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Calculation of the residual resistivity and the low-field Hall coefficient of 3*d* and 4*sp* impurities in aluminum

N. Papanikolaou and N. Stefanou

Solid State Section, University of Athens, Panepistimioupolis, GR-15784, Zografos, Athens, Greece

C. Papastaikoudis

Institute for Materials Science, National Centre for Scientific Research "Democritos," GR-153 10 Aghia Paraskevi, Athens, Greece

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We report systematic calculations of the residual resistivity and the low-field Hall coefficient of Al-based dilute alloys with 3*d* and 4*sp* impurities, by self-consistently solving the linearized Boltzmann equation. We employ the on-Fermi-sphere approximation, which allows us to combine the full anisotropy of the aluminum Fermi surface, obtained by the four-orthogonal-plane-wave method, with the phase shifts associated with isotropic impurity scattering, evaluated by self-consistent local-density-functional impurity-in-jellium calculations. Our results show that the anisotropic scattering increases the residual resistivity, thus obtaining better agreement with the experiment. Moreover, a consistent interpretation of the observed trends of the low-field Hall coefficient is presented.

I. INTRODUCTION

The transport properties of Al-based dilute alloys have been investigated experimentally[1–12] and theoretically.[11–22] Aluminum is a trivalent simple metal with a roughly spherical Fermi surface (FS), but there are strong deviations from the spherical shape near the Brillouin-zone boundaries. A satisfactory explanation of the various transport properties such as residual resistivity, low-field Hall coefficient, magnetoresistance, etc., in the low-temperature limit where impurity scattering is the dominant effect, requires the consideration of the full anisotropy of the Al FS in the description of impurity scattering.

Nowadays, transport properties of metallic dilute alloys can be reliably calculated, using the self-consistent computational formalisms developed in recent years. The Korringa-Kohn-Rostoker (KKR) Green's-function method, for instance, allows the evaluation from first principles of the transition amplitude between two states on the FS of a metallic host, due to impurity scattering. Transport coefficients can then be determined by solving the appropriate Boltzmann equation.[13,14] This method involves heavy computation and has not been applied so far to Al-based alloys.

In the case of dilute alloys of simple metals, a weak scattering approach has been used for the calculation of transport coefficients. In this framework, the four-orthogonal-plane-wave (4-OPW) model with the relevant pseudopotential parameters fitted to experimental de Haas–van Alphen (dHvA) data[22,24] is used for the Al host. The effective potential of a point defect is described by pseudopotential form factors to first-order Born approximation.[8,17,20] This method can be used only for weak scatterers, like *sp* impurities, where the Born approximation is justified.

As a generalization of the above procedure, an effective *t* matrix is used to describe the scattering, and the transition amplitude between two states on the FS is then obtained in terms of the phase shifts utilizing the so-called "on-Fermi-sphere approximation."[25] Within this approach the phase shifts can be determined independently, by some first-principles calculation for instance.[21,22] Thus, weak *sp* as well as strong *d*-resonance scattering can be treated on the same footing.

Alternatively, Coleridge[26] used a KKR scheme with three phase shifts to fit dHvA frequencies in Al. The FS dimensions and the anisotropy of the wave functions deduced from this fit were found similar to those obtained by the 4-OPW approach.

The residual resistivity of transition-metal impurities in simple-metal hosts exhibits a well-known parabolic behavior.[27] This behavior can be predicted by simple models like the free-electron model, or the spherical-band approximation, which takes into account some band-structure effects in terms of spherical averages.[13,15] In the case of the Cu host, the spherical-band approximation yields residual resistivities in very good agreement

with the experiment and with *ab initio* calculations.[13] However, the case of 3*d* impurities in Al seems to be more complicated since the residual resistivities calculated within the jellium model or the spherical-band approximation are too small compared with the experiment.[15,16]

Systematic experimental investigations of the low-field Hall coefficient of 3*d* impurities in Al have been reported by Papastaikoudis and co-workers.[5] The experimental results showed a parabolic behavior within the 3*d* series and were analyzed using the concept of the 3*d* impurity virtual-bound state moving across the Fermi level.

In this paper we study the effect of anisotropic scattering on the residual resistivity and the low-field Hall coefficient of Al-based dilute alloys with 3*d* and 4*sp* impurities. We have used the 4-OPW model for the FS of Al together with the on-Fermi-sphere approximation and obtained the scattering phase shifts by self-consistent impurity-in-jellium calculations within the framework of the density-functional theory.[28] The linearized Boltzmann equation is then solved self-consistently to obtain the anisotropic transport relaxation time, which is used to calculate the residual resistivity and the low-field Hall coefficient.

II. METHOD OF CALCULATION

The determination of transport properties like the resistivity and the low-field Hall coefficient in dilute alloys requires the solution of the linearized Boltzmann equation in the presence of homogeneous electric **E** and magnetic **H** fields,[29]

$$e(\mathbf{v}_\mathbf{k}\cdot\mathbf{E})\frac{\partial f_\mathbf{k}^0}{\partial E_\mathbf{k}}+\frac{e}{\hbar}(\mathbf{v}_\mathbf{k}\times\mathbf{H})\cdot\nabla_\mathbf{k}g_\mathbf{k}=-\int(g_\mathbf{k}-g_{\mathbf{k}'})P_{\mathbf{k}\mathbf{k}'}d^3k', \tag{1}$$

where $g_\mathbf{k}$ is the deviation from the Fermi-Dirac distribution function $f_\mathbf{k}^0$, $\mathbf{v}_\mathbf{k}=\nabla_\mathbf{k}E_\mathbf{k}/\hbar$ is the group velocity of Bloch electrons, and $P_{\mathbf{k}\mathbf{k}'}$ is the scattering probability rate between states $|\mathbf{k}\rangle$ and $|\mathbf{k}'\rangle$. In the low-field limit and at sufficiently low temperatures, the incoherent scattering of conduction electrons from isolated impurity atoms is the dominant effect. Therefore, assuming elastic scattering we have

$$P_{\mathbf{k}\mathbf{k}'}=\frac{2\pi Nc}{\hbar}|T_{\mathbf{k}\mathbf{k}'}|^2\delta(E_\mathbf{k}-E_{\mathbf{k}'}), \tag{2}$$

where N is the total number of atoms in the crystal, c is the atomic concentration of impurities, and $T_{\mathbf{k}\mathbf{k}'}$ is the T matrix describing the scattering by a single impurity atom.

In the low-field limit, the vector mean-free path $\mathbf{\Lambda}_\mathbf{k}$ is defined by the linear ansatz,

$$g_\mathbf{k}=-e\mathbf{E}\cdot\mathbf{\Lambda}_\mathbf{k}\left[\frac{\partial f_\mathbf{k}^0}{\partial E_\mathbf{k}}\right], \tag{3}$$

and is in general not parallel to the group velocity. However, following Böning *et al.*[11] we assume

$$\mathbf{\Lambda}_\mathbf{k}=\mathbf{v}_\mathbf{k}\tau_\mathbf{k}, \tag{4}$$

where the anisotropic transport relaxation time $\tau_\mathbf{k}$ does not depend on the magnetic field. Therefore, within the above approximation, Eq. (1) can be readily solved for $\mathbf{H}=0$, yielding the following integral equation for $\tau_\mathbf{k}$:

$$\tau_\mathbf{k}v_\mathbf{k}\frac{\Omega}{8\pi^3}\int_{\mathrm{FS}}P_{\mathbf{k}\mathbf{k}'}\frac{dS_{\mathbf{k}'}}{\hbar v_{\mathbf{k}'}}=v_\mathbf{k}+\frac{\Omega}{8\pi^3}\int_{\mathrm{FS}}\tau_{\mathbf{k}'}\frac{\mathbf{v}_\mathbf{k}\cdot\mathbf{v}_{\mathbf{k}'}}{v_\mathbf{k}}P_{\mathbf{k}\mathbf{k}'}\frac{dS_{\mathbf{k}'}}{\hbar v_{\mathbf{k}'}} \tag{5}$$

for points $\mathbf{k}$ of the FS. Ω is the volume of the crystal and $v_\mathbf{k}=|\mathbf{v}_\mathbf{k}|$.

The residual resistivity ρ is given in our case by

$$\frac{1}{\rho}=\frac{e^2}{12\pi^3\hbar}\int_{\mathrm{FS}}v_\mathbf{k}\tau_\mathbf{k}dS_\mathbf{k}, \tag{6}$$

and the low-field Hall coefficient is obtained from the expression[30]

$$R_H^0=\frac{12\pi^3}{e}\frac{\int_{\mathrm{FS}}(\overline{\kappa^{-1}})v_\mathbf{k}^2\tau_\mathbf{k}^2dS_\mathbf{k}}{\left[\int_{\mathrm{FS}}v_\mathbf{k}\tau_\mathbf{k}dS_\mathbf{k}\right]^2}, \tag{7}$$

where $(\overline{\kappa^{-1}})$ is the local mean curvature at point $\mathbf{k}$ of the FS:

$$(\overline{\kappa^{-1}})=\tfrac{1}{2}[(\kappa_1^{-1})+(\kappa_2^{-1})], \tag{8}$$

with $\kappa_1^{-1},\kappa_2^{-1}$ being the local principal radii of curvature.

The Bloch functions of the Al host are calculated using the 4-OPW model,[24]

$$\Psi_\mathbf{k}(\mathbf{r})=\frac{1}{\sqrt{\Omega}}\sum_{n=1}^{4}\alpha_n(\mathbf{k})e^{i(\mathbf{k}-\mathbf{K}_n)\cdot\mathbf{r}}, \tag{9}$$

where $\mathbf{K}_n$ are the reciprocal lattice vectors: (000), (111), $(11\bar{1})$, (200) in units of $2\pi/a$, $a=4.032$ Å being the lattice constant of Al. The expansion coefficients $\alpha_n(\mathbf{k})$ are evaluated from the corresponding 4-OPW secular equation, where the Fermi energy E_F and the pseudopotential matrix elements are fitted by Cole *et al.*[22] to the dHvA experimental data of Coleridge and Holtham.[23] The 4-OPW model gives a good description of the FS and also yields accurate wave functions.[31]

We proceed further using the on-Fermi-sphere approximation, according to which the crystal-lattice pseudopotential is ignored during the scattering of the electrons by the impurity atom. In this approximation $T_{\mathbf{k}\mathbf{k}'}$ is written as[17,25]

$$T_{\mathbf{k}\mathbf{k}'}=-\frac{4\sqrt{2}\pi^2\hbar^3}{m^{3/2}E_F^{1/2}\Omega}\sum_{lm}e^{i\delta_l}\sin\delta_l c_{lm}(\mathbf{k})c_{lm}^*(\mathbf{k}'), \tag{10}$$

where δ_l are the phase shifts at E_F describing the scattering of plane waves from a single impurity potential and the coefficients $c_{lm}(\mathbf{k})$ are given by

$$c_{lm}(\mathbf{k})=\sum_{n=1}^{4}\alpha_n(\mathbf{k})Y_{lm}^*(\mathbf{k}-\mathbf{K}_n), \tag{11}$$

Y_{lm} being the spherical harmonics.[32]

We obtain the scattering phase shifts by calculating the electronic structure of a single impurity in a jellium having the electron density of Al. Within this model, a sub-

stitutional impurity is described by cutting off a spherical hole in the jellium positive background equal to the Wigner-Seitz sphere and putting a positive point charge equal to the impurity atomic number at the center of this vacancy. The electronic structure is calculated self-consistently within the framework of the density-functional theory.[28] Exchange and correlation effects are included using the local-density approximation with the parametrization of Vosko, Wilk, and Nusair.[33] A range of impurity potential $S=10$ a.u. and an angular momentum cutoff $l_{\max}=3$ are sufficient to obtain adequate convergence in all the cases examined. The calculated phase shifts satisfy the Friedel's screening rule within a few percent. Details about our method of calculation can be found elsewhere.[34]

The FS of Al consists of the second-zone hole part and a third-zone toroidlike electron surface. The second zone is in most parts spherical and only in the regions of intersecting Brillouin-zone boundaries deviates from the spherical shape. In order to perform the surface integrals in Eqs. (5)–(7) a system of triangles is generated using 1000 points on the second zone and 656 points on the third zone of the FS. Special care has been taken in the highly curved regions of the surface using a more dense mesh. The Fermi velocity at point $\mathbf{k}$ is calculated analytically from[19]

$$\mathbf{v}_{\mathbf{k}}=\frac{\hbar}{m}\sum_{n=1}^{4}|\alpha_n(\mathbf{k})|^2(\mathbf{k}-\mathbf{K}_n)\ . \tag{12}$$

Within the so-called "three-group model," the FS of Al is divided into three parts according to their curvature:[35] (i) a free-electron-like portion in the second zone (S_-) with slightly negative curvature, which covers most of the FS; (ii) holelike cylinders also in the second zone just below the Brillouin-zone boundaries (S_{++}) with high positive curvature; and (iii) electronlike cylinders in the third zone (S_{--}) with high negative curvature.

We have tested the sensitivity of our results for the residual resistivity and the low-field Hall coefficient with other 4-OPW parametrizations of the Al FS,[24] and the differences are very small. Moreover, we have calculated some FS properties like the surface area, the density of states, and the optical mass. Our results are essentially the same with those obtained by other authors.[20] The integral equation (5) is solved by an iterative procedure. Using the Ziman's approximation as an initial guess for $\tau_{\mathbf{k}}$,[29]

$$\tau_{\mathbf{k}}^{-1}=\frac{\Omega}{8\pi^3}\int_{\mathrm{FS}}P_{\mathbf{k}\mathbf{k}'}\left[1-\frac{\mathbf{v}_{\mathbf{k}}\cdot\mathbf{v}_{\mathbf{k}'}}{v_{\mathbf{k}}v_{\mathbf{k}'}}\right]\frac{dS_{\mathbf{k}'}}{\hbar v_{\mathbf{k}'}}\ , \tag{13}$$

we obtain an adequate convergence in $\tau_{\mathbf{k}}$ in ~ 5 iterations in all cases examined.

III. RESULTS AND DISCUSSION

A. Residual resistivity

The results for the residual resistivity of the $3d$ and $4sp$ impurities in Al are shown in Fig. 1. The overall agreement between theoretical and experimental results is satisfactory. We obtain an important enhancement of the residual resistivity as a result of the anisotropic scattering, thus getting much better agreement with the experiment, compared with the free-electron model:

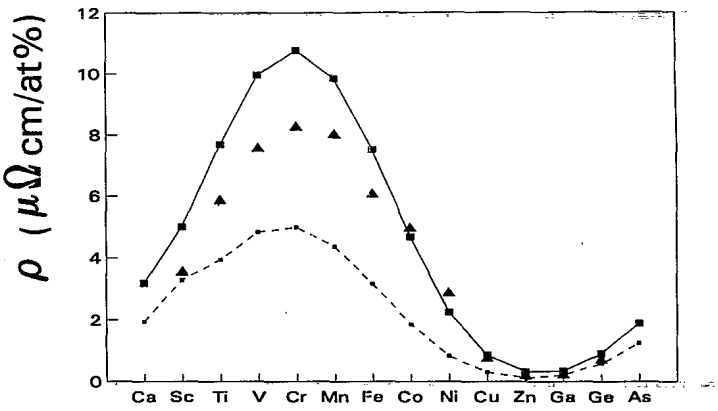

FIG. 1. The residual resistivity ρ of $3d$ and $4sp$ substitutional impurities in Al host. The squares show the theoretical results and the triangles the experimental data (Ref. 38). The broken line shows the results obtained by the jellium model [Eq. (14)].

$$\rho=\frac{4\pi\hbar^2 c}{Ze^2(2mE_F)^{1/2}}\sum_l(l+1)\sin^2(\delta_{l+1}-\delta_l)\ , \tag{14}$$

where Z is the valence of the host ($Z=3$ for Al), or the spherical-band approximation.[13,15] This anisotropy-induced enhancement was also reported by other authors, who calculated the residual resistivity of sp impurities in Al using multiple-plane-wave pseudopotential approach.[36,18] As first pointed out by Fukai,[36] the mixing of the plane waves near the Brillouin-zone boundaries causes an increase in the residual resistivity compared with a single plane-wave treatment.

The parabolic behavior of the residual resistivity within the $3d$ series is due to the d virtual-bound state [$\rho\sim\sin^2(\delta_2)$]. In the case of strong scatterers, i.e., impurities of the middle of the $3d$ series, the calculated values of ρ are larger than the experimental ones. This could be ascribed to the fact that we use the full, all-electron scattering potential for the impurity, whereas the host is described by a weak pseudopotential. This inconsistency might overestimate the impurity scattering for strong scatterers, thus leading to higher resistivity values.

Boerrigter, Lodder, and Molenaar[16] calculated the residual resistivity of $3d$ impurities in Al using several models to investigate the importance of the choice of the scattering potential in the determination of the phase shifts. Since the anisotropy of the FS was not taken into account in these calculations, the resistivities were too small and the calculated values were multiplied by a constant factor, accounting for Fermi-surface effects, to get better agreement with experiment. In the case of the late $3d$ and the $4sp$ impurities, the agreement with experiment is excellent and the residual resistivity can be described by the generalized Linde's rule[37]

$$\rho=\alpha\Delta Z^2+\beta\Delta Z+\gamma\ , \tag{15}$$

where ΔZ is the valence difference between impurity and host atoms, as shown in Fig. 2.

B. The low-field Hall coefficient

Figure 3 shows our results for the low-field Hall coefficient together with the experimental data of Papastaikoudis and co-workers,[5] for the $3d$ impurities. The overall agreement between experiment and theory is satisfactory.

Contrary to the residual resistivity, where the assumption of a spherical FS yields the correct trends and the anisotropy gives a more or less constant shift, the variation of the low-field Hall coefficient is entirely due to the anisotropy of the FS. A spherical FS yields $R_H^0 = 1/ne (\equiv R_H^{FE})$, where n is the free-electron density of the host, independently on the considered impurity ($R_H^{FE} = -3.47 \times 10^{-11}$ m^3/C for Al host). This is shown in Fig. 4, where R_H^0 is separated into three contributions by splitting the integral in the numerator of Eq. (7) in three surface integrals over S_{++}, S_{--}, S_-. The sign of each contribution to the low-field Hall coefficient is determined by the sign of the local mean curvature. It can be seen from Fig. 4 that the variation of R_H^0 comes essentially from the highly curved S_{++} and S_{--} parts of the FS, whereas S_- gives a constant contribution, roughly equal to the free-electron value R_H^{FE}.

As it can be seen from Fig. 3, the theoretical curve of R_H^0 shows almost the same dependence on the impurity atomic number as the experimental data. It exhibits a parabolic behavior in the beginning of the $3d$ series with the minimum at Ti and a subsequent monotonic increase up to Cu, at which R_H^0 becomes positive. Then R_H^0 abruptly decreases to a negative value for a Zn impurity.

It is reasonable to assume that the s and p phase shifts remain constant within the $3d$ series and the impurity is essentially screened by d electrons (see Fig. 5). Therefore,

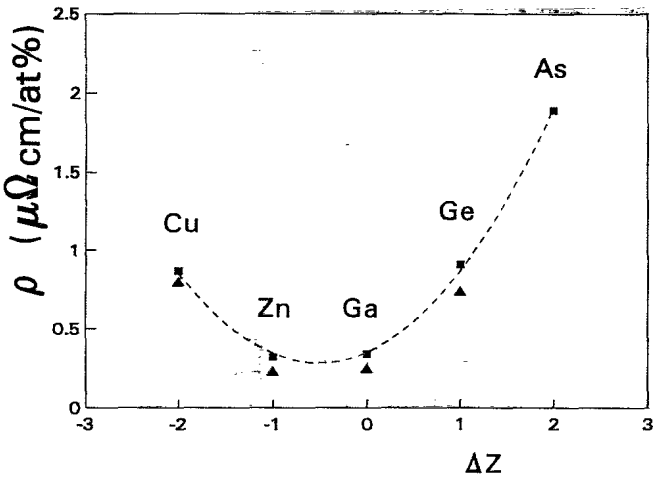

FIG. 2. The residual resistivity ρ of $4sp$ substitutional impurities in Al host vs the valence difference ΔZ. The squares show the theoretical results and the triangles the experimental data (Ref. 38). The broken line shows the interpolation based on the generalized Linde's rule: $\rho = \alpha \Delta Z^2 + \beta \Delta Z + \gamma$.

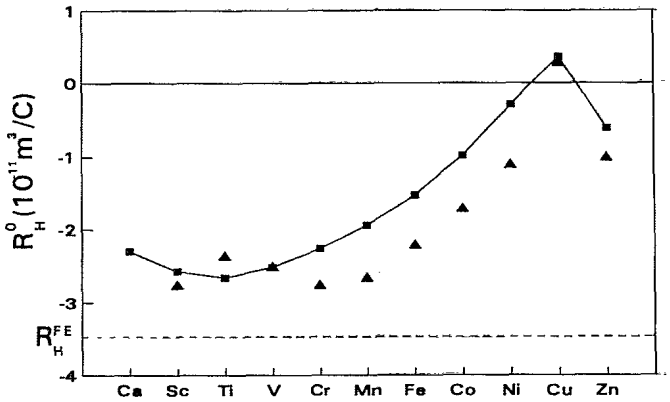

FIG. 3. The low-field Hall coefficient R_H^0 of $3d$ substitutional impurities in Al host. The squares show the theoretical results and the triangles the experimental data (Refs. 5 and 8).

and in order to isolate the effect of d scattering on the low-field Hall coefficient, we keep fixed the s and p phase shifts to a constant value (that of Cr impurity) for all the $3d$ impurities. We then calculate τ_k by solving Eq. (5) self-consistently and evaluate R_H^0 by Eq. (7). The low-field Hall coefficient calculated in this way exhibits a monotonic behavior, increasing with the impurity atomic number. Therefore, we conclude that the bending of the R_H^0 curve at the beginning and at the end of the $3d$ series is due to the anisotropic scattering of s and p electrons, whereas the monotonic increase within the series is essentially an effect of d scattering.

The behavior of R_H^0 can be discussed qualitatively in terms of the symmetry of the anisotropic parts of the FS. As reported by Pfändner, Böning, and Brenig,[19] the second zone S_{++} region has pd character while the S_{--} region in the third zone exhibits more sd admixture. Therefore, s scattering, for instance, is weak in the S_{++} anisotropic region. This means a long relaxation time in the parts of the FS with highly positive curvature, resulting in a positive contribution to R_H^0 [see Eq. (7)]. Follow-

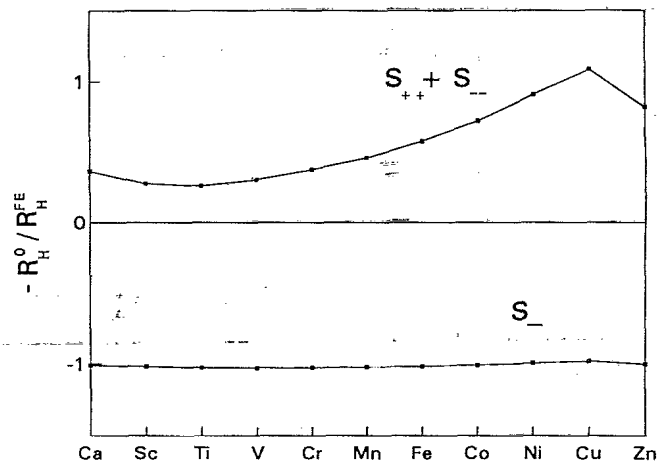

FIG. 4. Contributions of the different parts of the Al FS to the low-field Hall coefficient R_H^0 of $3d$ impurities, normalized to the free-electron value: $R_H^{FE} = -3.47 \times 10^{-11}$ m^3/C.

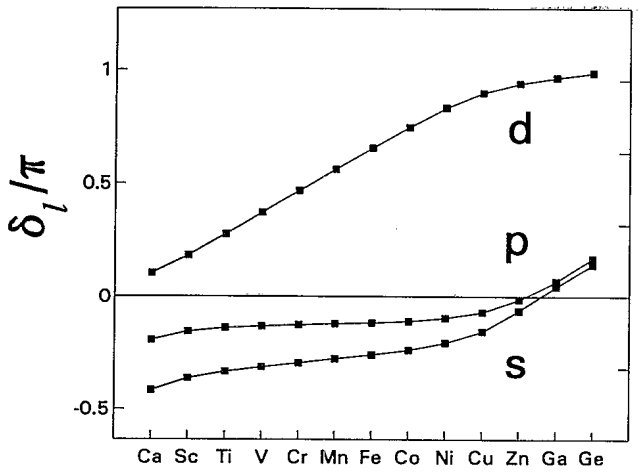

FIG. 5. Scattering phase shifts δ_l of $3d$ and $4sp$ substitutional impurities in Al-jellium.

ing similar arguments for a p scatterer, we can say, as a rule of thumb, that s scatterers give positive contributions to the low-field Hall coefficient while p scatterers give negative contributions. In the case of d scattering both S_{++} and S_{--} regions are involved. As it turns out from our calculations, the positive contribution dominates in this case.

While R_H^0 slowly increases within the $3d$ series, the case of the $4sp$ impurities seems to be more complicated. For a Zn impurity, we find a decrease in R_H^0 when compared with the continuous increase observed in the $3d$ series. This decrease is also observed by the experiment (see Fig. 3). However, for the next $4sp$ impurities Ga and Ge, we obtain negative values, far below R_H^{FE}, while the experiment reports positive values.[8,39] As it turns out from our calculations, R_H^0 is extremely sensitive to the choice of the phase shifts in the case of sp dominant scattering, in contrast to the $3d$ impurities, where it is quite insensitive to the phase shifts (see Figs. 3 and 5). This is demonstrated in Table I, where two different phase-shift parametrizations are used to calculate R_H^0 of AlGe. Using the impurity-in-jellium phase shifts we obtain a strongly negative low-field Hall coefficient ($=-8.57\times10^{-11}$ m^3/C), whereas the phase shifts obtained from Heine-Abarenkov-Animalu form factors in the Born approximation[17] give a high positive value of R_H^0 ($=5.78\times10^{-11}$ m^3/C). Thus, in order to obtain reliable R_H^0 values when sp scattering is dominant, it is essential to determine very accurately the distribution of the screening charge between s and p. Therefore, experimental measurement of the low-field Hall coefficient constitutes a very sensitive probe to check the accuracy in theoretical calculations of scattering properties of sp impurities in Al.

TABLE I. The low-field Hall coefficient (in 10^{-11} m^3/C) of AlGe, calculated according to different phase-shift parametrizations [A, impurity-in-jellium phase shifts; B, phase shifts obtained from Heine-Abarenkov-Animalu form factors in the Born approximation (Ref. 17)], together with the experimental result (Ref. 8).

	δ_s	δ_p	δ_d	δ_f	R_H^0
A	0.439	0.531	−0.043	−0.017	−8.6
B	0.622	0.223	0	−0.008	5.8
Experiment					1.8

IV. CONCLUSION

We have calculated the residual resistivity and the low-field Hall coefficient of Al-based dilute alloys with $3d$ and $4sp$ impurities by self-consistently solving the linearized Boltzmann equation. The FS of the Al host is calculated by the 4-OPW model while the impurity scattering enters through the phase shifts obtained from a self-consistent impurity-in-jellium calculation. Combining the anisotropy of the FS and the phase shifts within the on-Fermi-sphere approximation, we gain physical insight on the effect that the anisotropic impurity scattering has to the residual resistivity and the low-field Hall coefficient of Al-based dilute alloys. Our calculations indicate that the consideration of the anisotropic Al FS gives higher values for the residual resistivity, and thus, we obtain a better agreement with the experimental data. Moreover, the overall agreement between the calculated low-field Hall coefficient of the $3d$ impurities in Al and the experimental data is satisfactory, although the theoretical values are somewhat higher than the experimental ones.

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