ELECTRICAL RESISTIVITY AND ELECTRONIC STRUCTURE OF AMORPHOUS $Ni_{81.5}P_xB_{18.5-x}$ ALLOYS

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Accurate measurements of electrical resistivity of seven amorphous alloys $Ni_{81.5}P_xB_{18.5-x}$ (x = 0, 1.8, 3.7, 7.4, 13, 16.7 and 18.5) have been performed in the temperature range 4.2–300K. The increase of the residual resistivity with x is accompained with a decrease in the temperature dependent contribution to resistivity ($\Delta\rho$). The reduced resistivities ρ_r (see text) show that the decrease of $\Delta\rho$ with x is related to the decrease in the electronic density of states at the Fermi level $N(E_F)$.

The amorphous $Ni_{81.5}P_xB_{18.5-x}$ alloy system is interesting because it allows the investigation of the changes in the physical properties caused by replacing one metalloid (B) for another (P). The low temperature heat capacity measurements$^{1)}$ have shown that both $N(E_F)$ and the Debye temperature (θ) decrease strongly with x. Furthermore the $N(E_F)$ data for this system fit well within those for other Ni-based glasses when plotted vs effective magnetic valency z* (z* accounts, in a crude way, for the changes in the band structure due to hybridisation of the electronic s, p, and d-states). Here we report the results of our measurements of the electrical resistivities of these alloys. The details concearning the sample preparation$^{1)}$ and the measurement technique were reported earlier.

Fig. 1 shows the residual resistivities ρ (measured at 4.2K) and the relative changes in resistivity $\Delta\rho/\rho = (\rho_{295} - \rho_{4.2})/\rho_{4.2}$ of amorphous $Ni_{81.5}P_xB_{18.5-x}$ alloys vs x. A large increase of ρ with x, accompained with a decrease of $\Delta\rho/\rho$ is observed. A similar behaviour of ρ and $\Delta\rho/\rho$ is observed in amorphous $Ni_{100-x}P_x$ alloys$^{2)}$ ($15 \leqslant x \leqslant 25$) and described in terms of Ziman model$^{3)}$. Within the framework of this model ρ increases due to an increase of the value of the structure factor at $2k_F$ which is caused by alloying with polyvalent element (P). The increase in ρ is accompained with a decrease in the temperature dependent part of resistivity ($\Delta\rho$) caused by thermal smea-

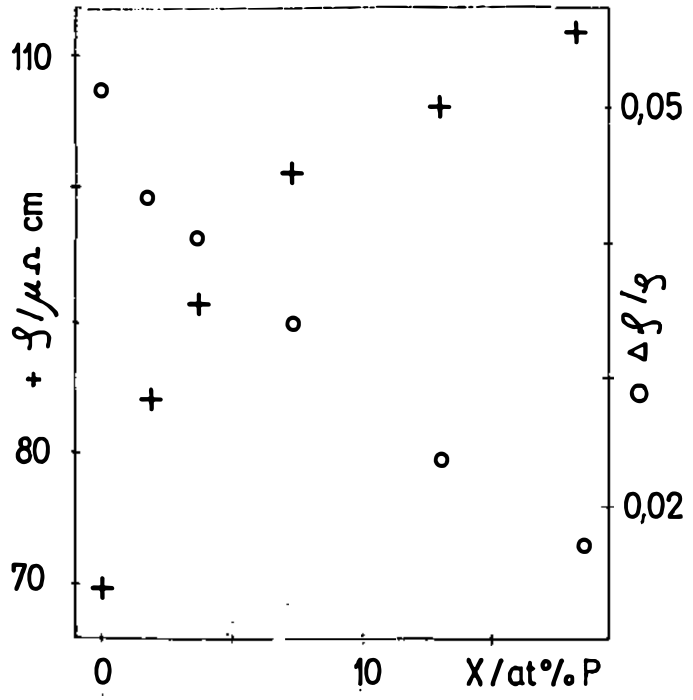

Fig. 1
Residual resistivity (ρ) and relative change in resistivity ($\Delta\rho/\rho$) of $Ni_{81.5}P_xB_{18.5-x}$ alloys vs x.

ring of the structure factor. In $Ni_{100-x}P_x$ alloys $\Delta\rho$ changes sign for $x \approx 24$ which could be interpreted with $2k_F$ being close to the position of the first peak of the structure factor.

However in order to reproduce the experimental resistivity results for $Ni_{100-x}P_x$ alloys a different number of conduction electrons per P atom had to be assigned[4] to different alloys (x) thus indicating the inadequacy of this simple donor model. Moreover, the Hall efect results for selected $Ni_{100-x}P_x$ alloys[5] yield the effective conduction electron concentrations quite different from those used for the explanation of their electrical resistivity[4]. In particular the effective electron concentration for $Ni_{76}P_{24}$ alloy was found[5] to be too small in order to account for a negative sign of $\Delta\rho$. On the other hand rather high resistivity of this alloy (160 μΩcm) seems to indicate that the incipient localization may be responsible for negative $\Delta\rho$. According to the above the Ziman model seems to be insufficient in order to explain both the size of the resistivity and its temperature variation in $Ni_{100-x}P_x$ and $Ni_{81.5}P_xB_{18.5-x}$ alloys. Therefore a proper understanding of resistivities of these alloys will probably have to await a detailed resistivity calculation starting from the hibridisied s, p and d-band (similar to those recently performed for liquid transition metals[6]).

We are not in the position to do such calculation but we can make some progress by relating the temperature dependent parts of the resistivity of $Ni_{81.5}P_xB_{18.5-x}$ alloys to their electronic structure. As mentioned earlier both $\Delta\rho$ and $N(E_F)$ in these alloys decrease rather rapidly and nonlinearly with x. In order to single out the electronic structure contribution to $\Delta\rho$ one can use the concept of the reduced resistivity[7]) defined by:

$$\rho_r = \Delta\rho \frac{M\,\theta^2 v^{1/3}}{T} \tag{1}$$

with M the molar mass, v the atomic volume and T = 295 K.

The reduced resistivity corrects crudely the change in resistivity for the lattice effects (assumed to be proportional to the square of the amplitude of ionic vibrations). This concept has been used[7]) for a pure crystalline metals in order to examine the difference in $\Delta\rho$ between the transition and simple metals. It was found that ρ_r for transition metals is of the order of unity while those for simple metals are about ten times smaller, thus clearly indicating the contribution of the electronic structure to $\Delta\rho$. It was also noted that the spread in ρ_r values is smaller for the metals with the same crystalline structure.

Compared with the crystalline metals and alloys the amorphous ones are to the first approximation isostructural and hence the relation between ρ_r and the electronic structure should appear even more clearly. The $Ni_{81.5}P_xB_{18.5-x}$ alloys have the additional advantage of being nonmagnetic so that the magnetic contribution to $\Delta\rho$ (which is not accounted for in ρ_r) is absent.

In Fig. 2 we show the reduced resistivities of our alloys vs corresponding $N(E_F)$ values. An approximately linear variation of ρ_r with $N(E_F)$ is observed. The ρ_r values are closer to those for simple (crystalline) metals than to those for transition

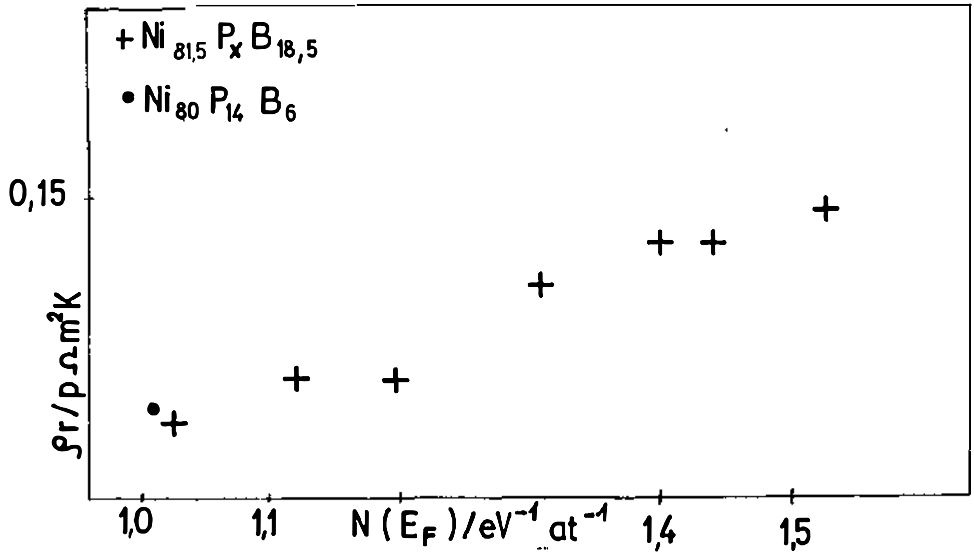

Fig. 2
Reduced resistivity (see text) of Ni-based metallic glasses vs $N(E_F)$

metals which is consistent with a rather low N(E_F) values of our alloys (but may also be a feature specific to amorphous alloys). For the comparison we also plotted in Fig. 2 the ρ_r value for the amorphous $Ni_{80}P_{14}B_6$ alloy which fits nicely within other data.

At the moment we have no detailed explanation for the observed linear variation of ρ_r with N(E_F) in Ni-based glasses. We note however that the increase in N(E_F) reflects a larger presence of Ni d-states at E_F and hence may imply an increase in the electron-phonon coupling which would enhance the variation of the electrical resistivity with temperature.

Summarizing the above we note that the available evidence suggest that the Ziman model is not sufficient to explain both the resistivity values and their temperature variations in Ni-based metallic glasses. Therefore for a proper description of ρ and $\Delta\rho$ a calculation of the electrical resistivity starting from the hybridised s, p and d bond is required. This view is supported by linear relation between the reduced resistivity and N(E_F) in NiPB alloys.

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