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

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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 θ_0 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, θ_0 varies smoothly with Z except at $Z = 3.00$, but γ , which is equal to $(2/3)\pi^2 k^2 N(E_F)$, 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 McMillan⁵ 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 $Z = 2.98, 3.00, \text{ and } 3.09$. Increases in $dN_{bs}(E_F)/dZ$ 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 contradictory⁶. Band-structure calculations⁷ suggest that for In the lowest energy β -arm states are 0.5 eV

or more below the lowest α -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 β -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 β and α 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 α arms at $Z = 2.98$, and different pockets of electrons appear at the ends (opposite the β arms) of the α 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.

McMillan⁵ has noted that for five cubic transition metals λ is proportional to a ratio of certain moments of the phonon spectrum with the dimensions $[\text{frequency}]^{-2}$, 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 λ and θ_0^{-2} . Figure 2 shows a test of the constancy of $\lambda\theta_0^2$ for the α -phase indium alloys, and also of the more commonly expected correlation--constancy of $\lambda/N_{bs}(E_F)$. It is clear that λ is more nearly proportional to $N_{bs}(E_F)$ than to θ_0^{-2} , but it is also clear that the contributions of an electronic state to λ and to $N_{bs}(E_F)$ are different.

It is expected⁸ 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 λ . 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 λ does increase more rapidly for higher Z , but not as rapidly as does $N_{bs}(E_F)$, which also occurs as a factor in λ .

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 θ_0 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 .

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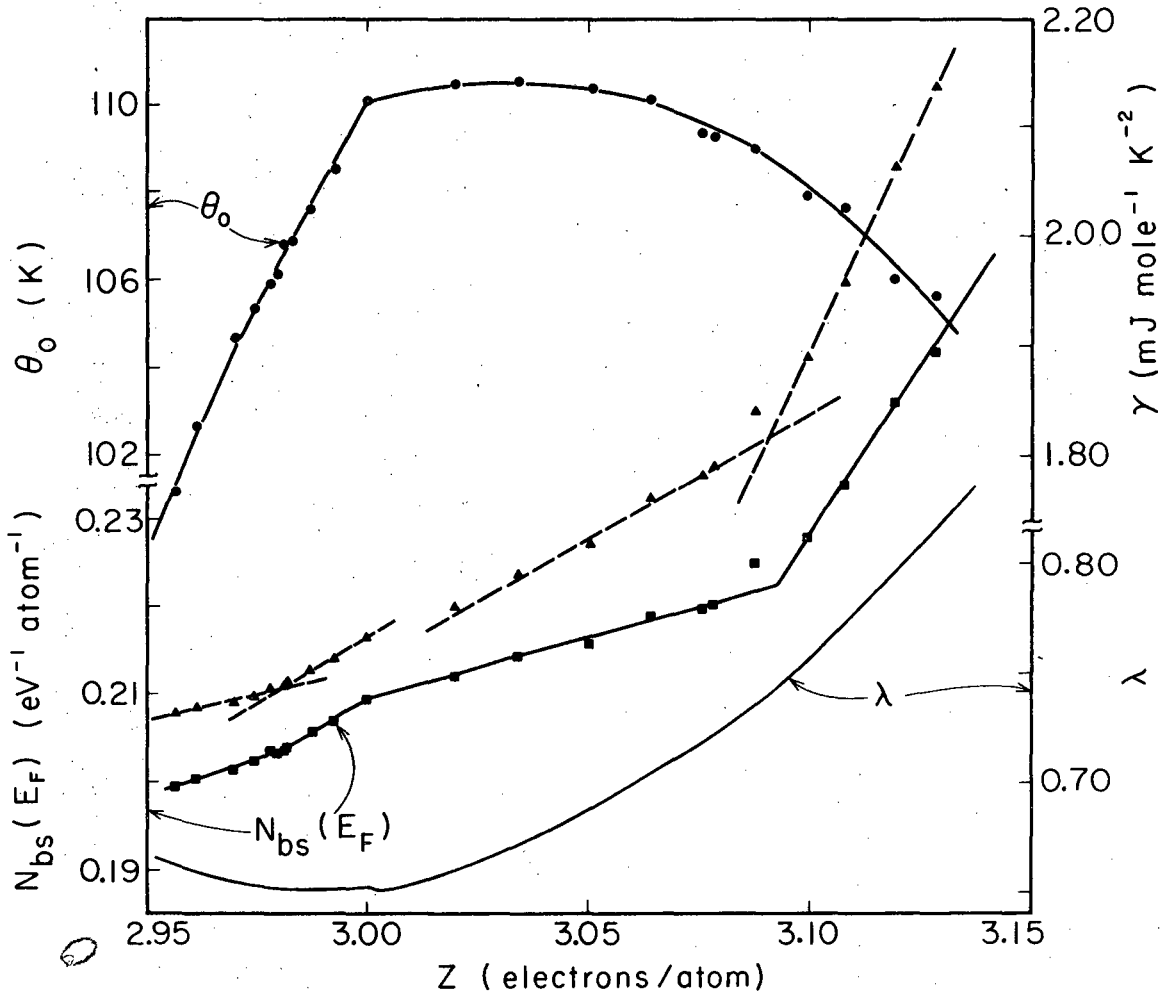
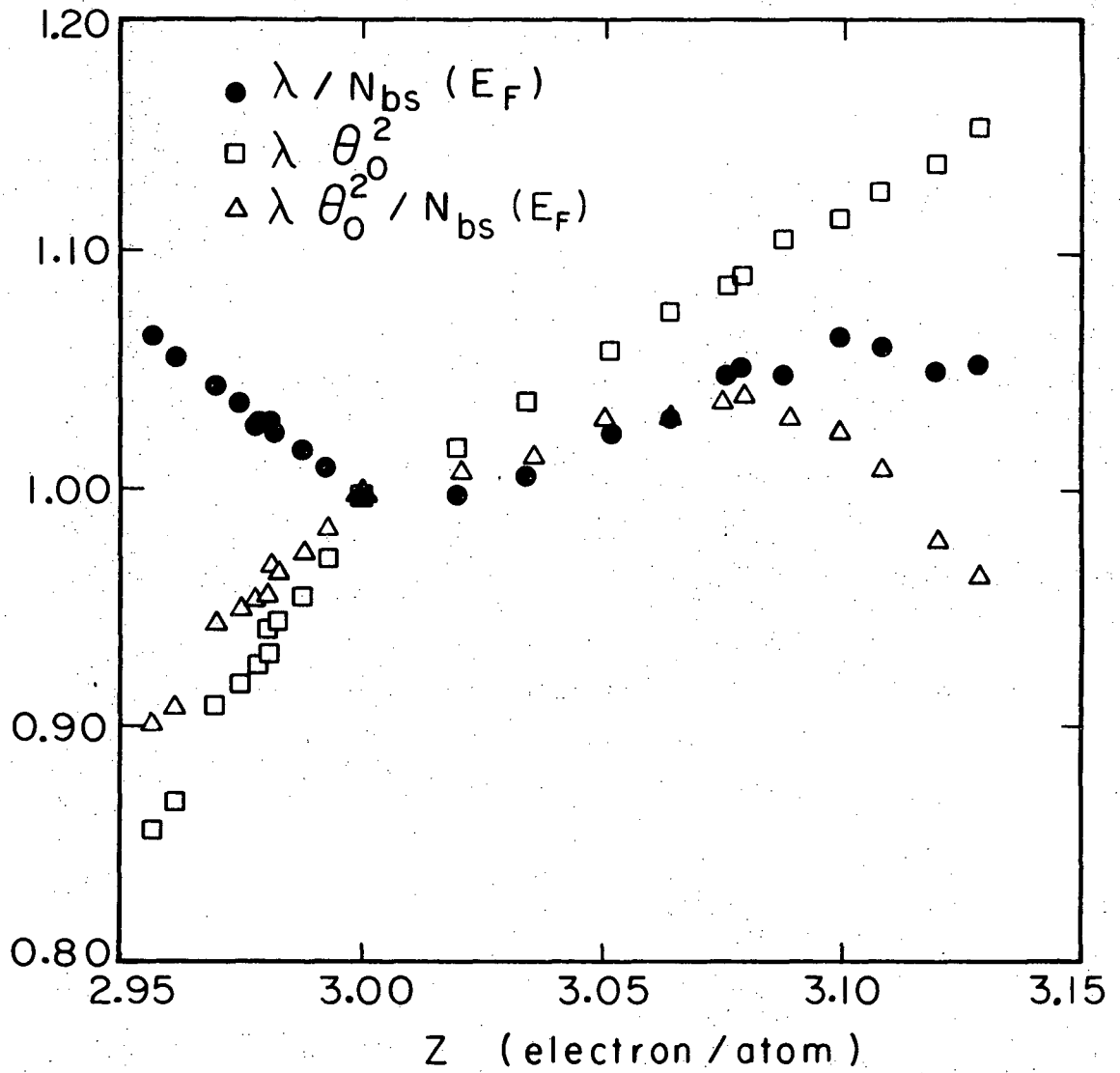


Fig. 1. Measured and derived parameters. The dashed lines are intended to emphasize the changes in slope of γ near $Z = 2.98$ and 3.09 .



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Fig. 2. Test of the constancy of $\lambda \theta_0^2$ and $\lambda / N_{bs} (E_F)$. Both quantities are plotted as ratios to their values at $Z = 3.00$.

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