting Eq. (7) into Eq. (6), we obtain

$$\langle f | H' | i \rangle = \frac{Z_1 e^2}{L} X_{n0} \ , \tag{8}$$

where

$$X = \sum_j \int_{-L/2}^{L/2} \frac{e^{iqz}}{[(x_0 - x_j)^2 + y_j^2 + (z-z_j)^2]^{1/2}}\, dz \ . \tag{9}$$

The energy loss per unit time is written as

$$\Delta E = - \frac{Z_1^2 e^4}{\hbar^2 VL} \int_{-\infty}^{\infty} \sum_n (E_n - E_0) |X_{n0}|^2 \delta\left(q - \frac{\omega_{n0}}{V} \right) dq \ , \tag{10}$$

where $\hbar\omega_{n0} = E_n - E_0$, the energy loss in the excitation to the nth states. Noting that Eq. (9) is rewritten for large L as

$$X = \sum_j \int_{-\infty}^{\infty} \frac{e^{iqz}}{[(x_0 - x_j)^2 + y_j^2 + (z-z_j)^2]^{1/2}}\, dz = 2 \sum_j e^{iqz_j} K_0(p_j q) \ , \tag{11}$$

where $p_j = [(x_0 - x_j)^2 + y_j^2]^{1/2}$ and $K_0(p_j q)$ is the modified Bessel function of the second kind. If we replace $\hbar\omega_{n0}$ in Eq. (10) by the average ionization energy I, we obtain

$$\sum_n (E_n - E_0) |X_{n0}|^2 \delta\left(q - \frac{\omega_{n0}}{V} \right) = \delta\left(q - \frac{I}{\hbar V} \right) \frac{i\hbar}{2} (\dot{X} X^\dagger - X^\dagger \dot{X})_{00} = \delta\left(q - \frac{I}{\hbar V} \right) \left(\frac{\hbar^2}{2m} \right) \left[\sum_j (\nabla_j X_j)(\nabla_j X_j^\dagger) \right]_{00} \ , \tag{12}$$

where

$$X_j = 2 e^{iqz_j} K_0(p_j q)$$

and m is the electron mass.

Inserting Eq. (12) into Eq. (10) and normalizing to unit flux, we have

$$\Delta E = - \frac{2 Z_1^2 e^4}{m V^2} \int q^2 [K_0^2(qp) + K_1^2(qp)]\, \rho(x,y,z)\, dx\, dy\, dz \ , \tag{13}$$

where $\rho(x,y,z)$ is the density of the atomic elec-

trons and $p = [(x_0 - x)^2 + y^2]^{1/2}$.

IV. CHANNELING STOPPING POWER FOR CONVENIENT ASSUMPTIONS

First we derive exactly the stopping power of ion beams with the impact parameter x_0 by one atom from Eq. (13):

$$\Delta E(x_0) = -\frac{2Z_1^2 e^4}{mV^2}\int_{-\infty}^{\infty} dz \int_0^{2\pi} d\theta \int_{p_{\min}}^{\infty} p\,dp \times q^2[K_0^2(qp) + K_1^2(qp)]\ \rho((z^2 + p^2 + x_0^2 - 2x_0 p\cos\theta)^{1/2}). \tag{14}$$

It is worthy to note that when the density $\rho(x, y, z)$ is constant the energy-loss function $\Delta E(x_0)$ becomes

$$\Delta E = -\frac{4\pi Z_1^2 e^4}{mV^2}\rho\left[\ln\left(\frac{2mV^2}{I}\right) - \gamma\right] dz\ , \tag{15}$$

which is the usual Bethe-Bloch formula, and γ is Euler's constant.

On the other hand, if we assume that the density function $\rho(r)$ changes slowly at small p compared with $K_0^2(qp)$ and $K_1^2(qp)$, we may put $\rho(r)$ in front of the integration. Thus we obtain

$$\Delta E(x_0) = -\frac{2Z_1^2 e^4}{mV^2}\int_{-\infty}^{\infty} dz\,\rho((z^2 + x_0^2)^{1/2}) \int_0^{2\pi} d\theta \times \int_{p_{\min}}^{\infty} p\,dp\ q^2[K_0^2(qp) + K_1^2(qp)]\ . \tag{16}$$

Since the factor $\int_{-\infty}^{\infty} dz\rho((z^2 + x_0^2)^{1/2})$ is proportional to the "string density," we may conclude that the stopping-power function is proportional to the local electron density.

It is easy to obtain[5,6] the planar-channeling stopping power $S(y_0)$ in terms of the energy-loss function $\Delta E(x_0)$ [Eq. (14)],

$$S(y_0) = -\frac{1}{\sigma}\int_{-\infty}^{\infty} \Delta E((y_0^2 + u^2)^{1/2})\,du\ , \tag{17}$$

where σ is the area of the unit mesh in the atomic plane and y_0 is the distance from the wall.

However, this assumption is not good in our case. Then we perform calculations [Eq. (14)] directly.

V. CONCLUDING REMARKS

We consider the electron-cloud distribution in the atom by Moliere[7] formula

$$\rho(r) = \frac{Z_2 b^2}{4\pi r}\,(0.35e^{-br} + 8.8e^{-4br} + 40e^{-20br})\ , \tag{18}$$

where $b = 0.3/a_{TF}$, a_{TF} is the Thomas-Fermi screening length, and Z_2 is the atomic number of the atom. Inserting Eq. (18) into Eq. (14), we may obtain the planar-channeling stopping power as

$$S^{pl}(\xi) = S(l - \xi) + S(l + \xi)\ .$$

Numerical calculations of $S^{pl}(\xi)$ are performed for 3-MeV He ions in the Au {100} channel and shown in Fig. 1 compared with the local-electron-density approximation given by Eq. (16). It is concluded that the local-electron-density approximation [Eq. (16)] is not valid at larger ξ, as expected.

At smaller ξ the local-electron-density approximation[8] is in very good agreement with our exact calculation, which means that the abnormal stopping power $S^{pl}(\xi)$ is represented by Eq. (2). However, as shown in Fig. 1, we could not distinguish the difference between expressions (1) and (2).

We could not explain the difference between the Robinson's expression and our result at large ξ. It is noted that the experiments by Datz *et al.* used by Robinson were performed for relatively low incident velocities compared with the core-electron velocities. Therefore, our perturbation theory [Eq. (10)] cannot be applied for lower-level core-electron excitations. In order to explain the Robinson's expression at large ξ, numerical calculations without perturbation theory are now in progress.

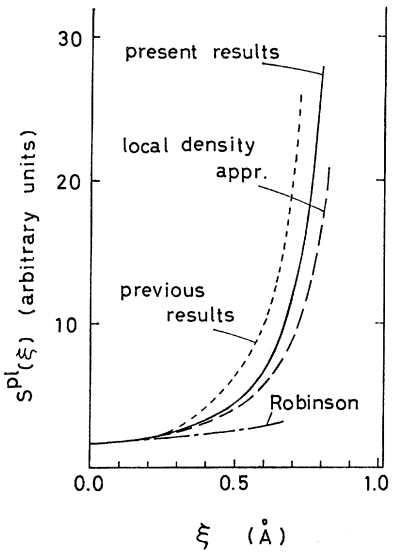

FIG. 1. Abnormal stopping power $S^{pl}(\xi)$ as a function of the distance ξ from the midpoint between the channeling planes for 3-MeV He ions in the Au {100} channel. The solid and dashed curves are our exact calculation and the local-electron-density approximation, respectively. The dotted curve is the result from the semiclassical calculation of our previous paper (Ref. 6) and the dot-and-dashed curve is Robinson's result.

[1]H. O. Lutz, S. Datz, C. D. Moak, and T. S. Noggle, Phys. Rev. Letters 17, 285 (1966).
[2]W. M. Gibson, J. B. Rasmussen, P. Ambrosius-Olesen, and C. J. Andreen, Can. J. Phys. 46, 551 (1968).
[3]S. Datz, C. D. Moak, T. S. Noggle, B. R. Appleton, and H. O. Lutz, Phys. Rev. 179, 315 (1969).
[4]M. T. Robinson, Phys. Rev. 179, 327 (1969).
[5]Y. H. Ohtsuki, Phys. Letters 34A, 104 (1971).
[6]Y. H. Ohtsuki, M. Mizuno, and M. Kitagawa, J. Phys. Soc. Japan 31, 1109 (1971).
[7]G. Moliere, Z. Naturforsch. 2a, 133 (1947).
[8]E. S. Machlin, S. Petrallia, A. Desalvo, R. Rosa, and F. Zignani, Phil. Mag. 22, 101 (1970).

PHYSICAL REVIEW B VOLUME 5, NUMBER 9 1 MAY 1972

Experimental Study of the Host NMR Linewidth and Spin-Lattice Relaxation Rate in Dilute *Cu*Fe Alloys below the Kondo Temperature*

J. E. Potts† and L. B. Welsh
Department of Physics, Northwestern University, Evanston, Illinois 60201
(Received 26 October 1971)

In order to determine the properties of single magnetic impurities in the Kondo state and the effects of these single magnetic impurities on the host-conduction-electron spin system, the Fe-impurity contributions to the Cu^{63}-host nuclear-magnetic-resonance (NMR) linewidth ΔH_i, and spin-lattice relaxation time T_{1i}, have been studied over a wide Fe-concentration range ($0 < c < 1260$ ppm) in *Cu*Fe. The NMR-linewidth measurements made from 1.65 to 77 °K and in magnetic fields from 2 to 16 kOe and in some cases up to 60 kOe, show the anomalous behavior of the slope $S = d\Delta H_i/dH$ originally observed by Heeger *et al.* and studied for a 480-ppm *Cu*Fe alloy by Golibersuch and Heeger exists over a wide Fe-concentration range. This anomalous behavior, which consists of the transition from a constant slope at low fields, S_L, to a smaller magnitude slope at high fields, S_H, occurs in a relatively narrow range of fields about some critical field H_c. This behavior clearly results from the single-impurity contribution to the NMR linewidth as evidenced by the linear concentration dependence of both S_L and S_H and also by the concentration independence of S_L/S_H. S_H has the same $(T+29)^{-1}$ temperature dependence as the bulk susceptibility, while S_L is enhanced for $H < H_c$ and $T < T_c \approx 6$ °K. At 1.65 °K, $S_H = (1.50 \pm 0.10) \times 10^{-6} c$, $S_L = (2.83 \pm 0.10) \times 10^{-6} c$ (c in ppm), and $S_L/S_H = 1.9$. These results show that the Ruderman-Kittel-Kasuya-Yosida-like oscillatory conduction-electron spin polarization existing about an impurity for $T \gg T_K$ is either enhanced for $T < T_c$ and $H < H_c$, or else an additional long-range oscillatory spin polarization is formed in the Kondo state. From the inverse concentration dependence of H_c we conclude that long-range interactions of sufficient strength exist between Fe spins via the d-d double-resonance mechanism to effectively saturate the extra oscillatory spin polarization in successively smaller applied fields as the Fe concentration increases. The impurity-induced host relaxation rate is linear in Fe concentration up to at least 300 ppm, decreasing from $T_{1i}^{-1} = 2.3 \times 10^{-3} c$ (c in ppm) for 2.65 kOe to $T_{1i}^{-1} = 2.5 \times 10^{-4} c$ for 15 kOe at 1.65 °K. The low-concentration data follow a single curve when plotted as $T(cT_{1i})^{-1}$ vs T/H ($0.1\ °\text{K/kOe} < T/H < 1.0\ °\text{K/kOe}$). Comparison of this curve with the existing high-temperature ($T \gg T_K$) theories would imply that the spin-lattice relaxation in the liquid-helium temperature range is dominated by a dipolar coupling of the nuclei to longitudinal dipolar fluctuations of the impurity spin. These results are discussed in the light of the T_{1i} data for $T > T_K$ which does not appear to be consistent with this mechanism suggesting that none of the $T \gg T_K$ relaxation mechanisms may be simply extended to the region $T < T_K$.

I. INTRODUCTION

Dilute alloys of magnetic impurities in a nonmagnetic host metal have for several years been the subject of considerable experimental and theoretical investigation.[1] The nature of the ground state or Kondo state of the magnetic impurity and the form of the correlations between the impurity d spin and nearby host-conduction-electron spins for temperatures below the Kondo temperature T_K have been of particular interest. The host nuclear magnetic resonance (NMR) has proved to be a particularly useful probe for determining the effects of the impurities upon the host-conduction-electron system, because the impurity spin induces a Ruderman-Kittel-Kasuya-Yosida (RKKY)-type spin polarization in the conduction-electron system which is sensed by the host nuclei via the contact interaction $(A\vec{I}\cdot\vec{\sigma})$. Information about the magnitude and form of the oscillatory spin polarization may then be obtained by observing the field and temperature dependence of the host NMR properties.

Several detailed investigations of the effect of