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ON THE THERMAL AND ELECTRICAL CONDUCTIVITY OF V_3Si AND V_5Si_3

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Abstract. - Thermal conductivity and electrical resistivity measurements have been performed on V_3Si and V_5Si_3 single crystals. Thermal conductivity anomalies are observed on both compounds and seem likely to be related to the resistivity "saturation" behaviour exhibited by these two compounds.

Introduction. - It is known that the electrical resistivity of a "d" band compound (transition elements and their alloys) deviates from linearity at high temperature exhibiting a negative curvature.

Several interpretations as anharmonicity, Fermi Smearing, T dependent band structure, phonon ineffectiveness etc. (1) were proposed to explain such a behaviour.

In this paper we report and discuss results of the electrical and the thermal conductivity measurements performed on two extremely different compounds belonging to the Vanadium-Silicon system : V_3Si , an A15 compound with a high superconductivity temperature ($T_c \approx 17$ K) and V_5Si_3 which is normal down to 0.2 K.

Finally a correlation between these two transport properties is outlined for these compounds.

Experimental results. - Figure 1 shows the resistivity of V_3Si and V_5Si_3 as a function of temperature, both of these curves displaying the classical saturation phenomenon. The temperatures where a change of curvature can be observed, are respectively 82 K for V_3Si and 130 K for V_5Si_3 .

Recently it has been shown that the thermal conductivity of V_3Si (2) is mainly due to the electrons (Fig.2) whereas that of V_5Si_3 is partly due to the phonons. In this later case this dependence appears clearly by plotting K_p/T as a function of T (Fig.3) and shows that the contribution of the phonons which reaches a maximum at 20 K, is important around this temperature. In fact it appears difficult in the case of V_5Si_3 to separate quantitatively the two contributions of electrons and phonons and one has to consider qualitative arguments in this particular case. The thermal conductivity goes through a minimum for V_3Si (Fig.2) like for V_5Si_3 (Fig.4). In the case of V_3Si the temperature of this minimum T_m is the same as the temperature of the inflexion point in the $\rho(T)$ curve. For V_5Si_3 the conductivity due to phonons decreases at high temperature because of the occurrence of anharmonic and umklapp process and then the increase of $K(T)$ after T_m is essentially due to the electrons. More

precisely for this compound the temperature T_m of the minimum of $K(T)$ (150 K) differs slightly from the temperature of the inflexion point on the resistivity curve (130 K). This would be a consequence of the important contribution of the phonons in the thermal conductivity for the temperature range investigated.

Discussion. - The semi classical treatment of Wilson (3) involves a minimum to occur in the thermal conductivity but it is likely that such a treatment is not realistic for complex compounds as V_3Si and V_5Si_3 . Furthermore the behaviour of the resistivity cannot be explained satisfactory in the framework of a semi classical theory of transport phenomena. The empirical relation of Wiesmann et al (4)

$$\frac{1}{\rho} = \frac{1}{\rho_{ideal}} + \frac{1}{\rho_{max}}$$

(parallel resistor) takes into account the occurrence of the saturation phenomena where $\frac{1}{\rho_{max}}$ appears as an excess of electrical conductivity arising at high temperature. Similarly the increase of the thermal conductivity after the minimum can be understood as an excess of thermal conductivity.

Correlating the simultaneous increase of both conductivities, we suggest that such a behaviour could be explained by a growing "collectivization" of "d" electrons (5) as the temperature increases beyond T_m . This phenomenon could be interpreted as a continuous delocalization of the "d" electrons in the conduction band leading to an increase of the number of carriers contributing to the observed excess of both conductivities. For the compound V_3Si , experimental evidence of charge transfer and its redistribution with temperature has been obtained (6). Such a general process can take into account the existence of an inflexion point in the resistivity curve of transition metals and their alloys (Al_{15} , Nb, V, La, Zr_2Rh , V_5Si_3 , etc...) and the above correlation appears to have a general validity extending to other systems than those presently studied (7).

Moreover in the low temperature range, V_3Si and V_5Si_3 exhibit a quite different behaviour : - the resistivity of V_3Si behaves as $\rho = a + bT^n$ with $n \approx 2$ contrarily to that of V_5Si_3 $\rho = c + dT^m$ with $4 < m < 5$

- in the case of V_3Si the electrons are responsible of the thermal conductivity (2) whereas for V_5Si_3 an important part of this property is due to the phonon. These differences emphasize the importance of a particular electron phonon interaction related to the occurrence of superconductivity in V_3Si .

Conclusion. - It has been shown that at high temperature a correlation arises between the thermal and the electrical conductivity for the two compounds V_3Si and V_5Si_3 . It seems likely that such a correlation could be extended to other alloys based on transition elements. These studies are in progress and more details will be published elsewhere.

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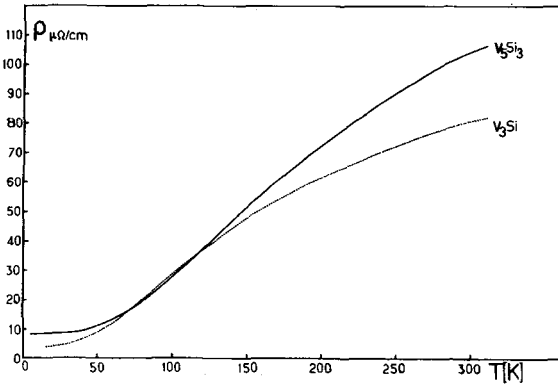


Fig. 1 - The resistivity of the V_3Si (MSi_2 , $[\bar{1}10]$, RRR = 20,4) and V_5Si_3 (151A, RRR = 11,6) single crystals.

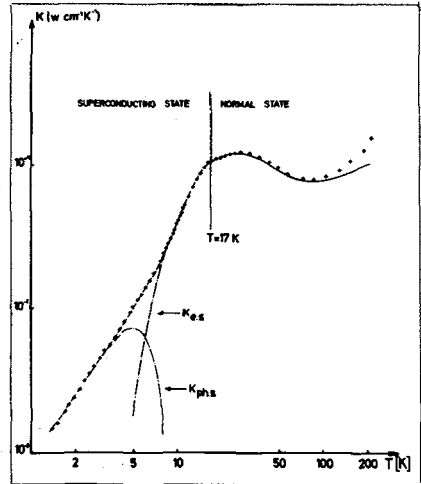


Fig. 2 - The thermal conductivity of the V_3Si sample (MSi_2) with the phonon (K_{phs}) and the electron K_{es} contributions.

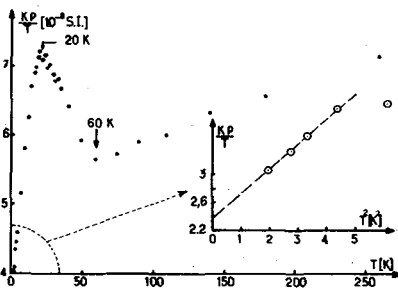


Fig. 3 - The parameter $\frac{K_p}{T}$ for the sample V_5Si_3 (151A) showing the extrapolation at $T = 0\text{ K}$ which gives the Lorentz number (insert).

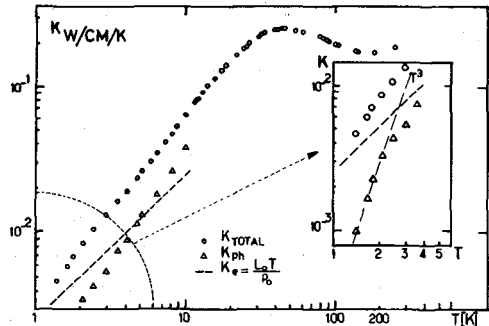


Fig. 4 - The thermal conductivity of the V_5Si_3 sample with the electron contribution calculated from $\text{WFL}^+ K_e = \frac{L_0 T}{\rho_0}$. The phonon contribution obeys the T^3 Law below 2 K (insert).

+ WFL = Wiedemann-Franz Law

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