res and C. T. De Dominicis, Phys. Rev. 178, 1097 (1969); S. Doniach and M. Sunjić, J. Phys. C 3, 285 (1970).

[22]D. M. Newns, Phys. Rev. 178, 1123 (1969).

[23]Observe that Eq. (3) is valid only if the band states above ϵ_F are excluded from the model.

Electron Lifetime Effects on Properties of *A*15 and bcc Materials

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(Received 3 August 1978)

Electron lifetime effects on several basic physical parameters of *A*15 and bcc materials are calculated using theoretical band structures and observed electrical resistivities. Notable changes in properties result from resistivities accessible thermally or by induced defects.

Many transition metals and alloys have interesting physical properties that may be strongly modified by electron scattering processes involving, for example, phonons, defects, and impurities. The materials scientist is often faced with the problem of establishing to what extent these properties are dependent on the sample quality. Theoretical treatments of this problem have been given previously.[1] We report in this Letter a simple model for estimating these effects in the *A*15 compounds and bcc transition metals and alloys with no adjustable parameters. The input to this model is a single experimental number (the electrical resistivity ρ) plus several band-theory results.[2] Application of the model provides the density of states $N(E)$, Fermi velocity v_F, Drude plasma frequency Ω_p, and other properties as a function of the thermal (ρ_{th}) and residual (ρ_0) resistivity. Finally, with one assumption, we obtain the relation between T_c for superconductivity and the residual resistivity.

For electrons near the Fermi level in an imperfect crystal, lifetime effects may be included in an *approximate* fashion[3] by using the uncertainty principle (see, for another example, Weismann *et al.*[1]). If $X(E)$ is a quantity whose energy dependence near the Fermi level is known for the perfect crystal, lifetime effects may be incorporated with the prescription

$$\langle X\rangle = \int X(E)S(E_b)\,dE, \tag{1}$$

where $S(E_b)$ is a broadening function which depends upon $E_b = \hbar/\bar{\tau}$. The mean electron lifetime $\bar{\tau}$ can be estimated with the Drude plasma frequency[2] Ω_p using

$$\rho^{-1} = \langle\Omega_p^2\rangle\bar{\tau}/4\pi. \tag{2}$$

The exact form of the broadening function is not too crucial when the broadening is large compared to any fine structure in $X(E)$. Dingle[3] has shown from a semiclassical argument that the proper weighting function may be a Lorentzian with half-width $\hbar/\bar{\tau}$. Another possible choice for S is the analogous (though physically different) one for thermal broadening where $S = -\partial f/\partial E$ and f is the Fermi-Dirac function with T replaced by $T_B \equiv \hbar/\kappa\bar{\tau}$. We have made calculations[4] with both forms of S and find the results differ by $\leq 10\%$ which is the estimated reliability of the calculations. (Calcultions given below are, in fact, with $S = -\partial f/\partial E$ to avoid complications from the broad Lorentzian wings).

One can thus obtain an approximate correction for lifetime broadening and calculate band-structure quantities at $T = 0$ as a function of ρ_0 by averaging such quantities using Eq. (1) with E_B or κT ($=\kappa T_B$) replaced by $\hbar/\bar{\tau}$. Furthermore, since T_B is considerably greater than T in all cases considered here we can, by these arguments, neglect the usual thermal broadening effects and use the results below to characterize, qualitatively, all sample states with the same resistivity, whether defect or thermally induced.

Normal-state properties.—Figure 1 shows the calculated bare density of states $\langle N\rangle$, Fermi velocity $\langle v_F\rangle$, and $\langle\Omega_p^2\rangle^{1/2}$ as a function of T_B and ρ for V_3Si and $V_{2.94}Si$, assuming a rigid-band model. The slight shift (~ 35 meV) in Fermi level between these two compositions leads to appreciable differences in $\langle N\rangle$ for the perfect crystal ($\rho = 0$) but an accurate determination of such fine structure is not possible in the present calculations. Indeed, $\langle N\rangle$ for nearly perfect V_3Si is experimentally found to be ~ 2.5 states/(eV spin V-atom). However, for $\rho > 25$ $\mu\Omega$ cm the calculated fine structure is largely washed out and at

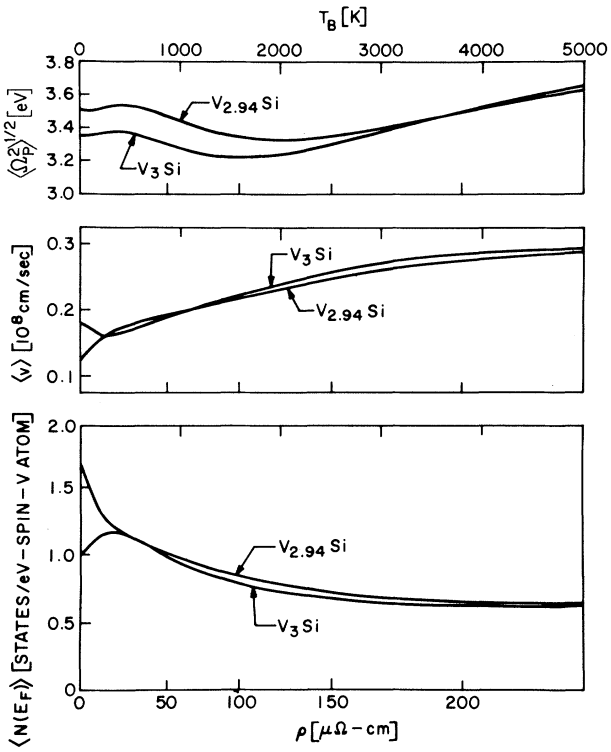

FIG. 1. $\langle N\rangle$, $\langle v_F\rangle$, and $\langle\Omega_p^2\rangle^{1/2}$ as a function of ρ (nonlinear scale) and the equivalent broadening temperature for V_3Si and $V_{2.94}Si$.

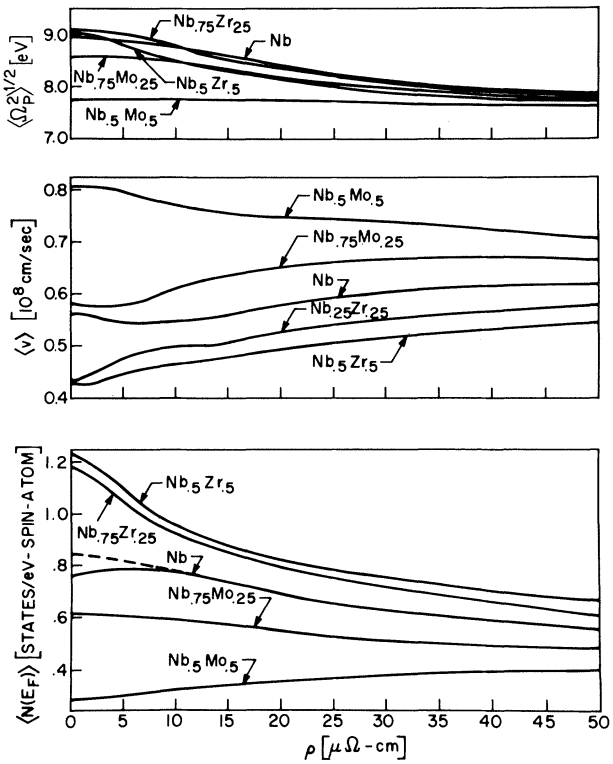

FIG. 2. $\langle N\rangle$, $\langle v_F\rangle$, and $\langle\Omega_p^2\rangle^{1/2}$ as a function of ρ for Nb and its alloys with Zr and Mo.

300 K where $\rho \approx 75$ $\mu\Omega$ cm one finds $\langle N\rangle \approx 1.0$ states/eV spin per vanadium atom. This large reduction in $\langle N\rangle$ with increasing T is in agreement with that obtained from magnetic-susceptibility (χ) measurements using values for the background paramagnetism and the Stoner enhancement factors which are within 10% of Clogston's estimates.[5] Thus, because of the high T_B of these materials, anomalous temperature dependences can arise from (calculable) fine structure in $\langle N\rangle$ on a scale of 500–1000 K instead of 50 K as assumed in many models.

A somewhat better test is provided by defect-induced resistivity. Recent measurements at low temperatures on single-crystal V_3Si show that neutron irradiations which lower T_c from 17 to ~7 K raise the residual resistivity ρ_0 to[6] ~92 $\mu\Omega$ cm and lower $\langle N\rangle$ to 0.93 (from specific heat)[6] and ~1.0 (from χ)[7] states/(eV spin V-atom). These are in reasonable agreement with the predicted value of 0.85 from Fig. 1. Finally, note that the calculated reduction of $\langle N\rangle$ with ρ gradually saturates for $\rho \geq 150$–200 $\mu\Omega$ cm. This is the range of resistivities experimentally observed in the defect saturation state,[8] and also proposed for the thermally induced saturation of ρ.[9]

Figure 2 exhibits corresponding results for Nb and its bcc alloys with Zr and Mo, assuming a rigid-band model. (Similar findings have been obtained for Ti-V-Cr alloys.) For pure Nb the calculated $\langle N\rangle$ at $\rho = 0$ is about 10%–15% below the experimental value.[10] It thus seems possible that a monotonic $\langle N\rangle$ vs ρ curve (see the dashed line) may replace the one with the calculated weak maximum. Lifetime-broadening effects are most pronounced for $Nb_{0.5}Zr_{0.5}$. $\langle N\rangle$ calculated for this alloy with $\rho = 0$ is about 60% larger than that for Nb while the experimental difference[10] is only several percent. However, this alloy has strong disorder scattering, and a typical[11] $\rho_0 \approx 40$ $\mu\Omega$ cm reduces $\langle N\rangle$ by 50% placing it within 10% of the value for Nb. Similar agreement is obtained with $Nb_{0.75}Zr_{0.25}$. For $Nb_{0.75}Mo_{0.25}$ and $Nb_{0.5}Mo_{0.5}$ the calculated $\langle N\rangle$ at the experimental ρ_0's are 0.60 and 0.34 states/(eV spin atom) in agreement with McMillan's values[10] of 0.65 and 0.34, respectively.

Further experimental tests of the defect-state

calculations come from Ginzburg-Landau κ. This quantity, however, is enhanced by electron-phonon renormalization and some estimate of McMillan's λ is required. For nearly defect-free V_3Si measurements of Guha *et al.*[7] give $\kappa_{obs} = 20.5$ while the calculated value $\kappa_{calc} \approx 15$ using the experimental estimate[6] $\lambda = 0.9$. However, following the neutron dose described above, $\kappa_{obs} = 57$ and $\kappa_{calc} = 55$ (using the experimental[6,7] $\lambda \approx 0.6$). Thus, again, the dirty state is easier to predict than the clean one. For a saturation $\rho_0 \approx 150$ $\mu\Omega$ cm from radiation-induced defects, the calculations predict $\kappa_{calc} \approx 70$ (with $\lambda \approx 0.52$; see below).

For thermally induced ρ we also calculate $\bar{\tau}^{-1}(300\text{ K}) = 1.45\times10^{14}$ sec^{-1} at $\omega = 0$ for intrinsic V_3Si which can be compared with the value $\sim 1.0\times10^{14}$ sec^{-1} obtained by Yao and Schnatterly[12] by extrapolation from near-infrared measurements. [For Nb the calculated and observed $\bar{\tau}^{-1}(300\text{ K})$ are 2.2×10^{14} and $(2.0-2.6)\times10^{14}$ sec^{-1}, respectively.] This experiment also yields $\Omega_p \approx 2.8\pm0.2$ eV compared to our calculated value (at 300 K) of 3.2 eV. The mean free path $l = \langle v_F\rangle\tau$ is calculated to be ~ 13 Å at 300 K, and $\sim 8-9$ Å at the saturation-state resistivity of 150 $\mu\Omega$ cm. The V-atom chain spacing is 2.36 Å.

Superconductivity.—Calculations for the defect state cannot be extended to superconductivity without additional assumptions relating T_c (or McMillan's λ) and a band-structure quantity. We therefore further assume that $\lambda \propto \langle N\rangle$ (see, for example, Dynes and Varma[13]) yielding $\lambda(\rho_0)$, and use McMillan's equation[10] to obtain $T_c(\rho_0)$. Following Labbé, Barišić, and Friedel[14] and Nettel and Thomas[14] we also take $\langle N\rangle$ to be averaged over an energy $\bar{\omega} \sim \Theta_D$. Since $\Theta_D \sim 400$ K in V_3Si, the inaccuracy of the fine details in $N(E)$ for the pure crystal is relatively unimportant when $\rho_0 \lesssim 20$ $\mu\Omega$ cm (see the equivalent scale of T_B in Fig. 1). Since $\rho(300\text{ K}) \sim 75$ $\mu\Omega$ cm in all $A15$ materials, this yields T_c independent of resistance ratios greater than $\sim 3-4$, in agreement with experiment.[8]

Figure 3 shows the calculated range of $\lambda(\rho)$ assuming $\bar{\omega} = 300-400$ K and, for the unnormalized scale, $\lambda = 0.90$ for perfect V_3Si. Again, for the neutron-damaged sample with $\rho_0 \approx 92$ $\mu\Omega$ cm the experimental estimates of $\lambda \approx 0.5$ (from χ)[7] and 0.62 (from specific heat)[6] are in reasonable agreement with the calculated range ($\sim 0.57-0.65$). The graph also shows the electron-phonon coupling coefficient for transport process $\lambda_{tr} = \hbar\bar{\tau}^{-1}/2\pi kT$ obtained from Eq. (2) and ρ_{th} at 300 and 100 K in intrinsic V_3Si. However, for the saturated defect state one finds $\rho_{th} \approx 0$, and therefore $\lambda_{tr} \approx 0$, even though superconductivity (at 2.2 K) persists. This relation, then, breaks down at high ρ.

The dependence of T_c on ρ_0, calculated from McMillan's equation, $\lambda(\rho_0)$, and assuming Θ_D to be a constant, is given in Fig. 3. The observed dependence, reflected in the T_c-resistance ratio correlation,[8] is also shown. While such close agreement is somewhat fortuitous (Θ_D varies by $\sim 15\%$), the combination of broadened-band calculations and the assumption $\lambda \propto \langle N\rangle$ yield, with no adjustable parameters, the rapid fall of T_c with ρ_0 up to $\rho_0 \approx 150-200$ $\mu\Omega$ cm, in general agreement with experiment.

Similar calculations for 3*d* and 4*d* bcc metals reveal appreciable lifetime effects also. Figure

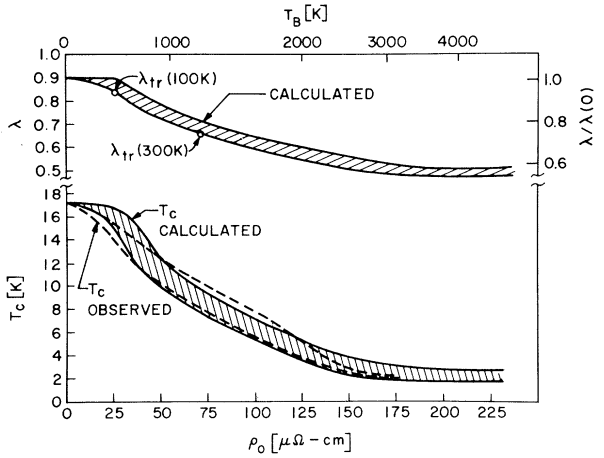

FIG. 3. Electron-phonon parameter λ and calculated and observed T_c vs ρ_0 for V_3Si.

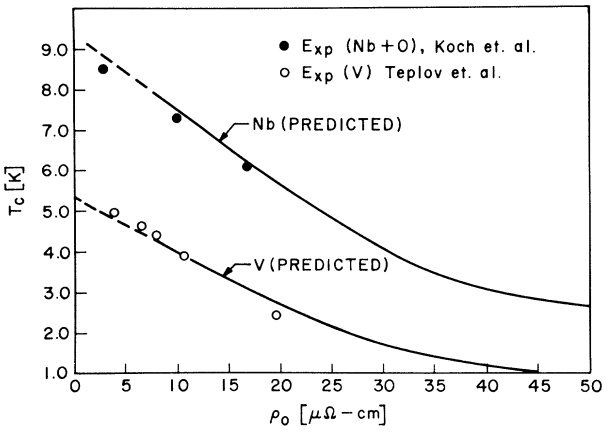

FIG. 4. Calculated and observed T_c vs ρ_0 for Nb and V.

4 gives the predicted dependence of T_c on ρ_0 for Nb and V calculated in a manner similar to that for V_3Si. The dashed lines in Fig. 4 correspond to the dashed-line extrapolation of $\langle N \rangle$ in Fig. 2. While some inaccuracy in the calculations again occurs at low ρ_0, the overall agreement with the data of Koch, Scarbrough, and Kraeger[15] and Teplov *et al.*[15] appears reasonable at higher ρ.

For the bcc metals, as for the $A15$ compounds, the broadened-band calculations predict $dT_c/d\rho_0 \sim -0.1$ to 0.2 K/$\mu\Omega$ cm. As an example of alloy scattering effects, ternary mixtures of Zr-Nb-Mo show[16] $dT_c/d\rho_0 \sim -0.12$ K/$\mu\Omega$ cm in qualitative agreement with the Nb results and a rigid-band model. Of greater importance is $Nb_{0.5}Zr_{0.5}$ where, as noted above, $\langle N \rangle$ may be reduced by ~50% due to the high ρ_0 from the solid-solution disorder. Without such scattering, and assuming $\lambda \propto \langle N \rangle$, the calculated T_c would be ~15–20 K.

A principal result of this model calculation is that lifetime effects from large ρ's, no matter how they are caused, can seriously alter the normal- as well as the superconductivity-state properties of these materials. It is a tentative conclusion that, for uniformly degraded samples, such effects may be calculated with reasonable accuracy by combining band calculations of moderate precision and a single, easily obtained, experimental number. The experimentalist may then be able to estimate to what extent T_c and other properties have been altered by poor sample quality.

[1]J. W. Garland, K. H. Bennemann, and F. M. Mueller, Phys. Rev. Lett. 21, 1315 (1968); J. Labbé and E. C. van Reuth, Phys. Rev. Lett. 24, 1232 (1970); S. J. Williamson, C. S. Ting, and H. K. Fung, Phys. Rev. Lett. 32, 9 (1974); H. Wiesmann, M. Gurvitch, A. K. Ghosh, H. Lutz, O. F. Kammerer, and Myron Strongin, Phys. Rev. B 17, 122 (1978); I. Nakayama and I. Tsuneto, Prog. Theor. Phys. 58, 1060 (1977).

[2]L. F. Mattheiss, L. R. Testardi, and W. W. Yao, Phys. Rev. B 17, 4640 (1978); L. F. Mattheiss, Phys. Rev. B 12, 2161 (1975).

[3]For additional references and more rigorous treatments, see R. B. Dingle, Proc. Roy. Soc. London, Ser. A 211, 517 (1952); P. B. Allen and V. Heine, J. Phys. C 9, 2305 (1976); and D. J. Huntley, F. J. Di Salvo, and T. M. Rice, to be published.

[4]The calculations have been done self-consistently, accounting for both the shift in Fermi level and the variation of $\langle \Omega_p \rangle$ with ρ.

[5]A. M. Clogston, Phys. Rev. 136, A8 (1964).

[6]R. Caton and R. Viswanathan, to be published; R. Viswanathan and R. Caton, Phys. Rev. B 18, 15 (1978).

[7]A. Guha, M. Sarachik, F. W. Smith, and L. R. Testardi, Phys. Rev. B 18, 9 (1978).

[8]J. M. Poate, L. R. Testardi, A. R. Storm, and W. M. Augustyniack, Phys. Rev. Lett. 35, 1290 (1975).

[9]Z. Fisk and G. W. Webb, Phys. Rev. Lett. 36, 1084 (1976).

[10]W. L. McMillan, Phys. Rev. 167, 331 (1968). We have taken $\lambda \approx 0.95$ for Nb.

[11]N. Morton, B. W. James, G. H. Wostenholm, and R. J. Nichols [J. Phys. F 5, 85 (1975)] report $\rho_0 \approx 20$ $\mu\Omega$ cm for $Nb_{0.75}Zr_{0.25}$. We linearly extrapolate to obtain $\rho_0 \approx 40$ $\mu\Omega$ cm in $Nb_{0.5}Zr_{0.5}$. W. DeSorbo [Phys. Rev. 130, 2177 (1963)] has shown that ρ_0 is proportional to solute concentration in Nb-Hf and Nb-Ti. For $Nb_{1-x}Mo_x$ ρ_0 has been obtained by extrapolating the data ($x = 0$–0.2) of R. A. French and J. Lomell, Phys. Rev. 173, 504 (1968).

[12]W. Yao and S. Schnatterly, to be published.

[13]R. C. Dynes and C. M. Varma, J. Phys. F 6, L215 (1976).

[14]J. Labbé, S. Barišić, and J. Friedel, Phys. Rev. Lett. 19, 1039 (1967); S. J. Nettel and H. Thomas, Solid State Commun. 21, 683 (1977).

[15]C. C. Koch, J. O. Scarbrough, and D. M. Kroeger, Phys. Rev. B 9, 888 (1974); A. A. Teplov, M. N. Mikheeva, V. M. Golyanov, and A. N. Gusev, Zh. Eksp. Teor. Fiz. 71, 1122 (1976) [Sov. Phys. JETP 44, 587 (1976)].

[16]R. Flukiger and M. Ishikawa, in *Proceedings of the Fourteenth International Conference on Low Temperature Physics, Otaniemi, Finland, 1975*, edited by M. Krusius and M. Vuorio (North-Holland, New York, 1976), Vol. 2, p. 63.