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Felienne Hermans, J.C. Ho, J. Boyer, N. Phillips. DENSITY OF ELECTRONIC STATES IN fcc T1-Pb-Bi ALLOYS. Journal de Physique Colloques, 1978, 39 (C6), pp.C6-477-C6-478. 10.1051/jphyscol:19786213 . jpa-00217633

HAL Id: jpa-00217633

<https://hal.science/jpa-00217633>

Submitted on 1 Jan 1978

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DENSITY OF ELECTRONIC STATES IN fcc Tl-Pb-Bi ALLOYS.*

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Résumé.- Nous avons mesuré la chaleur spécifique d'alliages cubiques du système Tl-Pb-Bi, et nous avons utilisé les valeurs de λ de Dynes et Rowell pour calculer $N(0)$. Le comportement de λ ne montre pas de corrélation simple avec $N(0)$ ou $\langle\omega^2\rangle$.

Abstract.- We have measured the heat capacity of fcc Tl-Pb-Bi alloys, and have used values of λ published by Dynes and Rowell to obtain $N(0)$ and the other component factors in λ . The behavior of λ shows no simple correlation with other properties.

The density of electronic states at the Fermi surface, $N(0)$, is of fundamental importance in determining many of the properties of metals including T_c , the critical temperature for superconductivity. It can be derived from the electronic heat capacity, γT , and the relation

$$\gamma = (2/3) \pi^2 k^2 (1 + \lambda) N(0), \quad (1)$$

if λ , the electron-phonon interaction parameter, is known. The latter quantity has generally been available only for pure metals, and the recent tunnelling measurements /1/ on fcc alloys of the Tl-Pb-Bi system provided the incentive for the heat capacity measurements reported here. This series of alloys is of particular interest because λ and T_c are strong functions of the electron/atom ratio z . Furthermore, the combination of tunnelling and heat capacity data permit a complete analysis of λ in terms of electronic and lattice properties through the relation /2/

$$\lambda = N(0) \langle \mathcal{Q}^2 \rangle / M \langle \omega^2 \rangle \quad (2)$$

where $\mathcal{Q}$ is a matrix element for the scattering of an electron, M is the atomic mass, and $\langle \omega^2 \rangle$ is a mean square phonon frequency. McMillan /2/ observed that for five transition metals $N(0) \langle \mathcal{Q}^2 \rangle$ was approximately constant and the values of λ and T_c were determined by the phonon spectrum. He suggested that this might be a more general relation, and since then the assumption $\lambda \propto 1 / \langle \omega^2 \rangle$, together with Eq.(2) and McMillan's expression /2/ for T_c (λ), has been widely used to interpret variations of T_c . This is in marked contrast to earlier practice, in which it was more often assumed that variations in T_c were determined primarily by electronic properties, and in particular by $N(0)$. As will be shown below,

neither of these simple correlations is consistent with the data now available for the Tl-Pb-Bi system.

Normal-state heat capacity data and zero-field data near T_c have been obtained for binary alloys with conduction electron/atom ratio z ranging from 3.4 to 4.2, and for three "pseudo leads," ternary alloys of the form $Pb_{1-2x}Tl_xBi_x$ with $x = 0.05, 0.10, 0.15$. Values of γ , T_c , and the Debye characteristic temperature, θ , were derived. Values of λ were derived from the published /1/ data, and used to calculate $N(0)$ from γ .

Fig.1 : Coefficient of electronic heat capacity and density of electronic states for the binary alloys, normalised to their values for Pb.

The results for both γ and $N(0)$ for the binary alloys are shown in figure 1. A striking feature of figure 1 is that although the slopes of γ vs. z are different for the Tl-Pb and Pb-Bi alloys, the values of $N(0)$ fall on a common straight line to within 0.5%, the apparent precision of the data. Furthermore, although the values of γ for $Pb_{0.9}$

* This work was supported by the Division of Materials Sciences, Office of Basic Energy Sciences, U.S. Department of Energy.

$\text{Ti}_{0.05}\text{Bi}_{0.05}$ and $\text{Pb}_{0.8}\text{Ti}_{0.1}\text{Bi}_{0.1}$ are 3.5 and 6.5 % greater than for Pb, the values of $N(0)$ are the same for all three to within 0.5%. In these respects the results are consistent with the rigid-band model, but in light of what is now known about the electronic structure of alloys, that must be regarded as either a coincidence or indicative of some hitherto unrecognized correlation. The slope of $N(0)$ vs. z , however, is not in agreement with that derived from band-structure calculations /3,4/ for Pb. (Earlier heat capacity data /5/ on binary alloys with $3.90 < z < 4.09$ were interpreted as being in agreement with the calculated Pb band structure and the rigid-band model. However, the γ values were of lower precision and the λ values used in the analysis were not in good agreement with the more recent results.

Fig.2: λ and its component factors for the binary alloys, normalised to their values for Pb.

Smooth curves representing the z dependence of λ and its component factors for the binary alloys are shown in figure 2. The x dependence of the same quantities for the ternary alloys is shown in figure 3. The curves are based on data reported by Dynes and Rowell /1/ for $\langle \omega^2 \rangle$ and on the values of $N(0)$ and λ derived above. $\langle \omega^2 \rangle$ was calculated from Eq.(2). Throughout the range of z studied $N(0)$ is essentially constant and the trends with z of $\langle \omega^2 \rangle$ and $\langle \omega^2 \rangle^{-1}$ are in opposite directions. The net effects for the two alloy systems are quite different, however: for Pb-Bi alloys and increasing z , the strong increase in $\langle \omega^2 \rangle^{-1}$ dominates the decrease in $\langle \omega^2 \rangle$ and produces the observed increase in λ ; for Ti-Pb alloys and $z > 3.8$ the two effects more nearly can-

cel and λ is essentially constant: for $z < 3.8$ the trends in $\langle \omega^2 \rangle$ and $N(0)$ dominate the behavior of λ . For Pb-Bi alloys, McMillan's correlation/2/ is approximately correct and the trend in λ is determined largely by changes in the phonon spectrum; for the Ti-Pb alloys on the other hand it is largely the electronic properties that determine λ .

Fig.3: λ and its component factors for the "pseudo leads", normalised to their values for Pb.

The dip in the λ vs. z curve at $z = 4$ (figure 2) and the positive slope of the λ vs. x curve (figure 3) reflect the softening of the lattice associated with alloying. The behavior of $\langle \omega^2 \rangle$ for the binary alloys near $z = 4$ and for the ternary alloys corresponds closely to that of the calorimetric values of Θ for this system, and is similar to that observed in many other alloy systems.

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