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DISORDERED PSEUDO ONE-DIMENSIONAL CONDUCTORS**

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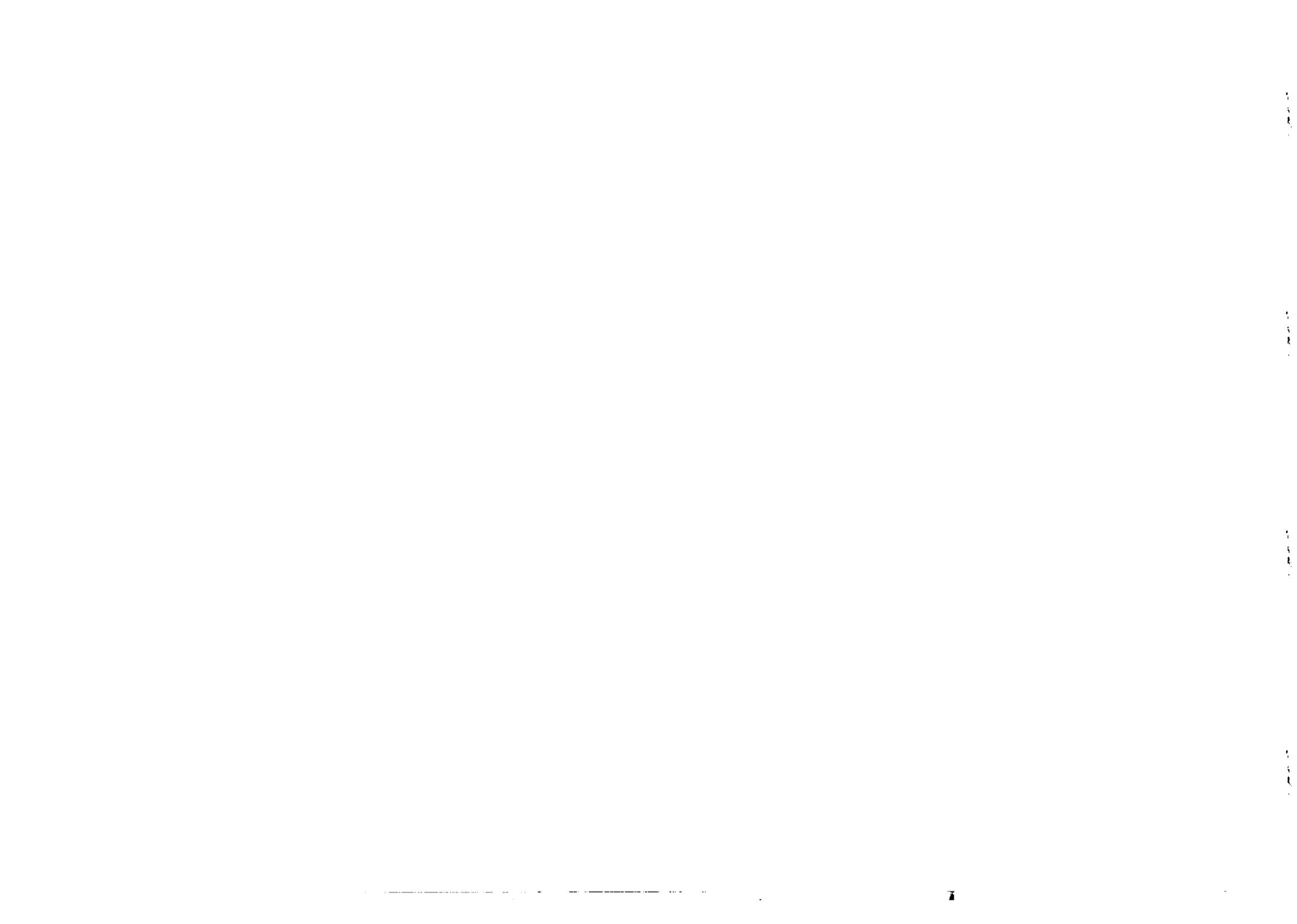


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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

PEIERLS INSTABILITY AND SUPERCONDUCTIVITY IN SUBSTITUTIONALLY
DISORDERED PSEUDO ONE-DIMENSIONAL CONDUCTORS*

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ABSTRACT

With CPA method the effect of the substitutional disorder in the pseudo one-dimensional conductors on the Peierls transition temperature (T_p) and superconductive transition temperature (T_c) has been calculated. The favourable condition for searching for somewhat high T_c superconductors in these systems has been discussed.

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1. INTRODUCTION

There has been a growing interest in the properties of materials with pseudo one-dimensional (1D) electronic systems for a long time [1]-[5]. Among all these materials the inorganic linear chain compounds such as the KCP-type conductors (e.g. $K_2Pt(CN)_4Br_{0.3} \cdot 3H_2O$), the linear chain trichalcogenides (e.g. $NbSe_3$) and the organic linear stacking compounds (e.g. TTF-TCNQ) are typical and have been widely studied. There are many different types of order that may occur in these systems - superconductive pairing, Peierls electron-hole pairing etc. From the theoretical point of view, one of the most interesting problems is the relation between the phonon softening associated with the Peierls instability and superconductivity [6]. On the other hand, it is also well known that disorder may arise in many ways in pseudo one-dimensional systems and plays an important role in many properties [3]. It is reasonable to discuss to what extent the disorder affects the relation between the phonon softening above the Peierls transition and superconductivity. In a previous paper [7] we confine ourselves to the pseudo 1D crystals containing a small amount of randomly positioned non-magnetic impurities. In this paper the calculation in the case of substitutionally disordered 1D conductors up to the moderate concentration is presented, and the favourable conditions for searching for somewhat high T_c superconductors are discussed.

2. MODEL AND CALCULATION

We have made calculation for a disordered binary substitutional alloy $A_x B_{1-x}$, using a tight binding Hamiltonian with single site energies ϵ_A and ϵ_B in correspondence with the kinds of atoms A and B occupying this site. The electrons are supposed to be in a single half-filled conduction band of 1D system. Besides, the phonon frequency ω and the electron-phonon coupling constant g are also considered to be site dependent.

As well known, the coherent potential approximation (CPA) has been shown to be a simple effective method in studying the disorder effects of alloys and applied to superconducting substitutional alloys successfully by A. Weinkauff and J. Zittartz [8]. Thus, I have treated the effect of atomic configurations on T_p and T_c by the CPA method introduced by B. Velicky [9]. The effects of spatially fluctuating of ω and g have only been treated by assuming a linear average procedure.

In the RPA we have the phonon self-energy

$$\Pi(i\omega_m, \mathbf{q}) = T g_f^2 \sum_n \sum_{\mathbf{k}} G(i\omega_n, \mathbf{k}) G(i\omega_n + i\omega_m, \mathbf{k} + \mathbf{q})$$

where $\omega_n = (2n+1)\pi T$, $n = 0, \pm 1, \dots$. Taking the average procedure by the method of B. Velicky one can write

$$\langle \Pi(0, \mathbf{q}) \rangle = T g_f^2 \sum_n \langle \sum_{\mathbf{k}} G(i\omega_n, \mathbf{k}) G(i\omega_n, \mathbf{k} + \mathbf{q}) \rangle \quad (1)$$

where $\langle \rangle$ means the average over the ensemble of atomic configurations of the substitutional alloys, g is the corresponding averaged electron-phonon coupling constant. According to the CPA treatment in reference [9] one can write the average on the right-hand side of (1) as follows:

$$\langle \sum_{\mathbf{k}} G(i\omega_n, \mathbf{k}) G(i\omega_n, \mathbf{k} + \mathbf{q}) \rangle = \sum_{\mathbf{k}} \bar{G}(i\omega_n, \mathbf{k}) \bar{G}(i\omega_n, \mathbf{k} + \mathbf{q}) + \sum_{\mathbf{k}} [\bar{G}(i\omega_n, \mathbf{k})]^2 \Lambda [\bar{G}(i\omega_n, \mathbf{k} + \mathbf{q})]^2 \quad (2)$$

where \bar{G} is the Green function in the presence of disorder,

$$\bar{G} = \frac{1}{z - \epsilon_{\mathbf{k}} - \Sigma(z)} \quad (3)$$

$\Sigma(z)$ is the coherent potential in CPA. $\epsilon_{\mathbf{k}}$ is the energy of the perfect system (pure B metal). The expression (2) is correct up to the terms of the second order.

The vertex function Λ can be obtained by the method of Leath [10],

$$\Lambda = \frac{\delta \Sigma}{\delta F} \quad (4)$$

We have calculated F by [9]

$$F(z) = \int_{-\infty}^{\infty} d\epsilon (z - \Sigma(z) - \epsilon)^{-1} g^0(\epsilon) \quad (5)$$

where $g^0(\epsilon)$ is the state density per atom for the pure B substance. The coherent potential $\Sigma(z)$ can be given by [9]

$$\Sigma(z) = x(\epsilon_A - \epsilon_B) + [\epsilon_A - \epsilon_B - \Sigma(z)] F(z) \Sigma(z) \quad (6)$$

In order to make the calculation be tractable, I have taken the assumption of a Lorentzian density [8],[11],

$$g^0(\epsilon) = \frac{1}{\pi} \frac{D}{1 + D^2 \epsilon^2} \quad (7)$$

here $D = \pi N(0)$, $N(0)$ is the density of states per spin at the Fermi level. Then one obtains

$$F(z) = (z - \Sigma(z) + iD^{-1}\eta)^{-1} \quad (8a)$$

$$\eta(z) = \text{Sgn} \{ \text{Im} (z - \Sigma(z)) \} \quad (8b)$$

Combining (6) with (8) it was found that,

$$\Sigma(z) = \frac{(z + i\eta(z)/D) x (\epsilon_A - \epsilon_B)}{z - [(\epsilon_A - \epsilon_B) - x(\epsilon_A - \epsilon_B)] + i\eta(z)/D} \quad (9)$$

The vertex function Λ can be calculated by (4).

Following [12], the symmetry relation of the electron dispersion $\epsilon_{\mathbf{k}+2\mathbf{k}_F} = -\epsilon_{\mathbf{k}}$ ($\epsilon_{\mathbf{k}}$ is measured from the Fermi level) was taken and then one has

$$\sum_k \bar{G}(i\omega_n, k) \bar{G}(i\omega_n, k+2k_f) = \frac{1}{i\omega_n - \Sigma(i\omega_n)} \cdot \frac{1}{i\omega_n - \Sigma(i\omega_n) + i\eta(i\omega_n)/D} \quad (10)$$

According to the experience of [8] [11] and [13], in the limit $D^{-1} \gg k_{B T_p}$, $\Sigma(z)$ (and thus $F(z)$) may be replaced approximately by their values at $z = i0$. We have

$$\text{Re } \Sigma(i0) \equiv a = \frac{x(\epsilon_A - \epsilon_B)}{1 + (1-x)^2 \delta^2} \quad (11a)$$

$$\text{Im } \Sigma(i0) \equiv -b\eta(i0) = -\frac{x(1-x)\delta(\epsilon_A - \epsilon_B)}{1 + (1-x)^2 \delta^2} \eta(i0) \quad (11b)$$

here $\delta = D(\epsilon_A - \epsilon_B)$ measuring the relative strength of the compositional disorder. It is easy to see that in the limit $x \ll 1$ one obtains

$$\text{Im } \Sigma(i0) = -\pi N(0) x (\epsilon_A - \epsilon_B)^2 \eta(i0),$$

$$\bar{G} = \frac{1}{i\omega_n - (\text{Re } \Sigma(i0) + \epsilon_f) + i\eta(i0)[\pi N(0)x(\epsilon_A - \epsilon_B)^2]}$$

Clearly, these are essentially the same results as shown by the formulae (4) and (5) in reference [7] except the apparent differences in symbols.

Using the similar techniques described in reference [7], after a detailed calculation I finally obtained the following results for 1D conductors,

$$\begin{aligned} \langle \Pi(0, 2k_f) \rangle &\approx T g^2 \sum_n \sum_k \bar{G}(i\omega_n, k) \bar{G}(i\omega_n, k+2k_f) \\ &= \frac{g^2 D}{\pi} \left[\text{Re } \Psi\left(\frac{1}{2} z_2'\right) - \text{Re } \Psi\left(\frac{1}{2} z_1'\right) \right] \end{aligned} \quad (12)$$

where

$$\begin{aligned} \frac{1}{2} z_1' &= \left(\frac{1}{2} + \frac{b}{2\pi T} + \frac{1}{D\pi T}\right) + i \frac{a}{2\pi T} \\ \frac{1}{2} z_2' &= \left(\frac{1}{2} + \frac{b}{2\pi T}\right) + i \frac{a}{2\pi T} \end{aligned} \quad (13)$$

This result is correct to the right-hand first term of equation (2). In the limit of pure substance ($x = 0$) and $D^{-1} \gg k_{B T_p}$, equation (12) reduces to

$$\langle \Pi(0, 2k_f) \rangle \approx \frac{g^2 D}{\pi} \left[\text{Re } \Psi\left(\frac{1}{2}\right) - \text{Re } \Psi\left(\frac{1}{D\pi T}\right) \right]$$

Making use of the asymptotic expansion, $\psi(z) = \ln z$ and $\psi\left(\frac{1}{2}\right) = -\gamma - 2\ln 2$ ($\gamma = 0.577$), one obtains the same formula of Rice and Strässler [14] for the Peierls transition temperature T_p^0 of the pure 1D Conductor, i.e.

$$T_p^0 = \frac{4}{\pi D} e^{\gamma} e^{-\omega^2/2g^2 N(0)}$$

Including the second term on the right-hand side of equation (2), the equation determining the Peierls transition temperature T_p of the disordered 1D alloys ($A_x B_{1-x}$) is

$$\frac{1}{\langle \lambda \rangle} = F(\delta, x, T_p) \quad (14)$$

where $\langle \lambda \rangle$ is the average normalized coupling constant given by the simplest approximation $x\lambda_A + (1-x)\lambda_B$, $\lambda_i = 2N(0)\epsilon_i^2 / \omega_i^0$ ($i = A, B$), and by detailed calculation one gets

$$F(\delta, x, T) = \frac{1}{2} S(x, \delta) \left\{ \text{Im } \Psi\left(\frac{1}{2} z_2'\right) - \text{Im } \Psi\left(\frac{1}{2} z_1'\right) \right\} - \left(1 + \frac{1}{2} R(x, \delta)\right) \left[\text{Re } \Psi\left(\frac{1}{2} z_2'\right) - \text{Re } \Psi\left(\frac{1}{2} z_1'\right) \right]$$

$$-\frac{1}{2} \frac{1}{D\pi T} \left[R(x, \delta) \operatorname{Re} \psi' \left(\frac{1}{2} Z_1' \right) - S(x, \delta) \operatorname{Im} \psi' \left(\frac{1}{2} Z_1' \right) \right] \\ + \frac{1}{4} \frac{1}{(D\pi T)^2} \left[R(x, \delta) \operatorname{Re} \psi'' \left(\frac{1}{2} Z_1' \right) - S(x, \delta) \operatorname{Im} \psi'' \left(\frac{1}{2} Z_1' \right) \right],$$

here, some dimensionless quantities of x and δ , which may be calculated numerically, are

$$R(x, \delta) = \frac{f_3(1+f_3)f_1 - f_2f_4}{f_2^2 + f_1^2f_3^2}, \quad S(x, \delta) = \frac{f_1f_3f_4 + (1+f_3)f_2}{f_2^2 + f_3^2f_1^2}$$

$$f_1 = \frac{1}{x^2(1-x)^2\delta^4} - \frac{(1-x)^2}{x^2} - \frac{[1+(1-x)^2\delta^2]^2}{\{[1+(1-x)\delta^2]^2 + x^2\delta^4\}(1-x)^2\delta^2},$$

$$f_2 = -\frac{2}{x\delta} + \frac{[1+(1-x)\delta^2][1+(1-x)^2\delta^2]}{(1-x)\delta\{[1+(1-x)\delta^2]^2 + x^2\delta^4\}},$$

$$f_3 = \frac{x(1-x)\delta^2}{1+(1-x)^2\delta^2},$$

$$f_4 = \frac{x\delta}{1+(1-x)^2\delta^2}$$

Following the procedure in reference [6], the electron-phonon coupling constant λ_{su} determining the superconductive critical temperature T_c in the McMillan's formula is given by

$$\lambda_{su} = \frac{1}{4} \frac{1}{\langle \lambda \rangle^{-1} + F} \quad (15)$$

Besides, the Debye temperature Θ of the $A_x B_{1-x}$ alloy is given in the usual approximation

$$\Theta = x\Theta_A + (1-x)\Theta_B$$

here Θ_A and Θ_B are the Debye temperature of the constituents A and B respectively. Finally making use of the McMillan's formula we calculated T_c .

The results of T_p and T_c are shown in Fig. 1, 2. Since the equation (2) is correct only to the second order, the above mentioned method of calculating T_p and T_c in substitutionally disordered pseudo one-dimensional alloys is valid only up to the moderate concentration of the second constituent.

3. RESULTS

From Fig. 1 and 2 we see that alloying with a very low concentration of the second constituent reduces DT_p and DT_c . However, if $\lambda_A > \lambda_B$, DT_p begins to increase as x increases to some value. This is in consistence with the results of C. Tannous et al. [11]. Furthermore, we have found that the reduced superconductive transition temperature DT_c may be higher or lower than DT_p , which depends on the values of electron-phonon coupling constant λ and the reduced Debye temperature $D\Theta$. For fixed values of λ_A and λ_B , DT_c will become lower than DT_p if the value of $D\Theta$ is relatively low, but for higher $D\Theta$, DT_c may be higher than DT_p . The magnitude of value of $D\Theta$ which make DT_c higher than DT_p varies with the values of λ_A and λ_B (see Fig. 1, 2). Anyway, it is important that DT_c will certainly become higher than DT_p for some appropriate range of the values of λ and Θ .

4. SUMMARY

Using CPA we have developed a method of calculating T_p and T_c in substitutionally disordered pseudo one-dimensional alloys up to the moderate concentration of the second constituent and thus discussed the effects of substitutional disorder on the relation between the phonon softening associated with the Peierls instability and superconductivity. The main point is that by introducing proper kind and amount of impurities or the second constituent in $A_x B_{1-x}$, there is the possibility that one may make the best use of the phonon softening above the Peierls transition in pseudo one-dimensional systems to obtain somewhat high value of superconductive transition temperature.

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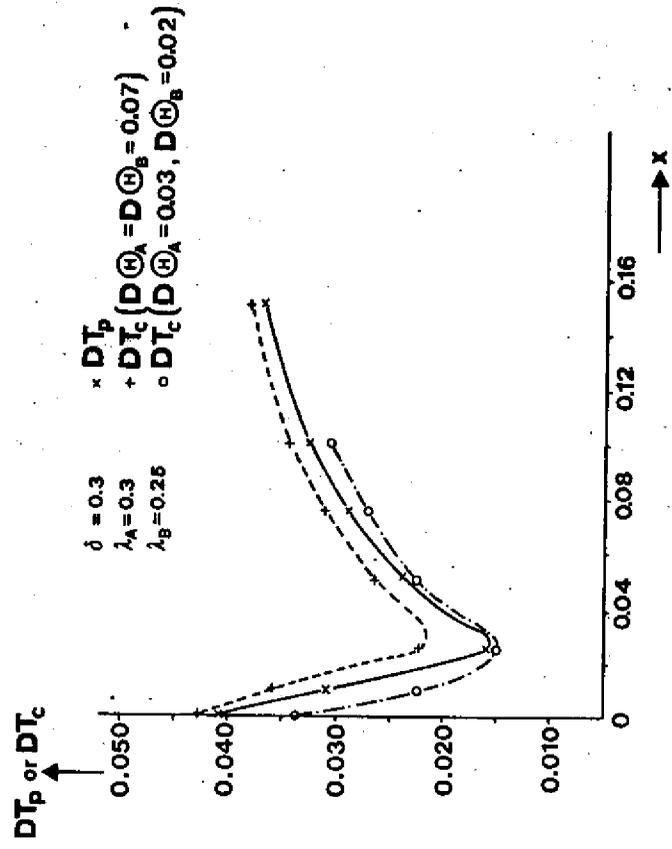


FIG. 1

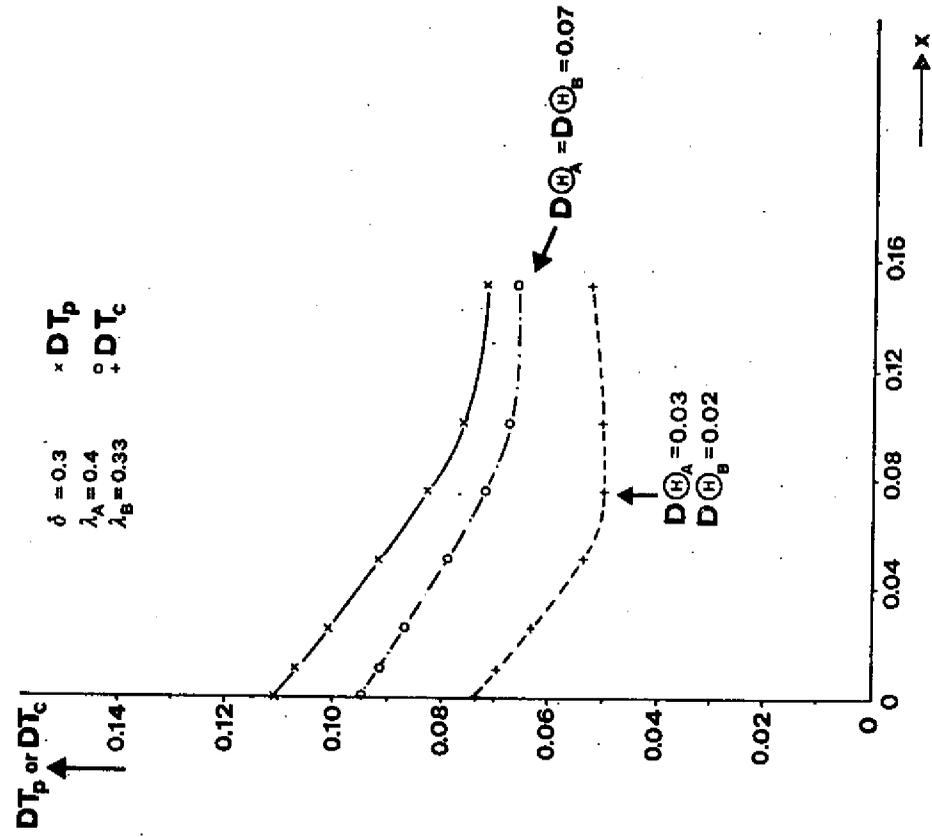


FIG. 2

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