Presented at 12th International
Conference on Low Temperature
Physics, Kyoto, Japan, Sept. 4-10,
1970.

UCRL-19681
Preprint





# DENSITY OF ELECTRONIC STATES IN α-PHASE IN ALLOYS CONTAINING Cd AND Sn

Norman E. Phillips, J. C. F. Brock
Marcel H. Lambert, and M. F. Merriam

Sept. 1970

AEC Contract No. W-7405-eng-48



LAWRENCE RADIATION LABORATORY
UNIVERSITY of CALIFORNIA BERKELEY

**DISCLAIMER**

# Density of Electronic States in α-Phase In Alloys Containing Cd and Sn*

Norman E. Phillips, J. C. F. Brock†,
Marcel H. Lambert‡, and M. F. Merriam

Inorganic Materials Research Division
of the Lawrence Radiation Laboratory,
University of California, Berkeley, California 94720

## Abstract

Low-temperature heat capacity measurements on α-phase In alloys were used to obtain the Debye characteristic temperature, the density of electronic states, and the electron-phonon coupling constant. The results show further evidence for Brillouin zone boundary - Fermi surface interactions, and are discussed from this point of view.

For certain values of Z, the conduction electron/atom ratio, the α-phase In alloys containing Cd or Sn exhibit rapid changes in the derivative with respect to Z of both axial ratio and $T_c$, the critical temperature for superconductivity.[1,2] These effects have been attributed to Brillouin zone boundary - Fermi surface interactions. We have measured the low-temperature heat capacity of these alloys to search for related effects in $N(E_F)$, the density of electronic state at the Fermi energy $E_F$, and to obtain values of the Debye characteristic temperature $\theta_o$ which make possible estimates of λ, the electron-phonon coupling constant. The measurements will be discussed in more detail elsewhere.[3,4]

As shown in Figure 1, $\theta_o$ varies smoothly with Z except at Z = 3.00, but γ, which is equal to $(2/3)\pi^2k^2\ N(E_F)$, shows rapid changes of slope near Z = 2.98 and 3.09, corresponding to the previously reported effects in $T_c$ and axial ratio. We have used an equation derived by McMillan[5] to estimate λ, and have calculated the "band density of states" $N_{bs}(E_F)$ on the assumption that $N_{bs}(E_F) = N(E_F)/(1 + \lambda)$. $N_{bs}(E_F)$ is well represented by four straight lines intersecting at Z = 2.98, 3.00, and 3.09. Increases in $d\ N_{bs}(E_F)/dZ$ occur at Z = 2.98 and 3.09 suggesting the appearance of new pieces of the Fermi surface at these Z values. From the "experimental" $N_{bs}(E_F)$, the increase in $E_F$ between Z = 2.98 and 3.09 is 0.25 eV.

The Fermi surface of pure In includes an extensive second-zone surface, possibly multiply connected, and third-zone "β arms". Additional third-zone pockets of electrons, the "α-arms", may exist but the available evidence is contradictory[6]. Band-structure calculations[7] suggest that for In the lowest energy β-arm states are 0.5 eV or more below the lowest $\alpha$-arm states. In the alloys the trend in axial ratio with $Z$ can be expected to increase this energy difference with increasing $Z$. Furthermore, it would be difficult to understand the positive $dN_{bs}(E_F)/dZ$ in the $2.95 < Z < 2.98$ region if the $\beta$-arms were not already in existence. It therefore seems unlikely that the increases in $dN_{bs}(E_F)/dZ$ are caused by the successive appearance of the $\beta$ and $\alpha$ arms. The band-structure calculations also suggest that fourth-zone states are too high in energy to be occupied in the alloys. A possible explanation of the increases in $dN_{bs}(E_F)/dZ$, suggested by the band-structure calculations, is that pockets of electrons appear at the center of the $\alpha$ arms at $Z = 2.98$, and different pockets of electrons appear at the ends (opposite the $\beta$ arms) of the $\alpha$ arms at $Z = 3.09$. The decrease in $dN_{bs}(E_F)/dZ$ just above $Z = 3.00$ could be associated with the disappearance of the second-zone connecting tubes.

McMillan[5] has noted that for five cubic transition metals $\lambda$ is proportional to a ratio of certain moments of the phonon spectrum with the dimensions [frequency]$^{-2}$, and he has suggested that such a correlation may apply for each class of superconductors. For the same metals there is a comparably good correlation between $\lambda$ and $\theta_o^{-2}$. Figure 2 shows a test of the constancy of $\lambda\theta_o^2$ for the $\alpha$-phase indium alloys, and also of the more commonly expected correlation--constancy of $\lambda/N_{bs}(E_F)$. It is clear that $\lambda$ is more nearly proportional to $N_{bs}(E_F)$ than to $\theta_o^{-2}$, but it is also clear that the contributions of an electronic state to $\lambda$ and to $N_{bs}(E_F)$ are different.

It is expected[8] that states close to strongly scattering Bragg planes, which are mixtures of several OPW's, will generally make relatively large contributions to the mean-square electron-phonon matrix element which occurs as a factor in $\lambda$. Our results do not seem to be consistent with this expectation. For example, it seems clear that new third-zone states begin to be populated at $Z = 3.09$. The value of $\lambda$ does increase more rapidly for higher $Z$, but not as rapidly as does $N_{bs}(E_F)$, which also occurs as a factor in $\lambda$.

It has been known for some time that the addition of small amounts (~ 1 at % or less) of Cd or Sn to In lowers $T_c$ by an amount related to the reduction in electron mean free path.[9] We note that $\theta_o$ for In is also higher than would be given by interpolation between alloys containing more than a few at % Cd or Sn -- and by an amount that could itself account for the higher value of $T_c$.

*Work supported by the U. S. Atomic Energy Commission.

†Present address: Department of Physics, University of the Witwatersrand, Jan Smuts Avenue, Johannesburg, South Africa.

‡Present address: Faculte des Sciences, Universite Libre de Bruxelles, Brussels, Belgium.

1. M. F. Merriam, Phys. Rev. Letters, 11, 321(1963); Phys. Rev. 144, 300(1966).

2. N. Ridley, Phys. Letters 25A, 134(1967).

3. M. H. Lambert, J. C. F. Brock, and N. E. Phillips, submitted for publication.

4. J. C. F. Brock, N. E. Phillips, and M. F. Merriam, to be submitted.

5. W. L. McMillan, Phys. Rev. 167, 331(1968).

6. See, for example, G. B. Brandt and J. A. Rayne, Phys. Letters 12, 87(1964), and A. J. Hughes and A. H. Lettington, Phys. Letters 27A, 241(1968).

7. N. W. Ashcroft and W. E. Lawrence, Phys. Rev. 175, 938(1968).

8. E. E. Havinga, Phys. Letters 26A, 244(1968).

9. G. Chanin, E. A. Lynton, and B. Serin, Phys. Rev. 114, 719(1959).

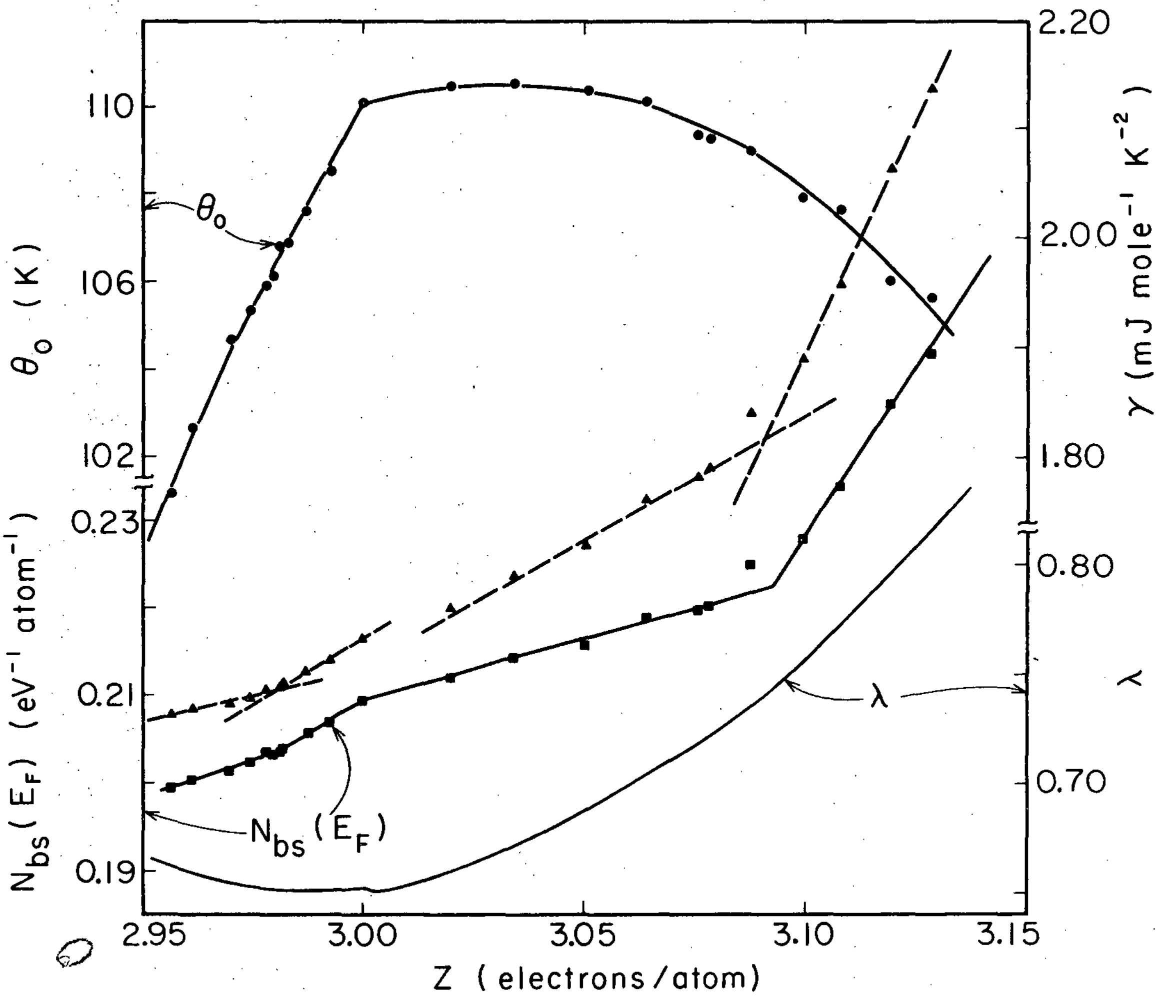


Fig. 1. Measured and derived parameters. The dashed lines are intended to emphasize the changes in slope of $\gamma$ near Z = 2.98 and 3.09.

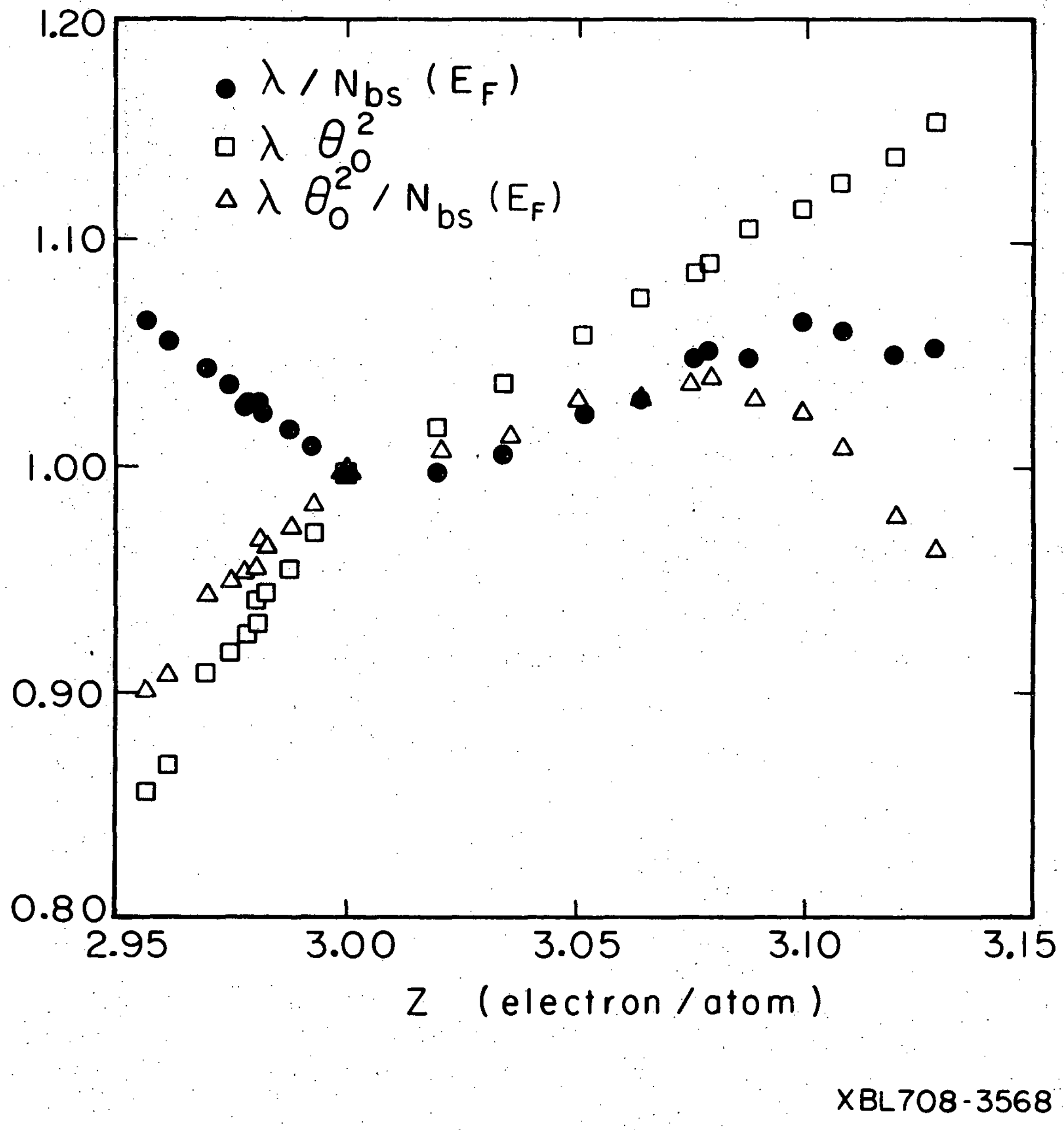


Fig. 2. Test of the constancy of $\lambda\theta_o^2$ and $\lambda/N_{bs}(E_F)$. Both quantities are plotted as ratios to their values at Z = 3.00.

*TECHNICAL INFORMATION DIVISION*
*LAWRENCE RADIATION LABORATORY*
*UNIVERSITY OF CALIFORNIA*
*BERKELEY, CALIFORNIA 94720*