Optical transitions connecting the spin-orbit split multiplets $\Gamma_{25}^{+} \rightarrow \Gamma_{15}^{-}$ would be expected to fall in the vicinity of 3 eV. Indeed, weak structure has been reported[7,8] in this region which could be interpreted with the assumption of a spin-orbit splitting of the Γ_{15}^{-} state of $\Delta(\Gamma_{15}^{-}) \sim 0.13$ eV. Unfortunately, the optical analysis and assignments are seriously hampered by, first, the weakness of the structure, so that the line shapes are obscured, and second, by uncertainty as to whether or not the observed transitions actually occur at the Γ point. It is hoped that the present measurement of $\Delta(\Gamma_{15}^{-})$ may assist in the future interpretation of the optical work.

Finally, we offer a speculative remark on situations where the q term would be expected to be greatly enhanced by larger spin-orbit interactions, one notable case being InSb. Here, if we assume that $\Delta(\Gamma_{15}) \sim 0.5$ eV,[6] we would estimate that $q \sim 0.2$ which might be observable in magneto-optical experiments.

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[10]In the subsequent discussion it is valid to replace $\vec{\pi} = \vec{p} + (\hbar/4mc^2)\vec{\sigma} \times \nabla V$ by $\vec{p}$. The error in q due to this approximation is estimated to be of the order of 0.001 or less.

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[13]As usual in this evaluation, the energy of the lower state Γ_{25}^{+} in the definition in Eq. (4) is taken to lie at the valence band edge which is, strictly speaking, the Γ_{8}^{+} state.

[14]J. C. Hensel and K. Suzuki, to be published. As a result of refinements in analysis, the values of the cyclotron resonance parameters previously quoted in Ref. 1 have been slightly revised: $\gamma_1 = 13.38 \pm 0.02$, $\gamma_2 = 4.24 \pm 0.02$, and $\gamma_3 = 5.69 \pm 0.02$.

NONLOCAL MODEL POTENTIAL AND LATTICE VIBRATIONS IN Li †

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Using the nonlocal and energy-dependent Heine-Abarenkov model potential we calculated the phonon spectrum of Li. A good agreement with the experimental values is obtained. We have also considered the importance of the l dependence of the model potential.

In a previous paper[1] a "first principles" calculation for the phonon frequencies of alkali metals was performed by using the Heine-Abarenkov model potential[2] (HA). The results were satisfactory, but, for Li, the discrepancies between the calculated and the experimental phonon spectrum[3] were up to 30%. However even in this case, the calculations reproduced the essential

feature of the experimental phonon frequencies, i.e., the crossing over of the transverse and longitudinal branch in the (100) direction.

Our aim is to show that the HA model potential gives, in fact, a better agreement with experiments once one avoids the local approximation used in Ref. 1 in building up the form factor from the HA model potential.

For our calculations we shall use the original HA model potential[2]

$$V_{\mathrm{HA}}(r)=\sum_l P_l A_l(E)\theta(r-R_M)+(Z/r)\theta(R_M-r),$$

where the symbols have the same meaning as in Ref. 2, and the "optimized HA model potential" recently introduced by Shaw.[4]

The form factor $V(\vec{q},\vec{k},\vec{k}',E(\vec{k}))$ is in general a function of the initial electron momentum and energy $\vec{k}$ and $E(\vec{k})$, the final momentum $\vec{k}'$, and the momentum transfer $\vec{q}$. In Ref. 1 the energy was taken equal to the Fermi energy E_{F}, the $\vec{k},\vec{k}'$ dependence was fixed by assuming scattering on the Fermi surface for $|\vec{q}|\leq|2\vec{K}_{\mathrm{F}}|$ and backward scattering with $|\vec{k}'|=|\vec{q}|-\vec{K}_{\mathrm{F}}|$ for $q>2K_{\mathrm{F}}$. Our results will show that the use of the energy-dependent and nonlocal form factor can sensitively modify the phonon frequencies and improve agreement with experiment.

In a second-order perturbation scheme, upon the use of a nonlocal and energy-dependent pseudopotential, the energy wave-number characteristic[4] takes the form[5,6]

$$\varphi(q)=\frac{2\Omega q^2}{(2\pi)^3(1+\alpha)^2}\,\frac{2\Omega}{4\pi(Ze)^2}\left[S\left(|V(\vec{q},\vec{k},\vec{k}',E(\vec{k}))|^2\right)+\frac{16\pi e^2}{q^2\epsilon(q)}S^2\left(V(\vec{q},\vec{k},\vec{k}',E(\vec{k}))\right)[1-f(q)]\right],$$

where

$$S(f(\vec{k},\vec{k}'))\equiv\mu^{(k)}(1+\alpha)\int_{\mathrm{B.Z.}}\frac{d^3k\,f(k,k')}{k^2-k'^2}.$$

$\mu(k)$ is the effective mass related to the k dependence of the pseudopotential[7] and α the orthogonalization hole.[7] Ω is the atomic volume, $\epsilon(q)$ is the dielectric function as in Ref. 2, and $f(q)$ represents the exchange correction term.[8]

The energy wave-number characteristic obtained with the HA model potential is exhibited in Fig. 1. The comparison with the energy wave-number characteristic of the local approximation (1) shows that the nonlocal effects in the pseudopotential are not negligible. The phonon frequencies calculated with the HA and Shaw potentials are drawn in Fig. 2.

The best agreement is obtained using the HA model potential and we can give reasons for the discrepancies obtained with Shaw's potential. We recall that in Shaw's procedure for lithium, only the $l=0$ component of the core potential is replaced by $A_l(E)$. But a semiclassical argument shows that this is not sufficient. The distance of closest approach to the ion of an electron is $l(l+1)/k^2=R^2$, and assuming that $k=k_{\mathrm{F}}$ and $R=R_M$, we have that for simple metals $k_{\mathrm{F}}R_M\sim 1$. Then for $l\geq 2$ $l(l+1)/k_{\mathrm{F}}^2>R_M$ is well satisfied

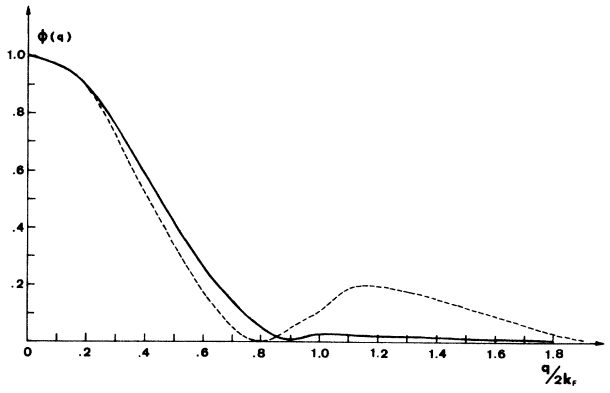

FIG. 1. Solid line, energy wave-number characteristic obtained with the nonlocal HA model potential. Dashed line, energy wave-number characteristic of the local approximation of Ref. 1.

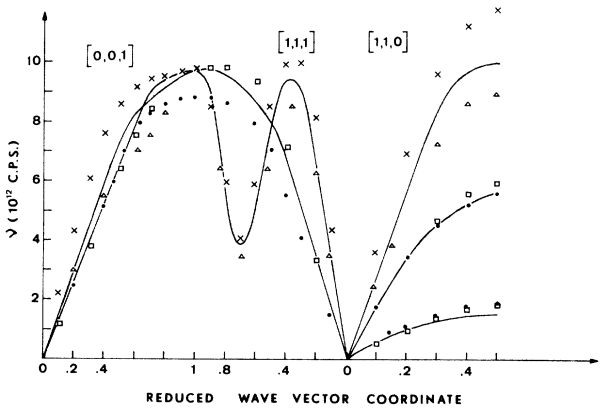

FIG. 2. Solid line, phonon frequency calculated with $\varphi(q)$ of formula (1). Open squares, experimental phonon frequencies (Ref. 3); dots, longitudinal and open triangles, transverse branches. Crosses, phonon frequency calculated with the Shaw's $\varphi(q)$.

and therefore the form of the potential is not expected to be important. Conversely for $l=1$ the wave function around R_M is not negligible and the l dependence of the potential must be taken into account. Now assuming, as Shaw did, a Coulomb potential for $l \geq 1$ and using the $l=0$ component of the HA model potential the importance of the $l=1$ component is evident, since the energy wave-number characteristic obtained is nearly coincident with the one calculated by Shaw. In the calculation of the form factor for $l \geq 1$, the core potential was further approximated by Z/R_M inside R_M because for $l \geq 1$ the pseudowave functions are sensibly different from zero only around R_M.

We performed the same calculations by taking the HA model potential up to $l=2$ and up to $l=3$, but the results did not change significantly from the ones obtained with the usual HA model potential. We then conclude that it is important only to model the $l=0$ and $l=1$ component of the potential.

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DECREASE OF MAGNETIZATION OF ITINERANT ELECTRONS BY SPIN-ORBIT SCATTERING ON IMPURITIES*

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The exchange-enhanced magnetic susceptibility of Sc and Ni_3Ga decreases strongly when small amounts of nonmagnetic impurities are added. The decrease is a linear function of the spectroscopic spin-orbit energy of the impurity at constant valency and has the same origin as the decrease of the Curie temperature of Ni in dilute Ni:Pd and Ni:Pt.

The effect of spin-orbit scattering on a system of conduction-electron spins is to reduce any spin polarization induced by an external field or electron-electron interactions. In nontransition metals, the spin susceptibility remains essentially unaffected by spin-orbit scattering even in the heaviest metals.[1] However, in some transition metals the effective mass of the d electrons is so large that their kinetic energy with respect to the lattice decreases to a few tenths of an electron volt, the order of magnitude of the spin-orbit energy in the atomic $4d$ and $5d$ shells, which therefore should bring about measurable effects.

We note that the static magnetic susceptibility decreases monotonically from the $3d$ to the $5d$ elements without exception (at constant valency) and that there are no ordered magnetic states in the $4d$ and $5d$ series. These trends are usually credited to an increase of the bandwidth in the heavier transition metals, but are certainly in part caused by spin-orbit scattering.[2] Several authors have included the spin-orbit energy in their band-structure calculations.[3] Especially interesting is the influence of spin-orbit interactions on magnetic order in metals. Lenglart[3] has recently studied the stability of the paramagnetic state of Pd with special attention to the intrinsic spin-orbit scattering. It is also noteworthy that the Curie temperature of weak itinerant ferromagnets like Sc_3In, Au_4V, Ni_3Al, and $ZrZn_2$ decreases very rapidly with increasing disorder of the lattice. One might ascribe this to spin-orbit scattering because the effective scattering cross section per ion should increase when the translational symmetry of the lattice breaks down.

In this Letter, we present data which we believe to be the first unambiguous manifestation of conduction-electron spin-orbit scattering by impurities. We have measured the static susceptibility of dilute alloys of Sc with the tetravalent elements Ti, Zr, Hf, and Th and with the pentavalent elements V, Nb, and Ta. We have also