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On the Transition Temperature of Superconducting Alloys

O temperaturze przejścia stopów nadprzewodzących

O температуре сверхпроводящего перехода в сплавах

Dedicated to Professor
Stanisław Szpikowski on occasion
of his 60th birthday

1. INTRODUCTION

The study of the superconductivity in disordered systems and particularly in alloys has its long history [1]. The early approaches of Anderson and Gorkov [2] have shown that nonmagnetic impurities have a little effect on the transition temperature. The problem of the concentration dependence of the transition temperature $T_c(x)$ remained opened. The experimental data show [3] a variety of behaviours, which roughly can be collected in three groups. In the first group the transition temperature T_c of an A_xB_{1-x} alloys interpolates linearly as a function of con-

centration x between the T_c 's of pure components $T_c(A)$ and $T_c(B)$. For other groups $T_c(x)$ possesses a minimum or a maximum for some concentration $0 < x < 1$, where the $T_c(x) \leq T_c(A)$, $T_c(B)$. The most interesting case is that corresponding to the maximum. Although the effect on the relative scale can be pretty large - transition temperature of an alloy can be two or three times as large as that for pure materials - its value is usually small of order of few K.

There exists in the literature number of papers [4-7] devoted to the study of the $T_c(x)$. Except of [4] all they use weak coupling BCS type of model interaction. Previously [8] we have formulated Eliashberg type of the theory for superconducting transition metal alloys formulated in Wannier representation. Coherent potential approximation (CPA) has been used to treat disorder. That approach was based on the following tight-binding Hamiltonian at a fixed configuration of ions

$$H = H_e + H_{ion} + H_{e-ion} \quad (1)$$

where

$$H_e = \sum_{i\sigma} \epsilon_i n_{i\sigma} + \frac{1}{2} \sum_{i\sigma} U_i n_{i\sigma} n_{i-\sigma} + \sum_{ij\sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} \quad (2)$$

$$H_{ion} = \sum_i p_i^2 / 2M_i + \frac{1}{2} \sum_{ij} \sum_{\alpha\beta} u_i^\alpha \phi_{ij}^{\alpha\beta} \cdot u_j^\beta \quad (3)$$

$$H_{e-ion} = \sum_{ij\sigma} \sum_{\alpha} T_{ij}^\alpha (u_i^\alpha - u_j^\alpha) a_{i\sigma}^+ a_{j\sigma} \quad (4)$$

$$T_{ij}^\alpha = \frac{q_0^i + q_0^j}{2} t_{ij} \frac{R_j^\alpha - R_i^\alpha}{|R_j - R_i|} \quad (5)$$

In the above formulae $n_{i\sigma} = a_{i\sigma}^+ a_{i\sigma}$ and $a_{i\sigma}^+ (a_{i\sigma})$ creates (annihilates) the d electron in the Wannier state $\psi_{i\sigma}$ with spin σ , the t_{ij} are hopping matrix elements. ϵ_i , U_i , M_i are random "energy levels", intrasite Coulomb matrix elements and ion masses, respectively. u_i^α denotes the α^{th} component of the displacement of an ion of the i^{th} site and q_0^i is the

Slater coefficient describing an exponential $\exp(-q_0^1 r)$ decrease of the d-electron wave function [9]. The presence of the atomic parameters of d electrons in hamiltonian (1) is the important feature of the theory [8] because the various correlations exist between superconducting and atomic parameters [3].

2. THE THEORY

In this section we shall briefly review the previous [8] theory. The starting point was the hamiltonian (1-5) defined on a Cubic lattices. Besides the usual Migdal-Eliashberg type of approximations [10] the another one has been used. It is so called contact approximation in which electron scattering processes caused by either electron-electron or electron-phonon interactions were taken into account only if the two electrons are initially both at the same site, say i and finally both at another site say j [4]. In the tight binding scheme this means the neglect of all off-diagonal (in site indices) matrix elements of the Greens functions and self-energies. The resulting Eliashberg equations has been configurationally averaged by means of the CPA [11] and then solved for T_c .

The resulting formula for the transition temperature is that of McMillan [12]

$$T_c = \frac{\theta}{1.45} \exp - \frac{1.04(1 + \lambda_{\text{eff}})}{\lambda_{\text{eff}} - \mu_{\text{eff}}^* (1 + 0.62 \lambda_{\text{eff}})} \quad (6)$$

with the parameters pertaining to the $A_x B_{1-x}$ alloy

$$\lambda_{\text{eff}} = \sum_{\alpha} \bar{v}^2 \frac{d^2}{d^2} \left\{ x N_A \tilde{D}_A^{\alpha} [x q_A^2 N_A + y/4 (q_A + q_B)^2 N_B] \right. \\ \left. + y N_B \tilde{D}_B^{\alpha} [y q_B^2 N_B + x/4 (q_A + q_B)^2 N_A] \right\} / N \quad (7)$$

$$\mu_{\text{eff}}^* = \mu_{\text{eff}} / (1 + \mu_{\text{eff}} \ln E/\theta) \quad (8)$$

where \bar{t} denotes the averaged hopping matrix element, Θ is the Debye temperature of the alloy, d is the distance between neighbouring atoms in a lattice, $y = 1 - x$.

$N_A(N_B)$, N denote, respectively, the partially and totally averaged electron densities of states at the Fermi level E_F and

$$\mu_{\text{eff}} = \langle U_i N_i^2 / N \rangle \quad (9)$$

$$\tilde{D}_1^{\alpha} = -\frac{2}{\pi} \int d\omega \frac{\text{Im } D_1^{\alpha}(\omega + i0)}{\omega}; \quad i=A,B \quad (10)$$

3. CONCENTRATION DEPENDENCE OF T_c

Equations (6)-(10) form a basis for the study of the concentration dependence of T_c . The problem has been previously studied numerically [5, 6] on the basis of similar theories. Here we want to study the concentration dependence of the transition temperature without numerical calculations. To this end let us simplify the expressions for effective parameters $\lambda_{\text{eff}}(x)$ and $\mu_{\text{eff}}(x)$. The parameters of the pure materials we are here interested in are collected in Table 1.

Table 1. Some of the parameters describing pure superconducting elements [3].

Element	Atomic structure	q_0 (\AA^{-1})	Work function (eV)	Θ (K)	T_c (K)	λ	μ	Ionic mass (m.u.)	Lattice
Ti	$3d^2 4s^2$	0.93	3.40	380	0.39	0.38	0.27	47.90	hex
V	$3d^3 4s^2$		4.25	390	5.43	0.60	0.26	50.94	bcc
Zr	$4d^2 5s^2$	0.91	3.15	250	0.53	0.41	0.25	91.22	hex
Nb	$4d^4 5s^1$		4.00	275	9.25	0.82	0.26	92.91	bcc
Mo	$4d^5 5s^1$	0.87	4.65	380	0.92	0.38	0.20	95.94	bcc
Ta	$5d^3 6s^2$		4.05	225	4.48	0.65	0.21	180.95	bcc

For we are interested in qualitative dependence $T_c(x)$ rather than quantitative one we can safely assume $q_A = q_B = q_0$. Similarly we neglect the α dependence in (7) and (10). These lead to the expressions

$$\lambda_{\text{eff}}(x) = t^2(x) [x N_A(x) \bar{D}_A(x) + (1-x) N_B(x) \bar{D}_B(x)]$$

$$\mu_{\text{eff}}(x) = [x U_A N_A^2(x) + (1-x) U_B N_B^2(x)] / N(x) \quad (11)$$

Exact numerical calculations in principle take into account the mutual influence of electrons on phonons. This has been neglected in (11).

The study of the concentration dependence of any quantity encounters one obvious problem. Namely the changes in the position of the Fermi level with concentration. This feature makes the determination of the function $N_{A(B)}(x)$ very difficult.

The simplest possibility is that none of the parameters in (12) is x dependent. Thus we get

$$\lambda_{\text{eff}}(x) = x \lambda_A + (1-x) \lambda_B$$

$$\mu_{\text{eff}}(x) = x \mu_A + (1-x) \mu_B \quad (12)$$

where the $\lambda_{A(B)}$, $\mu_{A(B)}$ are x -independent parameters characterising pure elements. This virtual crystal type of approximation describes quite well the $T_c(x)$ an $\text{Ta}_x\text{Nb}_{1-x}$ alloy. The comparison is shown in Figure 1.

Although the masses of Ta and Nb differ considerably (see Table 1) the neglect of the concentration dependence of \bar{D}_i seem to play a minor role. This may be related to the fact that \bar{D}_i is an integral quantity - its concentration dependence has been washed out by integration and also weighting factor $(1/\omega)$ in (10). So we retain this approximation and try $N_A(x) \approx x N_A^0$, $N_B(x) \approx (1-x) N_B^0$ where N_A^0 and N_B^0 are to be understood as the densities of states at the Fermi level of pure elements. Such an approximation nicely describes $T_c(x)$ for $\text{Mo}_x\text{Nb}_{1-x}$ alloy as seen from Figure 2.

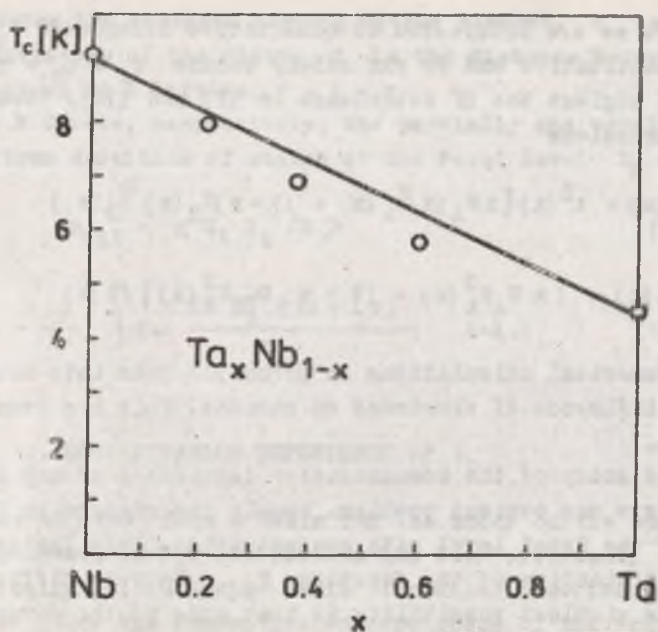


Fig. 1.

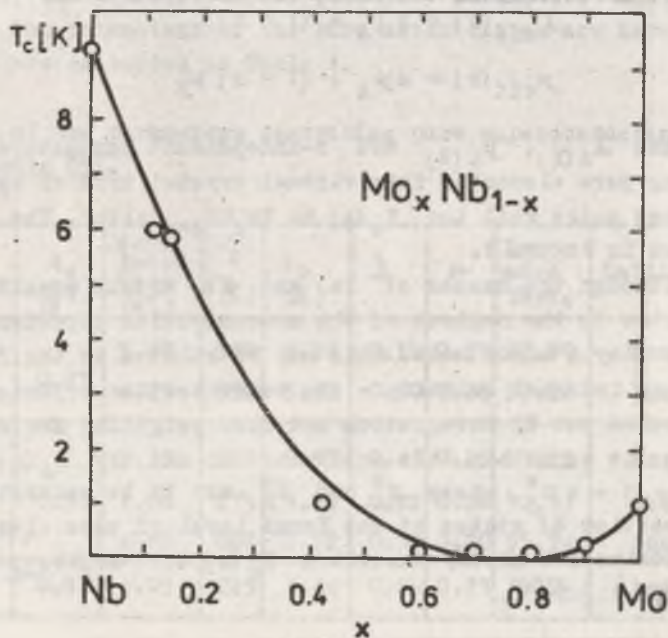


Fig. 2.

Similarly $T_c(x)$ for V_xNb_{1-x} and V_xTa_{1-x} can be described by taking $N_A(x) = \sqrt{x} N_A^0$. Then

$$\begin{aligned} \lambda_{\text{eff}}(x) &= x^{3/2} \lambda_A + (1-x)^{3/2} \lambda_B \\ \mu_{\text{eff}}(x) &= x^2 \mu_A + (1-x)^2 \mu_B \end{aligned} \quad (13)$$

The resulting comparison is shown in Figure 3.

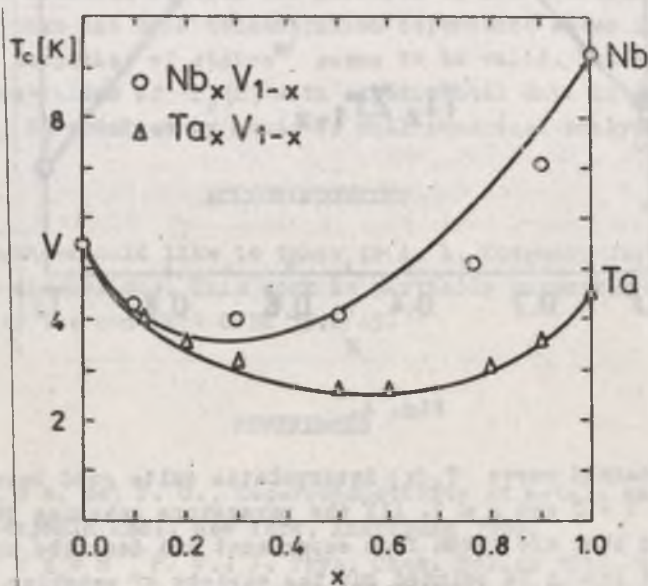


Fig. 3.

The most desirable type of dependence is given in Figure 4. Here $T_c(x)$ of an alloy Ti_xZr_{1-x} is for $0.35 < x < 0.7$ two or three times that of pure elements. This can be described by assuming the dependence

$$\begin{aligned} \lambda_{\text{eff}} &= x \lambda_A + (1-x) \lambda_B \\ \mu_{\text{eff}} &= x^2 \mu_A + (1-x)^2 \mu_B \end{aligned} \quad (14)$$

Suggesting that the product $N_A(x)D_A(x)$ is concentration independent while $N_A(x)/N(x)$ should be proportional to x .

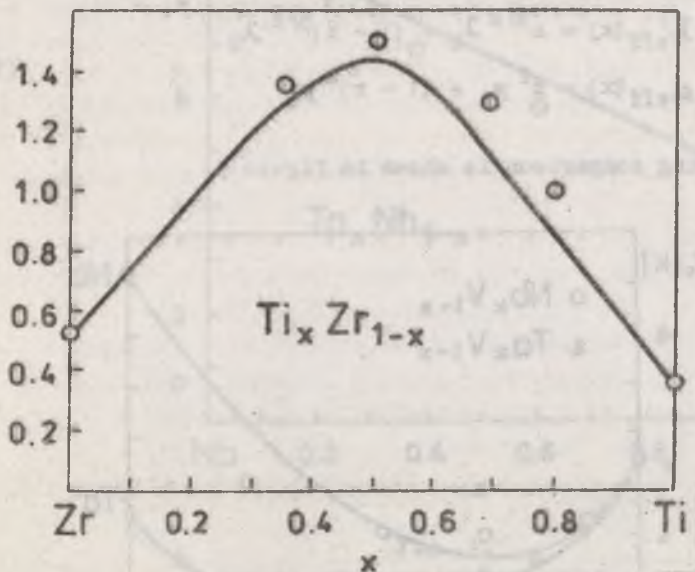


Fig. 4.

The obtained curve $T_c(x)$ interpolates quite good between the limits $x = 0$ and $x = 1$. All the parameters entering (6) are realistic as they are taken from experiment and describe the pure elements. It should be pointed out the variety of existing T_c formulae [13]. We have used here the most popular one and discussed the $T_c(x)$ in terms of the effective electron-phonon coupling λ_{eff} and Coulomb pseudopotential μ_{eff} . The independent experiments measuring the concentration dependence of λ would be very desirable as an independent check of the correctness of the above guess. (See however [14] for the examples of the concentration dependence of the (local and total) densities of states at the Fermi level calculated in CPA for a different purpose).

3. CONCLUSION

We have analyzed the concentration dependence of the superconducting transition temperature of substitutionally disordered transition metal alloys. Using the expressions for $T_c(x)$ obtained previously [8] we tried to extract the concentration dependence mainly of the electronic density of states. Although we have guessed (but see [14]) the explicit form of this dependence rather than obtained it from the solution of CPA equations, the conclusion that the main concentration dependence stems from the electronic densities of states^{*} seems to be valid. The agreement of the above values of $T_c(x)$ with experimental data is as good as that [5, 6] obtained by means of full numerical analysis.

ACKNOWLEDGEMENT

The authors would like to thank dr A. L. Kuzemsky for past and recent discussions. This work is partially supported by INTiBS under the contract CPBR 15.6/45.

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^{*} K.I.W. take the opportunity to thank prof. J. Appel for asking him that question some time ago.

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STRESZCZENIE

Dla szeregu stopów metali przejściowych obliczono zależność temperatury przejścia T_c w stan nadprzewodnictwa od koncentracji atomów. Okazało się, że poprawny opis funkcji $T_c(x)$ dla stopów Ta_xNb_{1-x} , Mo_xNb_{1-x} , V_xNb_{1-x} i V_xTa_x uzyskuje się uwzględniając jedynie zależność gęstości stanów $N_A(x)$ oraz $N_B(x)$ obliczonych w ramach przybliżenia potencjału koherentnego. Opis zależności $T_c(x)$ stopu Ti_xZr_{1-x} wymaga uwzględnienia zmian gęstości stanów fononów ze zmianą składu stopu. W pracy zaniedbano zależność od x innych parametrów stopu.

РЕЗЮМЕ

В работе вычислена температура сверхпроводящего перехода ряда сплавов. Хорошие согласье с экспериментом получено для сплавов Ta_xNb_{1-x} , Mo_xNb_{1-x} , V_xNb_{1-x} и V_xTa_{1-x} учитывая зависимость от x только плотности электронных состояний. Для сплава Ti_xZr_{1-x} надо также учесть зависимость от x плотности фононных состояний и константы связи.

