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EFFECT OF PRESSURE ON T_c AND BAND STRUCTURE IN
TRANSITION METAL ALLOYS

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Measurements on ten alloys of the series Zr-Nb-Mo show a close correlation of dT_c/dp with the d-band structure of these alloys and suggest that the d-band is virtually rigid with respect to pressure.

In an attempt to detect some unifying principle for the complex reaction of superconductivity of transition metals and their alloys to application of hydrostatic pressure, the alloy series Zr-Nb-Mo was chosen on the following grounds: 1) The series is homologous in structure [1]. 2) Data on the electronic specific heat coefficient γ and θ_D exist [2]. 3) Presumably no effects of electron-magnon interactions complicate the situation.

The main result is that for all 10 alloys the variation of T_c with pressure is strongly influenced by the shape of the d-band.

Pressure up to 75 kbar was generated in a piston-cylinder type cell [3]. At first sight, the results are rather complex. For Nb and Nb-rich alloys a pronounced kink near 20 kbar occurs in the otherwise $T_c(p)$ behaviour. For Nb-Zr alloys with 20, 40 and 60 at. % Zr and for Nb₇₃Mo₂₇ no kink is observed; $T_c(p)$ is nearly linear for all pressures.

The results on alloys are collected in fig.1, to-

gether with other relevant parameters. The occurrence of the kink in $T_c(p)$ for the Nb-rich alloys is represented by splitting of $d \ln T_c/dp$ into two branches for $p < 20$ kbar and $p > 25$ kbar, respectively. We discuss here the results for $p > 25$ kbar where the slope $d \ln T_c/dp$ decreases monotonically with increasing number n of valence electrons per atom at zero pressure*. One notes that $d \ln T_c/dp$ changes sign at a concentration near that at which $T_c(n)$ has a maximum. Since in these alloys $T_c(n)$ is closely related to the d-band structure, this suggests that $T_c(p)$ is likewise connected with the d-band. Analyzing the data in this respect it is found that a best data fit is obtained by the simple relation

* n is thus defined by the chemical composition. It is not to be confused with the actual electron concentration which may be pressure dependent.

$$\partial \ln T_c / \partial p = a (\partial \ln T_c / \partial n - \partial \ln \theta / \partial n) + b \quad (1)$$

with $a = 0.40 \times 10^{-6} \text{ bar}^{-1}$ and $b = 0.62 \times 10^{-6} \text{ bar}^{-1}$, $\theta =$ Debye temperature. Substitution of the BSC expression for T_c in eq. (1) yields

$$\partial \ln \theta / \partial p + (NV)^{-1} \cdot \partial \ln NV / \partial p = \quad (2)$$

$$= a (NV)^{-1} \cdot \partial \ln NV / \partial n + b$$

$V = V_{\text{BCS}}$. (We note that comparison of the detailed shape of $\theta(n)$ and $T_c(n)$ near $n = 5$ makes

interpretation in terms of the more recent analysis of McMillan [4] less favourable). For niobium $\partial \ln \theta / \partial p = \gamma_G \cdot \kappa$ can be calculated from the experimental data on γ_G (Grüneisen parameter) [5] and κ (compressibility) [6]. $\partial \ln \theta / \partial p$ becomes $0.65 \times 10^{-6} \text{ bar}^{-1}$ which equals our empirical term b within experimental error. Under the reasonable assumption that $\partial \ln \theta / \partial p$ does not change much with composition, eq. (2) thus reduces to

$$\partial NV / \partial p = a \cdot \partial NV / \partial n \quad (3)$$

with the solution

$$NV = f(ap + n) \quad (4)$$

Thus we arrive at the result that for $p > 25 \text{ kbar}$ the shape of the function $NV(n)$ remains unaffected by pressure, i.e. is rigid with respect to pressure.

Since in this alloy system V is a slowly varying function of n , the shape of $NV(n)$ is mainly determined by N . One is led to assume that this is also true for $NV(p)$, and to conclude from eq. (4) that the effect of the application of pressure is primarily a filling of the d-band. A simple mechanism which would provide this can be seen in a pressure-induced shifting of the broad s-band relative to the narrow d-band.

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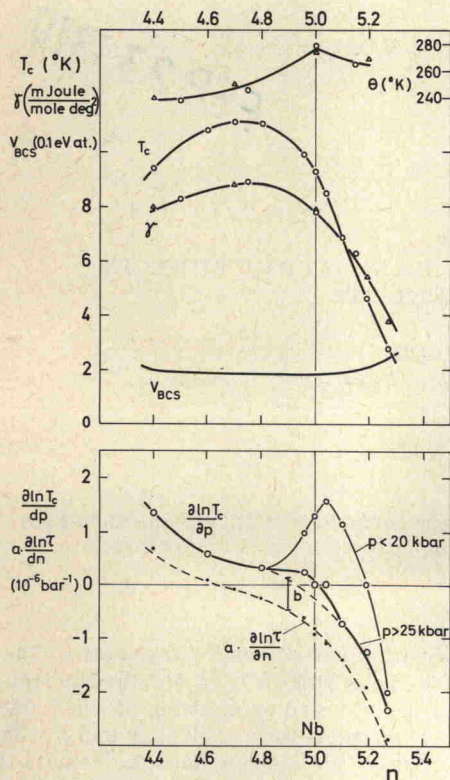


Fig. 1. Lower part: measured slopes $\partial \ln T_c / \partial p$. For $p > 25 \text{ kbar}$ comparison is made with $a \cdot \partial \ln T_c / \partial n \equiv a (\partial \ln T_c / \partial n - \partial \ln \theta / \partial n)$ (eq. (1) in the text). Relevant parameters are plotted in the upper part in the usual nomenclature. Data for θ and $\gamma \propto N$ were taken from ref. [2] and own measurements.

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