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AN APPROXIMATE METHOD FOR CALCULATING ELECTRON-PHONON MATRIX ELEMENT OF A DISORDERED TRANSITION METAL AND RELEVANT COMMENTS ON SUPERCONDUCTIVITY*

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1. INTRODUCTION

The superconductive properties of the disordered superconductors, such as homogeneous amorphous alloys and substitutional alloys have been studied for a long time [1-4]. The amorphous non-transition superconductors show an increase of transition temperature (T_c) and the strong-coupling behaviour revealed by an enlarged ratio $2\Delta_o/k_BT_c$. However, for transition metals and alloys, experiments have not shown the consistent enhancement of T_c [1]. Theoretical treatment of electron-phonon (E-P) interaction and T_c in a disordered metal is usually based on the free-electron model. As the d-electrons play the most important role in the superconductive properties of transition metals (TM), it seems to be appropriate to develop a method based on the tight-binding approximation to calculate the E-P matrix element for the disordered transition metals. With this method as a basis the experimental T_c data of the amorphous TM superconductors are re-analysed. Finally, some relevant comments on the superconductivity of the disordered materials are given.

2. MODEL AND CALCULATION OF E-P MATRIX ELEMENT

We deal with the disordered solids which are supposed to be "statically" perturbed crystal lattices [2]. The position of the nucleus of the j-th atom in real space is represented by R_j and the random variables (δR_j) which are the small deviations of the atomic positions from a presumed regular periodic atomic sites (R_j^0), are given by a Gaussian distribution with the root-mean-square "static" deviation of atomic positions from their presumed equilibrium lattice positions represented by δ. The statistically translational invariance was taken in the sense that the Gaussian distribution is preserved periodically from cell to cell. For the sake of simplicity, the unperturbed lattice was considered to be a simple cubic lattice. Under the tight-binding approximation it is natural to use the assumption of rigid d-function. Besides, for small δ and small "lattice wave" displacements u_j, it seems to be appropriate to suppose that the well-localized d-functions remain quasiorthogonal. Introducing a_j^+ as the operator creating the electron in the state $|d(r - R_j^0 - \delta R_j - u_j)\rangle$, we can extend the Hubbard Hamiltonian to describe the perturbed lattice, i.e.,

$$H = \sum_{j,\alpha,\xi,\sigma} J_{j,\xi_\alpha}\, a^+_{j,\sigma}\, a_{j+\xi_\alpha,\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow} \qquad (1)$$

where $J_{j,\delta_\alpha} \equiv J(a_{\delta_\alpha} + u_{j+\delta_\alpha} - u_j + \delta R_{j+\delta_\alpha} - \delta R_j)$ is the overlap integral between j and $j + \delta_\alpha$ lying on the lattice axis a_α and $a_{\delta_\alpha} \equiv R^0_{j+\delta_\alpha} - R^0_j$ [5]. We expanded J in a Taylor series and retained only terms to the order linear in $(u_{j+\delta_\alpha} - u_j)$, including the cross terms of the "static" deviation and $u_{j+\delta_\alpha} - u_j$,

$$\begin{aligned} J_{j,\xi_\alpha} &= J(a_{\xi_\alpha} + \delta R_{j+\xi_\alpha} - \delta R_j) + \left.\frac{\partial J}{\partial R}\right|_{R = a_{\xi_\alpha} + \delta R_{j+\xi_\alpha} - \delta R_j} \cdot (u_{j+\xi_\alpha} - u_j) \\ &= J(a_{\xi_\alpha} + \delta R_{j+\xi_\alpha} - \delta R_j) - \beta_o J(a_\alpha)\, \frac{a_{\xi_\alpha}}{a_\alpha} \cdot (u_{j+\xi_\alpha} - u_j) \\ &\quad + \sum_{i,k} J''_{j,\delta_\alpha,i,k} (\delta R_{j+\delta_\alpha,k} - \delta R_{j,k})(u_{j+\xi_\alpha,i} - u_{j,i}), \end{aligned} \qquad (2)$$

where $\delta R_{j,k}$ is the k-th component of δR_j, $u_{j,i}$ is the i-th component of u_j, $J''_{j,\delta_\alpha,i,k}$ is the k-th component of the gradient of $J'_{j,\delta_\alpha,i}$ which means the i-th component of the gradient J_{j,δ_α}, their values are all evaluated at the equillibrium site of the unperturbed crystal. q_o is the Slater Coefficient describing the exponential, $\exp(-q_o r)$, decrease of the d function.

For the simple model of the amorphous metal mentioned above, the momentum of electrons may still be a fairly good quantum number, at least in the long wavelength range. Besides, following the discussion in [6], we have assumed $u_j = \exp(i(q \cdot R_j^o - \omega t))$ in calculating the E-P matrix of the disordered metal. Because of the smallness of δ, the following average procedure has been used,

$$\begin{aligned} \sum_j \exp[-i\vec{k}\cdot R_j^o + i\vec{k}\cdot R_j - i\vec{k}'\cdot R_{j+i}] \propto\ & \langle \exp(i\vec{k}\cdot\delta R_j - i\vec{k}'\cdot\delta R_{j+i})\rangle \\ & \times \sum_j \exp[-(\vec{k} - \vec{k}' - \vec{q})\cdot R_j^o] \end{aligned} \qquad (3)$$

where $\langle\rangle$ means the average over the Gaussian distribution. We finally obtained the square of the E-P matrix element as follows,

$$\left|\langle k'\lambda'|H_{e-p}|k\lambda\rangle\right|^2 = \frac{1}{2}\sum_{\alpha}\left(q^2 J_\alpha^2 + J_\alpha^{*2}\delta^2\right)\left(\frac{a_\alpha\cdot e_\alpha}{a_\alpha}\right)^2 \frac{\hbar}{2NM\omega_{k,\lambda}}\left(\sin k_\alpha a_\alpha - \sin k'_\alpha a_\alpha\right)^2 \times\left\{\delta_{k'-k-g}\exp\left[-(k-k')^2\delta^2\right] + \frac{1}{N}\left(1-\exp\left[-(k-k')^2\delta^2\right]\right)\right\} \quad (4)$$

where $J_\alpha^{*2} = 2\sum_{k=1}^{3} J_{\alpha,k}^2$ and $J_{\alpha,k}$ is the k-th derivative of $(\nabla J)_\alpha$. When $\delta = 0$ the formula (4) reduces to Barišić's results [5].

Clearly, the term with the factor $\delta_{k'-k-g}$ is the electron-phonon process in which the conservation of momentum between the electrons and the phonons must be obeyed. The term without the factor $\delta_{k'-k-g}$ is the additional electron-phonon process which does not conserve the momentum. The first term inside the first bracket on the right-hand side of (4) denotes the usual electron-phonon process due to the lattice vibration of a periodic crystal and the second term in the same bracket means an additional term in the perturbed cyrstal, which was obtained in the limit $k\delta \ll 1$, i.e. in the long wavelength range. It is important to stress that the factor $\exp[-(k-k')^2\delta^2]$ in the term of the momentum conservative processes corresponds physically to the degradation of the coherent part of electrons and phonons into the incoherent part of them.

3. ANALYSIS OF T_c OF THE AMORPHOUS TM SUPERCONDUCTORS

The electron-phonon matrix elements calculated in the preceding section are rather complicated due to the momentum non-conservative process. However, when we analysed the experimental T_c data of the disordered 4d transition metal films [1] it was found that these experimental data can be interpreted quantitatively in the limit $\delta \to 0$, i.e. the quasi-crystal approximation (QCA). In this case, the original Barišić formula [5] may be used,

$$\eta = N(E_F)\langle I^2\rangle \simeq g^2 E_c$$

where E_c represents the contribution of the tight-binding d-electrons to the cohesive energy which has been calculated by [7] for the crystals of 3d and 4d TM. As well-known, the cohesive energy is only weakly dependent on the crystal structure [8], it is reasonable to suppose that the theoretical data calculated by [7] can be used in the QCA model for calculating η.

According to the viewpoint of QCA, it was expected that Lindemann's formula [9] for Θ_D may also be applied to our disordered model with the Lindemann's constant determined by the experimental Debye temperature of the amorphous Pd alloy [10] (see table 1) with the atomic volume (Ω), atomic weight and the melting temperature (T_m) of the corresponding crystals taken from [11] we obtained Θ_D for the amorphous 4d TM. Then making use of McMillan's formula, we finally calculated the transition temperature of the amorphous 4d elements which is consistent with experimental curve as shown in Fig. 1.

Table 1

Materials	Θ_D of crystal state (K)	Θ_D of amorphous state (K)
Pd [11]	283 ± 16	257*
$Pd_{0.775}Si_{0.165}Cu_{0.06}$ [10]	290	252

* This value was calculated in this paper with $\Theta_D = \alpha\left(\frac{1}{\Omega}\right)^{1/3}\left(\frac{T_m}{M}\right)^{1/2}$.

α was determined to be 128.7 from Θ_D of the amorphous Pd alloy [10].

4. THE RELEVANT COMMENTS

Under the tight-binding approximation we have shown in section 2, 3 that the momentum non-conservative E-P process still exists in the disordered transition metals just like in the disordered simple metals [2]. However, it turned out to be a good enough approximation to explain the experimental T_c data of the amorphous TM in the limit $\delta \to 0$ in which the momentum non-conservative process has a negligible effect on superconductivity. Therefore, the smearing of the electronic density of states and the softening of phonons are still the dominant factors resulting in the regular variation of T_c across the amorphous TM series. In view of the above mentioned fact we take the view that there is not much potentiality for increasing T_c by using the amorphous TM alloys.

In an article written by us [12] we proposed a principle of "the significant heterogeneous coordination" which would be a necessary condition for intensifying the electron-phonon coupling. According to this principle, what we want to emphasize now is that such kinds of disordered materials having striking differences with the corresponding crystal materials in respect of the coordination number (e.g. by introducing vacancies) and the kind of atoms in the first coordination shell of the structure are very important. We hope that experimentalists will prepare these kinds of disordered materials in order to study the effect of various "significant heterogeneous coordination" elements (including vacancies) on T_c.

Finally, it is worth making granular superconductors with very fine "clusters" of different ordered materials. In these systems there are a lot of heterometal interfaces, and according to the rule of "Distant Hybridization Superiority" suggested by us [13], there will be the favourable conditions for high T_c superconductivity if the different granules are made of constituents that have a large difference in valence electronic structure.

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REFERENCES

[1] Collver, M.M. and Hammond, R.H., Phys. Rev. Lett. 30 (1973) 92-95.
[2] Bergmenn, G., Physics Reports 27c (1976) 159-185.
[3] Agyeman, K., Müller, R. and Tsuei, C.C., Phys. Rev. B19 (1979) 193-198.
[4] Giorgi, A.L. and Matthias, B.T., Phys. Rev. B 17 (1978) 2160-2162.
[5] Barišić, S., Labbé, J. and Friedel, J., Phys. Rev. Lett. 25 (1970) 919-922.
[6] Bergmann, G., Phys. Rev. B3 (1971) 3797-3801.
[7] Gelatt, C.D., Ehrenreich, H. and Watson, R.E., Phys. Rev. B15 (1977) 1613-1628.
[8] Pettifor, D.G., J. Phys. C 3 (1970) 367-377.
[9] Pines, D., Elementary Excitations in Solids (W.A. Benjamin, INC., New York, Amsterdam, 1963).
[10] Golding, B., Bagley, B.G. and Hsu, S.L. Phys. Rev. Lett 29 (1972) 68-70.
[11] Gschneidner, K.A., Solid State Physics 16 (1964) 275-426.
[12] Yin, Dao-le and Zhang, Li-yuan, Acta Physica Sinica 29 (1980) 677-685.
[13] Zhang Li-yuan and Yin, Dao-le, Proc. of 4-th Inter. Conf. on Surface Science and the 3rd European Conf. on Surface Science (Sep 22-26, 1980 Cannes, France), Vol. 1 188-191.

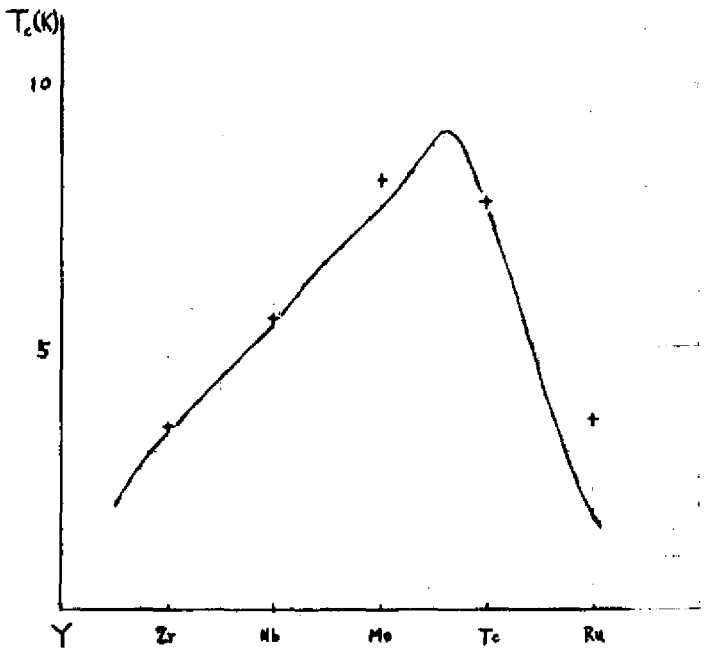

Fig. 1

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