spin-lattice relaxation rate was found to be ten times faster than predicted. This enhancement might be associated with the strong electron-electron interactions in this metal. This conclusion, however, is quite tentative since electric-quadrupole and paramagnetic-impurity processes may also contribute significantly. The impurity mechanism may be important despite the high purity of our samples, because of the long range of indirect spin couplings in palladium. It is hoped that nuclear resonance studies in the Rh-Pd and Pd-Ag alloy systems, presently in progress, will make it possible to interpret the spin-lattice relaxation rates in pure palladium with greater certainty.

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Absorption of Light Due to Interband Transitions in Sodium*

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The intrinsic absorbing power due to interband transitions in Na is calculated, using orthogonalized plane waves to evaluate the matrix elements appearing in the oscillator strengths, and a realistic band structure, obtained from a pseudopotential interpolation scheme, to perform the sum over k space. It is found that for a pseudopotential form factor V_{110} in reasonable agreement with the results of Fermi-surface measurements and band calculations, the calculated absorbing power is an order of magnitude smaller than that indicated by the experimental data of Mayer and co-workers, or by the data of Ives and Briggs.

INTRODUCTION

RECENT experiments by Mayer and co-workers[1] on the optical spectra of the alkali metals from the near infrared to the near ultraviolet, performed under conditions of high surface purity and in high vacuum, have demonstrated the existence of resonance behavior in the absorptivity at energies below the band-theoretically predicted onset of interband absorption. In K and Cs this resonance is sufficiently large and broad to mask completely the interband threshold. On the other hand, in Na one can clearly distinguish the Drude absorption in the infrared region, the resonance near 1.7 eV, and the interband absorption region beginning near the value 2.0 eV, predicted by theory. At low temperature, −183°C, the resonance disappears, and only the Drude and interband contributions to the absorptivity are present in Na. The origin of the resonance is as yet poorly understood, and for this reason it was felt that any comparison of the band-theoretically calculated absorptivity with experiment was most likely to succeed for a metal where this resonance was weakest. For this reason we will concentrate on Na throughout the remainder of this paper.

Butcher[2] has calculated the absorptivity of the alkali metals using the one-electron approximation and a nearly free-electron band model. In his calculation he leaves as an adjustable parameter the pseudopotential form factor V_{110}, [$V_{110}=V(\mathbf{G})$, $\mathbf{G}=(1,1,0)2\pi/a$, where a is the lattice constant], which he uses to fit the experimental results of Ives and Briggs.[3] Fitting the Ives-Briggs data for Na he obtained $V_{110}=0.323$ eV; when Butcher's results are fitted to Mayer's data for Na one obtains $V_{110}=0.457$ eV. This value for V_{110} is in marked disagreement with those inferred from the band calculations of Ham and others[4] and from Fermi-surface data.[5]

Examining Butcher's work one comes to the conclusion that within the one-electron approximation there are a number of deficiencies in Butcher's band model which might account for the discrepancy.

Primary among these is Butcher's use of plane waves to calculate the oscillator strengths. While it is known that Na is an excellent "nearly free-electron" metal to the extent that its Fermi surface is nearly spherical, it is by no means true that its one-electron wave functions are plane waves. A serious deficiency in the choice of plane waves is their lack of orthogonalization to the core states. As Herring[6] has shown, the use of orthogo-

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† NASA Predoctoral Fellow.

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nalized plane waves (O.P.W.) assures that the wave functions used will be orthogonal to the core states. The use of O.P.W. functions changes qualitatively the structure of the oscillator strengths. Before the addition of the core terms the wave function had not only the required translation symmetry under the crystal space group, but complete symmetry under infinitesimal translations. This added symmetry leads to the stringent requirement that only plane waves with the same k vectors will give nonvanishing contributions to the oscillator strengths. With the addition of the core terms the wave functions no longer have infinitesimal translation symmetry, and the matrix element in the oscillator strength will be nonzero for wave functions with k vectors differing by a reciprocal lattice vector.

In light of the above analysis it was decided to redo Butcher's calculation using orthogonalized plane waves instead of plane waves, and to refine further the calculation by using a band structure as given by a pseudopotential calculation, using six plane waves and two adjustable parameters, V_{110} and V_{200}, which could be chosen to yield bands in agreement with those calculated by Ham, rather than a free-electron energy spectrum, as assumed by Butcher.

In Sec. I, an expression will be derived for the matrix element entering the oscillator strength using O.P.W. In Sec. II, we discuss the computational technique used for evaluating the absorbing power, and the procedures used to ensure its accuracy. Section III contains the results of our calculation and a discussion of these results.

I. THEORY

The intrinsic absorbing power of a homogeneous isotropic medium $\sigma(\omega)$ is defined by $\langle R\rangle_{\mathrm{av}}=\sigma(\omega)\langle\mathbf{E}^2\rangle_{\mathrm{av}}$, where $\langle R\rangle_{\mathrm{av}}$ is the mean rate of absorption of electromagnetic energy per unit volume and $\mathbf{E}$ is the incident electric field. The absorbing power is given by

$$\sigma(\omega)=\frac{h}{\omega}\left(\frac{2e}{\pi m}\right)^2\int\frac{|\langle 2\mathbf{k}|\nabla_r|1\mathbf{k}\rangle|^2}{|\nabla_{\mathbf{k}}\Omega_{21}(\mathbf{k})|}dS_{21}, \qquad (1)$$

where $|1\mathbf{k}\rangle$ and $|2\mathbf{k}\rangle$ are the wave functions of the conduction band, denoted by 1, and the next highest state, denoted by 2, respectively. $\hbar\Omega_{21}(\mathbf{k})$ is the energy difference between bands 2 and 1, while dS_{21} is the surface element on the surface $\Omega_{21}(\mathbf{k})=\omega$, where ω is the frequency of the incident photon. The surface integral need be performed over only 1/48 of the surface $\Omega_{21}(\mathbf{k})=\omega$, for reasons of symmetry. All other symbols have their usual meaning. Now

$$\Psi_{1\mathbf{k}}=\textstyle\sum_{\mathbf{G}} a_{\mathbf{k}-\mathbf{G}}^{(1)}\chi_{\mathbf{k}-\mathbf{G}} \qquad (2a)$$

$$\Psi_{2\mathbf{k}}=\textstyle\sum_{\mathbf{G}} a_{\mathbf{k}-\mathbf{G}}^{(2)}\chi_{\mathbf{k}-\mathbf{G}}, \qquad (2b)$$

where $a_{\mathbf{k}-\mathbf{G}}^{(i)}$, satisfying

$$\textstyle\sum_{\mathbf{G}} a_{\mathbf{k}-\mathbf{G}}^{(i)}a_{\mathbf{k}-\mathbf{G}}^{(j)}=\delta_{ij} \qquad (3)$$

are obtained from the pseudopotential calculation. In the sum over $\mathbf{G}$, as in all such future sums, $\mathbf{G}$ ranges over the six reciprocal lattice vectors (0,0,0), (1,1,0), (1,0,1), (0,1,1), $(1,\bar{1},0)$, and $(1,0,\bar{1})$. We have set $2\pi/a$, where a is the lattice constant, equal to 1. The $\chi_{\mathbf{k}}$ are O.P.W., given by

$$\chi_{\mathbf{k}}=\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(N\Omega_0)^{1/2}}-\frac{1}{N^{1/2}}\sum_{nlm}\sum_{\nu} e^{i\mathbf{k}\cdot\mathbf{R}_\nu}u_{nlm}(\mathbf{r}-\mathbf{R}_\nu)B_{nlm;\mathbf{k}}. \qquad (4)$$

Ω_0 is the atomic volume, equal to $4\pi^3$ in our units; N is the number of atoms; $u_{nlm}(\mathbf{r}-\mathbf{R}_\nu)$ is the atomic wave function, with the usual quantum number n,l,m, measured from a lattice site $\mathbf{R}_\nu$.[7] The $B_{nlm;\mathbf{k}}$, chosen so that $\chi_{\mathbf{k}}$ are orthogonal to the core states (which we have assumed are represented by tight-binding wave functions), are given by

$$B_{nlm;\mathbf{k}}=i^l f_{nl}(k)Y_{lm}^*(\theta_k,\varphi_k); \qquad (5)$$

$$f_{nl}(k)=\frac{4\pi}{\Omega_0^{1/2}}\int u_{nl}(r)j_l(kr)r^2dr, \qquad (6)$$

where Y_{lm} are the usual spherical harmonics and $j_l(kr)$ are spherical Bessel functions of order l.

The $\chi_{\mathbf{k}}$ have a norm given by

$$(\chi_{\mathbf{k}}|\chi_{\mathbf{k}})=1-\sum_{nl}\frac{2l+1}{4\pi}f_{nl}^2(k).$$

A straightforward although somewhat tedious calculation gives

$$\langle\psi_{1\mathbf{k}}|\nabla|\psi_{2\mathbf{k}}\rangle=\textstyle\sum_G\sum_{G'} a_{\mathbf{k}-\mathbf{G}}^{(1)}a_{\mathbf{k}-\mathbf{G}'}^{(2)} \times\langle\chi_{\mathbf{k}-\mathbf{G}}|\nabla|\chi_{\mathbf{k}-\mathbf{G}'}\rangle, \qquad (7)$$

$$\begin{aligned}\langle\chi_{\mathbf{k}'}|\nabla|\chi_{\mathbf{k}}\rangle={}&-i[-\tfrac{1}{2}k\delta_{\mathbf{k},\mathbf{k}'}+B(\mathbf{k},\mathbf{k}')+A(\mathbf{k},\mathbf{k}')]\hat{k}'\\&-i[-\tfrac{1}{2}k\delta_{\mathbf{k},\mathbf{k}'}+B(\mathbf{k}',\mathbf{k})+A(\mathbf{k}',\mathbf{k})]\hat{k}, \qquad (8)\end{aligned}$$

where, specializing to the case of Na,

$$\begin{aligned}A(\mathbf{k},\mathbf{k}')={}&(k/4\pi)[f_{10}(k)f_{10}(k')+f_{20}(k)f_{20}(k')\\&+3f_{21}(k)f_{21}(k')\cos\gamma_{\mathbf{k}\mathbf{k}'}], \qquad (9)\end{aligned}$$

$$B(\mathbf{k},\mathbf{k}')=(1/4\pi)[af_{10}(k')+bf_{20}(k')]f_{21}(k) \qquad (10)$$

and

$$a=\int_0^\infty u_{21}(r)\frac{\partial}{\partial r}u_{10}(r)r^2\,dr,$$

$$b=\int_0^\infty u_{21}(r)\frac{\partial}{\partial r}u_{20}(r)r^2\,dr, \qquad (11)$$

$$\cos\gamma_{\mathbf{k}\mathbf{k}'}=\hat{k}\cdot\hat{k}'.$$

We have used $\hat{k}$ to denote $\mathbf{k}/|\mathbf{k}|$.

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[7] The radial part of $u_{nlm}(r)$, $u_{nl}(r)$, was represented in the form $\Sigma_i A_i r^{n_i}e^{-\lambda_i r}$, where A_i, n_i, and λ_i were chosen to obtain a good fit to the numerically tabulated $u_{nl}(r)$ given by F. Herman and S. Skillman [*Atomic Structure Calculations* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963)].

It should be noted that (1) is derived on the assumption that $\Psi_{1\mathbf{k}}$ and $\Psi_{2\mathbf{k}}$ are orthgonal and normalized to unity. The norm of $\chi_{\mathbf{k}}$ is a slowly varying function of $\mathbf{k}$ and was assumed constant and equal to its value at $k=0.62$, which is 0.932. The norm of $\Psi_{1\mathbf{k}}$, assuming $\chi_{\mathbf{k}}$ are normalized to unity, is approximately 1.1 while that of $\Psi_{2\mathbf{k}}$ is approximately 0.9, also assumed independent of k. The product of the norms of $\Psi_{1\mathbf{k}}$ and $\Psi_{2\mathbf{k}}$ is very close to one. We have therefore taken care of the normalization requirements of the $\Psi_{1\mathbf{k}}$ and $\Psi_{2\mathbf{k}}$ by dividing the norm of $\chi_{\mathbf{k}}$ before inserting $|\langle\Psi_{1\mathbf{k}}|\nabla|\Psi_{2\mathbf{k}}\rangle|^2$ into (1). $\Psi_{1\mathbf{k}}$ and $\Psi_{2\mathbf{k}}$ are not strictly orthogonal, with

$$(\Psi_1|\Psi_2)\approx 0.01\,.$$

This was felt to be sufficiently small compared to the core orthogonality terms themselves (≈ 0.1) not to introduce significant errors in the calculation. [This lack of orthogonality reflects the nonlocal character of the pseudopotential, which is neglected here.]

II. NUMERICAL PROCEDURES

The integral in (1) was evaluated by numerical techniques on an I.B.M. 7094 electronic computer. Because of cubic symmetry it is possible to restrict the integral to only that part of the surface $\Omega_{21}(\mathbf{k})=\omega$ contained in the wedge-shaped region shown in Fig. 1. This restriction is already reflected in (1). The procedure for performing the integral over a surface of constant $\Omega_{21}(\mathbf{k})=\omega$ was the following: A spherical net of 5000 points between $k=0.62$ and $k=0.5$ for $\Omega_{21}(\mathbf{k})$ was defined within the wedge. It was then simple for the machine to perform the integral over surfaces of constant $\Omega_{21}(\mathbf{k})=\omega$. Because a fixed net was used, the points on the planes bounded by Λ and Σ and Σ and Δ were weighted by a symmetry factor $\frac{1}{2}$, since each point on these planes also occurs on an adjacent wedge.[8] The accuracy of the program for doing the above integration was tested by assuming that $\Omega_{21}(\mathbf{k})$ and $|\langle\Psi_{1\mathbf{k}}|\nabla|\Psi_{2\mathbf{k}}\rangle|^2$ were in closed forms as given by Butcher.[2] When this was done it was found that the machine-calculated $\sigma(\omega)$ agreed with the $\sigma(\omega)$ obtained from Butcher's analytic solution within a few percent.

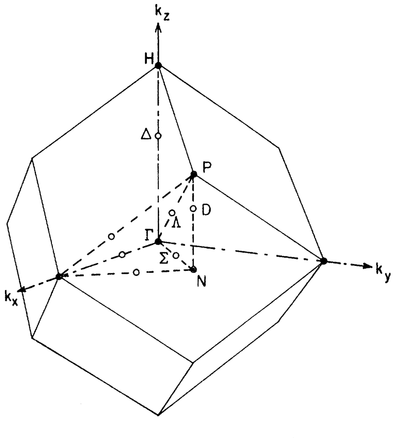

FIG. 1. The Brillouin zone of sodium showing the wedge-shaped region within which Eq. (1) was evaluated.

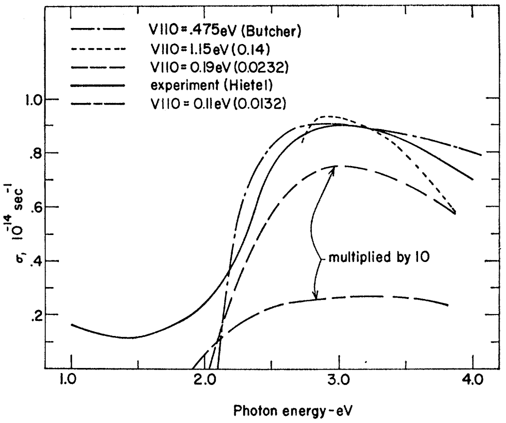

FIG. 2. The absorbing power σ is plotted against incident photon energy. The experimentally observed σ is compared with that determined by Butcher (Ref. 2) and the author for various values of V_{110}. Note carefully that σ for $V_{110}=0.11$ eV, $V_{110}=0.190$ eV have been multiplied by 10.0.

To test that the correct $f_{nl}(k)$ were being used, those given by Woodruff[9] for Si were scaled down by using the general result that

$$f_{nl}\propto(\Omega_{\text{core}}/\Omega_0)^{1/2}\,,\qquad(12)$$

where Ω_{core} is the volume occupied by the core states. The f_{nl} scaled properly within the approximation.

III. RESULTS AND DISCUSSION

We have calculated $\sigma(\omega)$ for $V_{110}=0.0132$, $V_{200}=0.066$; $V_{110}=0.0232$, $V_{200}=0.066$; and $V_{110}=0.140$, $V_{200}=0.066$, in units where $\hbar^2/2m=1$ and $2\pi/a=1$. In these units 1 eV$=0.122$. The results of these calculations are shown in Fig. 2. Our first choices for V_{110} and V_{200}, 0.0132 and 0.66, respectively, were governed by the requirement that the bands calculated from our pseudopotential interpolation scheme should agree with the bands given by Ham[4] along symmetry directions for the region of the Brillouin zone (B.Z.) $0.5\leq k\leq 0.62$. Outside this region $\hbar\Omega_{21}(k)>4.0$ eV, and since we were interested in calculating $\sigma(\omega)$ between 2.0 and 4.0 eV, there was no need to insist that our bands agree throughout the zone. In general, the pseudopotential form factors are energy- and momentum-dependent; it is only because we restrict $\mathbf{k}$ to a relatively narrow region of the B.Z. that we are able to obtain accurate bands from our simple pseudopotential interpolation scheme. As Fig. 2 shows, for this choice of parameters $\sigma(\omega)$ is more

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[8] The plane bounded by Λ and Δ was not weighted by a symmetry factor since the net was randomly distributed in respect to this plane and the region near this plane was of little importance in the evaluation of $\sigma(\omega)$ in the energy region we were interested in.

[9] T. O. Woodruff, Solid State Phys. 4, 367 (1957).

than an order of magnitude too small. The discrepancy is also present in Butcher's work when the same V_{110} is used. The core terms do not supply the hoped-for oscillator strength to reconcile theory and experiment. In fact, they suppress our $\sigma(\omega)$ in comparison with the $\sigma(\omega)$ calculated by Butcher.

That the core terms contribute so little and even suppress $\sigma(\omega)$ is rather surprising, but can be seen in retrospect as follows. We first restrict ourselves to the two equivalent vectors $\mathbf{k}$ and $\mathbf{k}-(1,1,0)$, since most of the contribution to $\sigma(\omega)$ comes from the region in k space near the Σ direction, where we need let $\mathbf{G}$ take on the values (0,0,0) and (1,1,0) in (2a, 2b) to obtain an adequate representation of $\Psi_{1\mathbf{k}}$ and $\Psi_{2\mathbf{k}}$. We set $\mathbf{k}'=\mathbf{k}-(1,1,0)$. Now $\langle\chi_{\mathbf{k}'}|\nabla|\chi_{\mathbf{k}}\rangle$ is made up of three contributions: $A(\mathbf{k},\mathbf{k}')$, which comes from a matrix of the form $\langle$plane wave $|\nabla|$core$\rangle$; $B(\mathbf{k},\mathbf{k}')$, which comes from a matrix of the form $\langle$core$|\nabla|$core$\rangle$; and $-k/2\delta_{\mathbf{k},\mathbf{k}'}$, which comes from a matrix of the form $\langle$plane wave $|\nabla|$ plane wave$\rangle$. For $k=0.62$ and $k'=0.8$, $A(\mathbf{k},\mathbf{k}')=0.0258$ and $B(\mathbf{k},\mathbf{k}')=-0.022$. We see that the core-core and core-plane-wave terms almost completely cancel each other in the region of k space of interest. The core terms are further weakened because $\mathbf{k}$ and $\mathbf{k}'$ are approximately antiparallel for $\mathbf{k}$ near Σ and the first and second terms on the right-hand side of (8) partially cancel each other.

When one considers $\langle\chi_{\mathbf{k}}|\nabla|\chi_{\mathbf{k}}\rangle$, we find $A(\mathbf{k},\mathbf{k})=0.044$ and $B(\mathbf{k},\mathbf{k})=-0.022$. This change in A results from the change in the sign of $\cos\gamma_{\mathbf{k}\mathbf{k}'}$ as we go from the case where the two $\mathbf{k}$ vectors are antiparallel to parallel. For $\mathbf{k}=\mathbf{k}'$ a core contribution of ≈ 0.022 survives and interferes with the -0.31 contribution due to the $k/2\delta_{\mathbf{k}\mathbf{k}'}$ term. We assume $k=0.62$. This explains why $\sigma(\omega)$ is suppressed by the addition of the core terms to the plane waves.

We have also calculated $\sigma(\omega)$ for $V_{110}=0.0232$, $V_{200}=0.066$; and $V_{110}=0.14$, $V_{200}=0.066$. While both these choices give band structures in disagreement with Ham's calculation, the former choice for V_{110} falls within the upper limit for V_{110} determined below. It was chosen to show how $\sigma(\omega)$ changes with V_{110}. The latter set of parameters indicates how large a V_{110} is needed to obtain a $\sigma(\omega)$ which agrees with $\sigma(\omega)_{\text{exp.}}$ insofar as its magnitude is concerned. Inspection of Fig. 2 indicates that as we increase V_{110} from 0.0132 to 0.0232, $\sigma(\omega)$ near its maximum increases roughly like $V_{110}{}^2$. Note that the shape of $\sigma(\omega)$ calculated for $V_{110}=0.0232$ agrees with $\sigma(\omega)_{\text{exp.}}$, but its magnitude is much too small. As was stated above, a $V_{110}=0.14$ was needed to obtain a $\sigma(\omega)$ which roughly agrees in magnitude with $\sigma(\omega)_{\text{exp.}}$, but which, as Fig. 2 clearly shows, has the wrong shape.

Before drawing any conclusions from this calculation it would be appropriate to review the experimental and theoretical work which throws light on the "best" choice for our parameters, V_{110} and V_{200}. Our aim will be to correlate the experimental and theoretical results so as to place an upper limit on V_{110}. We shall not be concerned with V_{200}, since its influence upon $\sigma(\omega)$ is very small compared to V_{110}.

TABLE I. Energies in electron volts.

	Na		K	
	V_{110}	V_{200}	V_{110}	V_{200}
Ham	0.11	0.90	−0.24	−0.33
Heine Abarenkov	0.242	···	−0.055	···
Ashcroft[a]	0.18	···	−0.23	−1.16

[a] Ashcroft obtains V_{110} and V_{200} for K from the work of Shoenberg and Stiles (Ref. 5) V_{110} for Na was estimated by Ashcroft from an analysis of the specific-heat effective mass.

Two of the most recent and refined band calculations for the alkali metals have been done by Ham and by Heine and Abarenkov (HA).[4] Using Ham's results for Na one obtains $V_{110}=0.115$ eV, if we make the assumption that V_{110} equals one-half the band gap at N (see Fig. 1). HA obtain $V_{110}=0.245$ eV. There is, however, strong evidence favoring the value obtained by Ham. As is clear from Table I, both Ham and HA are in good agreement as to the change in V_{110} as one goes through the alkali metals; HA's values, however, are shifted by ~ 0.20 eV compared to Ham's.

Now Ashcroft,[10] using the experimentally[5] determined shapes of the Fermi surfaces of K and Rb, determined V_{110} in these metals. His results for K are in excellent agreement with those of Ham. Ashcroft obtains $V_{110}=0.23$ eV compared to Ham's 0.24 eV. The excellent agreement between Ham's and Ashcroft's results for K, together with the agreement between HA and Ham as to the proper trend of V_{110} in the alkalis strongly supports the contention that the value obtained from Ham's work for Na is correct.

Furthermore, de Haas-Van Alphen experiments by Shoenberg and Stiles (SS) and cyclotron-resonance experiments by Grimes and Kip (GK) obtain for the Fermi surface anisotropy in Na values in substantially better agreement with those predicted by Ham than by HA. Shoenberg and Stiles estimate that $\Delta r/r$, the variation of the radius of the Fermi surface r, is less than 5.0×10^{-4}, while GK are unable to detect any anisotropy. This should be compared with Ham's prediction of no detectable anisotropy and HA's prediction of between 1.0×10^{-3} and 4.5×10^{-3} for $\Delta r/r$.

One final point remains: V_{110} obtained from Ham was evaluated at N, while it might be more appropriate to evaluate V_{110} at the Fermi energy E_F. This variation, as HA show, is expected to be only a few hundredths of an eV (≈ 0.04 eV) for Na. Keeping this in mind and the fact that the above analysis is only accurate to within a few hundredths of an eV, we can safely set an upper limit of 0.2 eV on V_{110}.

If we accept the experimental values of Mayer and Hietel or of Ives and Briggs, then the above calculation

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[10] N. Ashcroft, Phys. Rev. **140**, A935 (1965).

shows that the one-electron theory may not be capable of obtaining the correct magnitude of interband absorption in alkali metals. A similar conclusion was previously reached[11] for Al. There r_s (the mean interelectronic spacing in Bohr units) is 2.0 and the calculated absorption was three times smaller than that observed. In Na we have $r_s=3.96$ and the calculated absorption appears to be at least ten times smaller than observed. Possibly the anomalously large interband absorption indicates breakdown of the one-electron theory at short wavelengths. This breakdown could also lead to the observed resonance behavior. Because interband absorption refers to fixed momentum transfers $\mathbf{q}=\mathbf{k}-\mathbf{k}'=\mathbf{K}$, rather than a range of momentum transfer (as would arise in resonance formation), it may form a suitable starting point for theoretical research in the intermediate density regime $r_s \gtrsim 1$.

Note added in proof. Further de Haas–Van Alphen experiments on Na by M. J. G. Lee tentatively indicate a somewhat larger value of $|V_{110}|$ than quoted in this paper (the new value is slightly above our upper limit of 0.2 eV). While further work is expected to add a second significant figure to this result, we do not believe that this slightly larger value will alter the conclusions of this paper. We are grateful to Dr. D. Shoenberg for permission to mention Lee's preliminary results.

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I would like to thank Professor J. C. Phillips for suggesting this problem, as well as for his guidance throughout its execution.

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Resistivity Recovery of Dilute Alloys of Silver, Copper, and Gold, Proton-Irradiated at 80°K*

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Ag-Be, Ag-Li, Cu-Be, Au-Mg, and Au-Al were irradiated by 12-MeV protons at 80°K. High-resolution isochronals were then obtained from −130 to 90°C and activation energies were determined every 10°C using the change-of-slope method. The order associated with the reaction kinetics was determined at temperatures appropriate for the various annealing peaks by fitting 240-min isothermal anneals to first or second order. The recovery of the silver and copper alloys showed remarkable similarity to pure silver and copper, but the gold-alloy recovery was markedly altered as compared with pure gold. Activation energies for the stage-III defect in silver, copper, and gold alloys were found to be 0.64, 0.71, and 0.70 eV, respectively. The copper and silver alloys had a small first-order recovery stage near the low-temperature side of the main stage-III annealing peak. The main stage-III peak obeyed second-order kinetics in all cases. In the gold alloys the stage-III recovery was composed of a main second-order annealing peak with a small second-order annealing peak on each side of the main peak. These annealing results have been fitted to the various models for the recovery of damage, and some conclusions are drawn.

I. INTRODUCTION

At present the basic nature of the annealing processes occurring in stage I (10 to 100°K) is reasonably well understood. In both fcc and bcc metals a series of close interstitial vacancy pairs recombine.[1–3] At a temperature a little above temperatures associated with these close pairs, one has demonstrated long-range migration of an interstitial in copper and aluminum.[2–5] The geometrical arrangement of atoms constituting the interstitial defect which migrates in stage I is still being discussed.

Gold appears to be an anomalous material. The close-pair annealing peaks in copper and silver as seen by Palmer, Magnuson, and Koehler[1] in stage I are remarkably similar. However, Ward and Kauffman[6] and later Bauer, DeFord, Koehler, and Kauffman[7] found a very complex annealing spectrum for gold in stage I. Koehler and Leibfried[8] have attempted to explain the difference by supposing that the interstitial structure in gold differs from that existing in copper and silver.

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