Atomic ordering and T_c of narrow-band superconducting alloys

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We present a theoretical discussion for the transition temperature T_c of superconducting alloys taking into account both the effects of composition and of atomic order. T_c is found from the ensemble-averaged vertex equation for a Cooper pair written in the atomic representation. The application to new experimental data on the effect of long-range order on T_c of Nb_3Sn, V_3Au, and V_3Ga yields good agreement between theory and experiment.

I. INTRODUCTION

The effect of composition and of atomic ordering on T_c of the binary alloys A_xB_{1-x} is of considerable experimental interest. In particular, high-T_c A-15 substances have been investigated by producing different degrees of atomic disorder by high-energy neutron irradiation,[1,2] oxygen-ion bombardment of thin films,[3] and quenching of alloys from high temperatures followed by subsequent annealing.[4-6] In the new experiments on A-15 substances it is found that large changes in T_c accompany the changes of *long-range* order as measured by the Braggs-Williams parameter S. Furthermore, there are alloys between two transition metals where a small difference in the atomic sizes of the constituents leads to *short range* order as indicated by solid-solution hardening.[7] For these alloys, too, T_c will depend not merely on the composition, but also on Bethe's order parameter σ that measures the extent of local order between nearest-neighbor atoms.[8]

We wish to present a theory of T_c for superconducting alloys that takes both the effects of composition *and* of atomic order into account. We presume alloys with narrow energy bands, where the electrons responsible for superconductivity have atomic character in the sense that they revolve several times around an atom before the itinerant band motion carries them to a neighbor atom. To determine T_c, we start from the integral equation for the vertex part of a Cooper pair Γ written in the Wannier representation.[9] The temperature T_c is defined by the ensemble-averaged vertex equation, the kernel of which contains the pair Green's function F and the electron-electron interaction I owing to the short-range Coulomb repulsion and the frequency-dependent exchange of lattice excitations. For the kernel, we presume the contact model, which means physically that we consider those interactions in which the two electrons of a pair are initially at one and the same site and finally again at one site. Using the contact model, we calculate T_c as a function of composition and ordering. In the alternative coherent-potential-approximation treatment of superconducting alloys, random disorder is an essential presumption.[10-12]

II. ELECTRON-PHONON MODEL

For a particular alloy, we presume the following model: The electrons occupy a partly filled band whose eigenstates κ are given by

$$\psi_\kappa(\vec{r}) = N^{-1/2} \sum_\alpha \sum_{\vec{n}_\alpha} a_\kappa(\vec{n}_\alpha) w_{\vec{n}_\alpha}(\vec{r}) \quad (\kappa = 1, \ldots, N), \tag{1}$$

where $\vec{n}_\alpha$ labels the lattice sites occupied by α atoms ($\alpha = A, B$), $w_{\vec{n}_\alpha}$ denotes the Wannier function at $\vec{n}$, and N is the number of atoms. The coefficients a_κ connect the κ and $\vec{n}$ representations, by a unitary transformation. In the Wannier representation, the Green's function at $T=0$ has the form

$$G_0(\vec{n}_\beta', \vec{n}_\alpha; \epsilon) = N^{-1} \sum_\kappa \frac{a_\kappa(\vec{n}_\beta') a_\kappa^*(\vec{n}_\alpha)}{\epsilon - \epsilon_\kappa + i\delta_\kappa}, \tag{2}$$

where ϵ_κ is the band energy with respect to the Fermi surface and $\delta_\kappa = \pm\delta$ for $\epsilon_\kappa \gtrless 0$. In terms of G_0 the density of states per atom is given by

$$N(\epsilon) = -(\pi N)^{-1} \operatorname{sgn}\epsilon \sum_\alpha \sum_{\vec{n}_\alpha} \operatorname{Im} G_0(\vec{n}_\alpha, \vec{n}_\alpha; \epsilon) = \sum_\alpha N_\alpha(\epsilon). \tag{3}$$

The model for the normal modes is analogous to that for the electrons.[13] The modes l have the eigenfrequencies ω_l ($l = 1, \ldots, 3N$) and the displacement eigenvectors $u_{\vec{m}_\alpha i; l}$ ($i = 1, 2, 3$, corresponding to the three Cartesian coordinates). The lattice Green's function L_0 describes the propagation of a lattice distortion between $\vec{m}_\alpha$ and $\vec{m}_\beta'$ at $T=0$; this function is given by

$$L_{0ij}(\vec{m}_\beta', \vec{m}_\alpha; \omega) = (M_\alpha M_\beta)^{-1/2} \sum_l \frac{u_{\vec{m}_\beta' i; l} u_{\vec{m}_\alpha j; l}}{\omega^2 - \omega_l^2}, \tag{4}$$

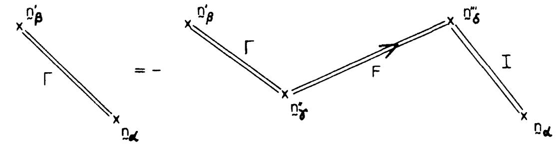

FIG. 1. Graphical representation of the vertex equation for an alloy in the contact model.

where M_α is the mass of an α atom. Using Eq. (4), we write the density of states as

$$g(\omega) = (6N\pi i)^{-1} \sum_i \sum_\alpha \sum_{\vec{m}_\alpha} M_\alpha \times [L_{0ii}(\omega^2 + i\delta) - L_{0ii}(\omega^2 - i\delta)] = \sum_\alpha g_\alpha(\omega). \tag{5}$$

We find the partial densities of states $N_\alpha(\epsilon)$ and $g_\alpha(\omega)$ by substituting the corresponding Green's functions into Eqs. (3) and (5).[14] In the framework of this electron-phonon model, we formulate the vertex equation for a Cooper pair.

III. ENSEMBLE-AVERAGED VERTEX EQUATION

The vertex part Γ satisfies at T_c a homogeneous integral equation of the form $\Gamma = -\Gamma GGI$, where G is the thermal Green's function (cf. Eq. 2) and I is the irreducible interaction. In the contact model, I depends on two sites only, since both electrons of a pair are taken to be at one site. The interaction can scatter the pair to a new site. In this model, the explicit form of the vertex equation is given by (cf. Fig. 1)

$$\Gamma(\vec{n}'_\beta, \vec{n}_\alpha; \omega_\nu) = -\beta_c^{-1} \sum_{\nu'} \sum_{\vec{n}''_\gamma, \vec{n}'''_\delta} \Gamma(\vec{n}'_\beta, \vec{n}''_\gamma; \omega_{\nu'}) \times F(\vec{n}''_\gamma, \vec{n}'''_\delta; \omega_{\nu'}) I(\vec{n}'''_\delta, \vec{n}_\alpha; \omega_{\nu'} - \omega_\nu), \tag{6}$$

where $\omega_\nu = i\pi(2\nu+1)/\beta$ and $\beta = 1/k_B T$. Eq (6) represents a system of N^2 equations. For large N, the value of T_c given by Eq. (6) should apply not only to just this particular alloy but to an ensemble of alloys of which this one is a representative. All of the alloys in the ensemble have the same value of the order parameter, S or σ. We wish to determine T_c from the proper ensemble average of Eq. (6).

To this end, we first introduce some quantities to describe the alloy statistics. The probability distribution for r atoms, $p(\vec{n}_1, \ldots, \vec{n}_r)$, is the probability that the sites $\vec{n}_1, \ldots, \vec{n}_r$ are occupied by the constituents $\alpha_1, \ldots, \alpha_r$. For convenience, we write below the pair distribution $p(\vec{n}_1\vec{n}_2)$ as $p(\vec{n}_\alpha\vec{n}'_\beta)$, $= p(\vec{n}_\alpha - \vec{n}'_\beta)$, etc. The conditional probability distribution $p(\vec{n}_1, \ldots, \vec{n}_r | \vec{n}_{r+1}, \ldots, \vec{n}_N)$ gives the probability for the constituents at the sites $\vec{n}_{r+1}, \ldots, \vec{n}_N$ if the constituents at $\vec{n}_1, \ldots, \vec{n}_r$ are fixed. This probability is defined by the following factorization:

$$p(\vec{n}_1, \ldots \vec{n}_N) = p(\vec{n}_1, \ldots, \vec{n}_r) p(\vec{n}_1, \ldots, \vec{n}_r | \vec{n}_{r+1}, \ldots, \vec{n}_N). \tag{7}$$

In terms of the conditional probability, we define the restricted averages of any quantity which depends on the alloy configuration [cf. Ref. 15, Eq. (2.15)].

We write the restricted ensemble average of Eq. (6), taking α and β atoms at the lattice sites $\vec{n}$ and $\vec{n}'$, respectively, and averaging over all of the possible alloy configurations at the other $N-2$ sites. We get

$$\begin{aligned} p(\vec{n}'_\beta \vec{n}_\alpha)\langle\Gamma\rangle_{\vec{n}'_\beta \vec{n}_\alpha} = -\sum_{\gamma,\delta} \sum_{\vec{n}'', \vec{n}'''} \langle \Gamma F I\rangle_{\vec{n}'_\beta \vec{n}''_\gamma \vec{n}'''_\delta \vec{n}_\alpha} \big[& p(\vec{n}'_\beta \vec{n}''_\gamma \vec{n}'''_\delta \vec{n}_\alpha) + \delta_{\vec{n}'\vec{n}''} p(\vec{n}'_\beta \vec{n}'''_\delta \vec{n}_\alpha) + \delta_{\vec{n}''\vec{n}'''} p(\vec{n}'_\beta \vec{n}''_\gamma \vec{n}_\alpha) + \delta_{\vec{n}'''\vec{n}} p(\vec{n}'_\beta \vec{n}''_\gamma \vec{n}'''_\delta) \\ & + \delta_{\vec{n}'\vec{n}'''} p(\vec{n}'_\beta \vec{n}''_\gamma \vec{n}_\alpha) + \delta_{\vec{n}'\vec{n}} p(\vec{n}'_\beta \vec{n}''_\gamma \vec{n}'''_\delta) + \delta_{\vec{n}'\vec{n}''} \delta_{\vec{n}''\vec{n}} p(\vec{n}'_\beta \vec{n}'''_\delta) \\ & + \delta_{\vec{n}'\vec{n}'''} \delta_{\vec{n}''\vec{n}} p(\vec{n}'_\beta \vec{n}_\alpha) + \delta_{\vec{n}'\vec{n}''} \delta_{\vec{n}'\vec{n}'''} p(\vec{n}'_\beta \vec{n}_\alpha) + \delta_{\vec{n}''\vec{n}'''} \delta_{\vec{n}'''\vec{n}} p(\vec{n}'_\beta \vec{n}''_\gamma) \big] \end{aligned} \tag{8a}$$

and ($\vec{n} = \vec{n}'$)

$$p(\vec{n}_\alpha)\langle\Gamma\rangle_{\vec{n}_\alpha} = -\sum_{\gamma,\delta} \sum_{\vec{n}'', \vec{n}'''} \langle \Gamma F I\rangle_{\vec{n}_\alpha \vec{n}''_\gamma \vec{n}'''_\delta} \big[p(\vec{n}_\alpha \vec{n}''_\gamma \vec{n}'''_\delta) + \delta_{\vec{n}''\vec{n}'''} p(\vec{n}_\alpha \vec{n}''_\gamma) + \delta_{\vec{n}\vec{n}'''} p(\vec{n}_\alpha \vec{n}''_\gamma) + \delta_{\vec{n}\vec{n}''} p(\vec{n}_\alpha \vec{n}'''_\delta) + \delta_{\vec{n}\vec{n}''} \delta_{\vec{n}''\vec{n}'''} p(\vec{n}_\alpha) \big]. \tag{8b}$$

Here the Kronecker $\delta_{\vec{n}'\vec{n}''} \equiv \delta_{\vec{n}'_\beta \vec{n}''_\gamma}$; the subscripts $\alpha, \beta, \gamma, \delta = \mathrm{A, B}$.

Equation (8) is exact within the contact model. To proceed, we employ an approximation, namely, the chain factorization of the probability distributions containing three and four different sites into a chain of pair distributions. For three sites we have, for example,

$$p(\vec{n}_\alpha \vec{n}'_\beta \vec{n}''_\gamma) = \frac{p(\vec{n}_\alpha - \vec{n}'_\beta)}{p_\alpha} \frac{p(\vec{n}'_\beta - \vec{n}''_\gamma)}{p_\beta} \frac{p(\vec{n}''_\gamma - \vec{n}_\alpha)}{p_\gamma}, \tag{9}$$

where $p_\alpha = p(\vec{n}_\alpha)$. This approximation is used in the tight-binding theory of the electronic structure of liquid and amorphous metals.[16] In a corresponding manner, the restricted ensemble average of $\langle \Gamma F I\rangle$ is factorized into a product of three averages,

$$\langle \Gamma F I\rangle_{\vec n_\beta'\vec n_\gamma''\vec n_\delta''' n_\alpha} = \langle \Gamma\rangle_{\vec n_\beta'-\vec n_\gamma''}\langle F\rangle_{\vec n_\gamma''-\vec n_\delta'''}\langle I\rangle_{\vec n_\delta'''-\vec n_\alpha}. \tag{10}$$

This type of chain approximation is reasonable if, e.g., the quantity $\Gamma(\vec n_\beta'\vec n_\gamma'')$ does not fluctuate much about its restricted average $\langle\Gamma\rangle_{\vec n_\beta'-n_\gamma''}$.[17]

We now substitute Eqs. (9) and (10) in Eq. (8). By summing the new equation over $\vec n', \vec n$ we eventually get

$$\langle\Gamma\rangle_{\beta\alpha} = -\sum_{\gamma,\delta}\langle\Gamma\rangle_{\beta\gamma}\frac{\langle F\rangle_{\gamma\delta}}{p_\gamma p_\delta}\langle I\rangle_{\delta\alpha}, \tag{11}$$

where

$$\langle I\rangle_{\delta\alpha} = N^{-1}\sum_{\vec n',\vec n}[\,p(\vec n_\delta' - \vec n_\alpha)\langle I\rangle_{\vec n_\delta'-\vec n_\alpha} + \delta_{\vec n'\vec n}p_\alpha\langle I\rangle_\alpha]. \tag{12}$$

The quantities $\langle\Gamma\rangle_{\beta\gamma}$ and $\langle F\rangle_{\gamma\delta}$ are defined correspondingly. The subscript β enters Eq. (11) as a common label and, therefore, it may be dropped. Hence Eq. (11) represents a system of two coupled integral equations.

To arrive at the simple form of Eq. (11) we have exployed one additional approximation, besides the chain factorization. This approximation concerns those paths $\vec n'$-$\vec n''$-$\vec n'''$-$\vec n$ which are not self-avoiding, Fig 1. In this case, where at least two of the four sites are identical, the corresponding terms in Eqs. (8) and (11) are accompanied by different pair distributions.[18] This difference is neglected, the reason being that the number of non-self-avoiding paths is by a factor $1/N$ smaller than the number of self-avoiding paths. We have now clearly stated the approximations made in the averaging procedure leading to Eq. (11). The chain factorization, Eqs. (9) and (10), is the pertinent approximation made in this context.

Next, we calculate the quantities $\langle F\rangle_{\gamma\delta}$ and $\langle I\rangle_{\delta\alpha}$, Eq. (11). The irreducible electron-electron interaction is given by

$$\langle I\rangle_{\delta\alpha} = \langle I^c\rangle_{\delta\alpha} + \langle I^{\mathrm{ph}}(\omega_\mu)\rangle_{\delta\alpha}, \tag{13}$$

where $\omega_\mu = 2\pi i\mu/\beta$. The short-range Coulomb part is

$$\langle I^c\rangle_{\delta\alpha} = \delta_{\delta\alpha}p_\alpha\langle U\rangle_\alpha, \tag{14}$$

where $\langle U\rangle_\alpha$ is the intra-atomic Coulomb integral for the α atoms. The interatomic Coulomb interactions are assumed to be small compared to $\langle U\rangle_\alpha$ and they are therefore ignored. The phonon part in Eq. (13) is given by

$$\begin{aligned}\langle I^{\mathrm{ph}}(\omega_\mu)\rangle_{\delta\alpha} = N^{-1}\sum_{\vec n',\vec n}\sum_{\vec m}\sum_\gamma \langle L(\omega_\mu)\rangle_\gamma\langle J^2\rangle_{\vec n_\delta'\vec m_\gamma\vec n_\alpha} \\ \times[\,p(\vec n_\delta'\vec m_\gamma\vec n_\alpha) + \delta_{\vec m\vec n}p(\vec n_\delta\vec n_\alpha) + \delta_{\vec m\vec n}p(\vec n_\delta'\vec n_\alpha) \\ + \delta_{\vec n'\vec n}p(\vec m_\gamma\vec n_\alpha) + \delta_{\vec m\vec n}p_\alpha],\end{aligned} \tag{15}$$

where

$$J^2 \equiv \sum_i |(\vec n_\delta'|\nabla_i V_{\vec m_\gamma}|\vec n_\alpha)|^2 \tag{16}$$

is the squared matrix element of the ion-potential gradient at $\vec m$ between Wannier functions centered at $\vec n'$ and $\vec n$. Presuming cubic symmetry, we get the restricted average of L for γ atoms as

$$\langle L(\omega_\mu)\rangle_\gamma = \frac{1}{3}\sum_i\langle L_{ii}(\omega_\mu)\rangle_\gamma = M_\gamma^{-1}\int_0^{\omega_0}\frac{g_\gamma(\omega)}{\omega_\mu^2-\omega^2}\,d\omega, \tag{17}$$

where $g_\gamma(\omega)$ is defined by Eq. (5).[19] For sufficiently localized Wannier functions, the three-center matrix elements in Eq. (15) can be neglected and the two-center matrix elements between nearest neighbors can be considered to be dominant. Equation (15) then becomes

$$\begin{aligned}\langle I^{\mathrm{ph}}(\omega_\mu)\rangle_{\delta\alpha} = \sum_\gamma\langle L(\omega_\mu)\rangle_\gamma z[\langle J^2{}_{\delta\delta\alpha}p_{\delta\alpha}(\delta_{\delta\gamma}+\delta_{\alpha\gamma}) \\ + \langle K^2\rangle_{\alpha\gamma\alpha}p_{\gamma\alpha}\delta_{\delta\alpha}],\end{aligned} \tag{18}$$

$\langle J^2\rangle_{\gamma\gamma\alpha} \equiv \langle J^2\rangle_{\vec m_\gamma\vec m_\gamma\vec n_\alpha}$, $\langle K^2\rangle_{\alpha\gamma\alpha} \equiv \langle J^2\rangle_{\vec n_\alpha\vec m_\gamma\vec n_\alpha}$,

$p_{\gamma\alpha} = p(\vec m_\gamma - \vec n_\alpha)$, and $\vec m = \vec n + \vec d_j$, where $\vec d_j$ is a vector between nearest-neighbor sites, $j = 1, 2, \ldots, z$.

The quantity $\langle F\rangle_{\gamma\delta}$ has the form of Eq. (12). To calculate this quantity, we take the ensemble average of the pair Green's function $\langle F\rangle = \sum_{\gamma\delta}\langle F\rangle_{\gamma\delta}$ to be equal to the arithmetic mean value of F for a given macroscopic alloy. The two averages will be identical if we restrict ourselves to homogeneous alloys without clusters of either constituent. We get

$$\begin{aligned}\langle F(\omega_\nu)\rangle_{\delta\gamma} &= N^{-1}\sum_{\vec n_\delta',\vec n_\gamma}F(\vec n_\delta', \vec n_\gamma; \omega_\nu) \\ &= \int_{\epsilon_{\min}}^{\epsilon_{\max}}\frac{N_\delta(\epsilon)N_\gamma(\epsilon)}{N(\epsilon)}\frac{d\epsilon}{|\omega_\nu - \Sigma(\omega_\nu,\epsilon)|^2 - \epsilon^2},\end{aligned} \tag{19}$$

where $\epsilon_{\min}$ and $\epsilon_{\max}$ are the band extrema with respect to the Fermi surface and Σ is the electron-phonon self-energy,

$$\Sigma(\omega_\nu, \epsilon) = \begin{cases} -\lambda\omega_\nu, & \text{if } |\omega_\nu| \le \omega_0 \\ 0, & \text{otherwise;}\end{cases} \tag{20}$$

λ is the coupling parameter given below, Eq. (21). The partial density of states $N_\gamma(\epsilon)$ depends on both the composition and the atomic order.

IV. COMPARISON BETWEEN THEORY AND EXPERIMENT

The transition temperature T_c can now be obtained from Eq. (11). By parametrizing the frequency dependence of $I^{ph}(\omega_\mu)$ in the manner of BCS, we get

$$k_B T_c = 1.13\omega_0 \exp[-(1+\lambda)/(\lambda-\mu^*)],$$

where

$$\mu^* = \mu/[1+\mu\ln(\epsilon_b/\omega_0)],$$

$$\lambda = -\sum_{\alpha,\beta} \frac{N_\alpha(0)N_\beta(0)}{N(0)} \frac{\langle I^{ph}(|\omega_\nu|=0)\rangle_{\alpha\beta}}{p_\alpha p_\beta}, \qquad (21)$$

$$\mu = \sum_{\alpha,\beta} \frac{N_\alpha(0)N_\beta(0)}{N(0)} \frac{\langle I^c\rangle_{\alpha\beta}}{p_\alpha p_\beta}. \qquad (22)$$

The energy ϵ_b is an effective "half-width" of the band defined by

$$\ln\epsilon_b = \tfrac{1}{2}(\ln|\epsilon_{max}| + \ln|\epsilon_{min}|).$$

The parameters λ and μ depend, first of all, on the composition $x = p_a$. For random disorder, x is the single-alloy parameter. For the more interesting cases with atomic order, λ and μ depend in addition on an order parameter. There are two different types of alloy order. The long-range order S measures the order of A and B atoms upon A and B sites over the entire lattice. The short-range order σ is not connected with A and B sites but with the local configuration of nearest-neighbor atoms. For both of these types of order, expressions for the partial-structure factor $p_{\alpha\beta}$ in terms of S and σ, respectively, can be found in the literature.[20] The parameters λ and μ depend on the $p_{\alpha\beta}$ via the interaction $\langle I\rangle_{\alpha\beta}$. Furthermore, $N_\alpha(0)$ and

$$\langle\omega^2\rangle_\alpha^{-1} = \int_0^{\omega_0} \frac{g_\alpha(\omega)d\omega}{\omega^2}$$

depend on the atomic order. These parameters may be considered as "experimental quantities," since a quantitative theory for their dependence on S or σ is not yet available. In fact, for a number of A-15 substances, the electronic specific heat and the Debye temperature Θ have been measured as functions of S.[21,22]

Using these data, we calculate $T_c(S)$ for Nb_3Sn, V_3Si, V_3Au, and V_3Ga, and compare the results with experiment. We presume the linear-chain model.[23] The long-range order S is determined by r_A, that is, the probability of a chain site being occupied by an A atom; $S = 4r_A - 3$ for stoichiometric A_3B. The parameter λ is given by

$$\lambda \equiv \lambda_{AA} = \lambda_0\left(\frac{S+3}{4}\right)^2 \frac{N_A(0,S)}{N_A(0,1)} \frac{\langle\omega^2(1)\rangle_A}{\langle\omega^2(S)\rangle_A}, \qquad (23)$$

TABLE I. Parameter values used to calculate $T_c(S)$.

Substance	λ_0	μ_0^*	Θ_0 (°K)	T_{c0} (°K)	Reference
Nb_3Sn	1.12	0.12	290	18	4
	1.55	0.18	240	18	26
V_3Au	0.71	0.18	340	4.6	5, 6
V_3Si	1.10	0.18	409	18.4	27, 28
V_3Ga	1.18	0.18	302	15.6	27, 29

where $\lambda_0 = \lambda(S=1)$. The parameter $\mu = \mu_{AA} \gg 1$ by virtue of the large values of the densities of states at the Fermi surface and of the Coulomb interaction $\langle U\rangle_A$; hence we take $\mu^* = 1/\ln(\epsilon_b/\omega_0)$ and neglect the S dependence of $\ln(\epsilon_b/\omega_0)$; $\mu^* = \mu_0^*$.

In calculating T_c vs S, we use McMillan's formula, which has been applied with remarkable success to strong-coupling superconductors.[24] The parameter values used for λ_0, μ_0^*, and Θ_0 are summarized in Table I. To get $\lambda(S)$, we determine $N_A(0,S)/N_A(0,1)$ from the corresponding experimental ratio between the low-temperature specific heats, taking into account the electron-phonon renormalization.[21,22,25] The phonon parameters Θ and $\langle\omega^2\rangle_A$ are assumed to be independent

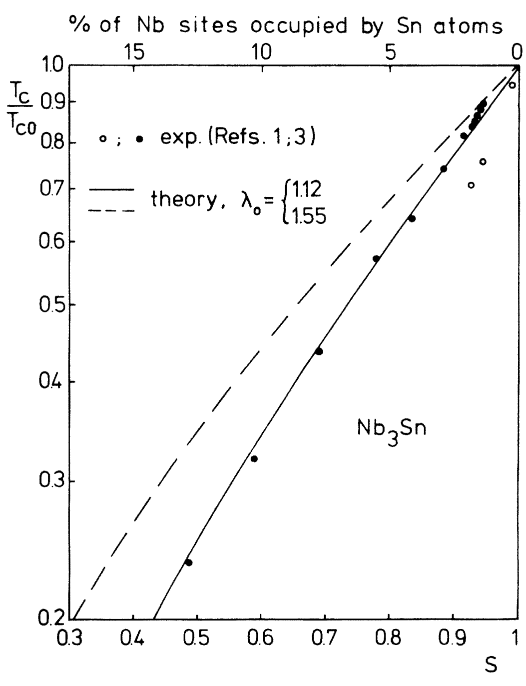

FIG. 2. Reduced transition temperature T_c/T_{c0} vs the long-range-order parameter S; $T_{c0} = T_c(S=1)$.

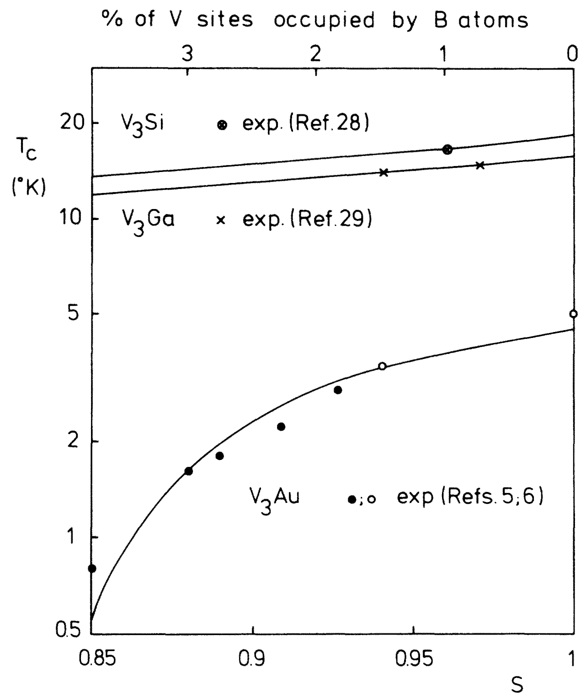

FIG. 3. Transition temperature T_c vs S; ○ denotes extrapolated experimental values of Ref. 6.

of S. This assumption is justified for V_3Au where the observed change of the phonon specific heat is negligible for $0.8 \leq S \leq 1$ (Ref. 5); for the other three substances, experimental results are not available.

A comparison between the experimental and theoretical results for T_c vs S is shown in Figs. (2) and (3). The large decrease of T_c with decreasing long-range order S is due equally to the density of states $N_A(0, S)$ and the partial structure factor $p_{AA} = \frac{1}{16} p_A^2 (S+3)^2$. For Nb_3Sn, the quantitative agreement for $\lambda_0 = 1.12$ with the new experimental results of Besslein *et al.*[3] must be taken with certain reservations. The Braggs-Williams parameter S is determined from the ion fluence and not by x-ray-diffraction methods. Furthermore, the lattice constant has not been measured as a function of S. It is certain, however, that the samples are not contaminated by oxygen. The oxygen ions whose initial energy is 24 MeV leave the target with the high energy of 8 MeV. Sweedler, Schweitzer, and Webb,[1,2] in their neutron-irradiation experiments, also determine S from the fluence. Because of the exponential dependence of S on the fluences of ions or neutrons, the difference between the experimental results of Refs. 1 and 3 could stem from the scaling of S. For V_3Si, $S = 0.96$ was recently obtained by Staudemann[28] with x-ray diffraction. For V_3Au, the S values corresponding to the experimental values of T_c given in Ref. 5 (cf. Fig. 3) have also been determined by x-ray diffraction.[6] Finally, for V_3Ga the two values of $S = 0.97$ and 0.94, corresponding to $T_c = 14.9$ and 13.8 °K, have been obtained by neutron diffraction with an uncertainty of less than 1%.

In this paper, the theoretical result for T_c is used to discuss the effect of long-range order S on high-T_c A-15 substances. The effect of short-range order σ on T_c of transition-metal alloys with different atomic sizes of the constituents will be discussed in a future paper.

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[14]The result for the partial densities of states is given by

$$N_\alpha(\epsilon) = \lim_{\Delta\epsilon \to 0} \frac{1}{\Delta\epsilon} \frac{1}{N^2} \sum_{\substack{\kappa \\ (\epsilon < \epsilon_\kappa < \epsilon + \Delta\epsilon)}} \sum_{\vec{n}_\alpha} |a_\kappa(\vec{n}_d)|^2 ,$$

$$g_a(\omega) = \lim_{\Delta\omega \to 0} \frac{1}{\Delta\omega} \frac{1}{3N} \sum_{\substack{l \\ (\omega < \omega_l < \omega + \Delta\omega)}} \sum_{\vec{m}_\alpha} \sum_i u^2_{\vec{m}_\alpha i ; l} .$$

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[18] An example for a non-self-avoiding path with three different sites is given by $\vec{n}'-\vec{n}''-\vec{n}'''-\vec{n}''$. The substitution of the chain approximation in Eq. (8a) yields the pair-distribution product $p(\vec{n}'-\vec{n}'')p(n''-\vec{n}''')$ together with the term $\langle\Gamma\rangle_{\vec{n}'-n''}\langle F\rangle_{\vec{n}''-n'''}\langle I\rangle_{\vec{n}'''-n''}$. In Eq. (11), this term is accompanied by the triple product $p(\vec{n}'-\vec{n}'')p(\vec{n}''-\vec{n}''')p(\vec{n}'''-\vec{n}'')$.

[19] In Eq. (17), $L_{ii}(\omega_\mu)\equiv L_{ii}(\vec{m}_\gamma, \vec{m}_\gamma; \omega_\mu)$; cf. Ref. 9, Eq. (3.15).

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