

## SPIN WAVE STIFFNESS CONSTANT IN THE FERROMAGNETIC B. C. C. TRANSITION METAL ALLOYS\*

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The spin wave stiffness constant  $D$  of ferromagnetic b. c. c. transition metal alloys is calculated. The numerical results are presented for Fe alloys.

### 1. Introduction

In the previous papers [1-2] the spin wave stiffness constant  $D$  was calculated for the ferromagnetic f. c. c. alloys. The results were obtained using the simple model in which the magnetic moment of alloy was constant at the whole region of concentration. Now we analyse a group of b. c. c. alloys. There are some experiments [3-5] in which the dependence of the stiffness constant  $D$  on the concentration are examined. Recently Edwards and Hill [6] calculated the stiffness constant for b. c. c. ferromagnetic alloys and their results are compared with ours. Morkowski and Jezierski [7] analysed the stiffness constant in the f. c. c. and b. c. c. alloys using the method of effective Hamiltonian [8]. In this paper the spin wave stiffness constant  $D$  was calculated using a one band model of ferromagnet and the exact expression for  $D$  obtained by Edwards and Fisher [9].

The method of calculations is similar as presented in the paper [1] but it is extended to weak itinerant ferromagnets.

### 2. The magnon energy in itinerant electron b. c. c. ferromagnetic alloys

We consider the binary ferromagnetic alloys  $A_{1-c}B_c$ , where  $c$  is the concentration of the impurity  $B$ . For the system of itinerant electrons we used the one-band Hamiltonian

$$H = \sum_{i\sigma} \epsilon_i n_{i\sigma} + \sum_{ij\sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} + \sum_i I_i n_{i+} n_{i-}, \quad (1)$$

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here the operators  $n_{i\sigma}$ ,  $a_{i\sigma}^+$  and  $a_{i\sigma}$  are the occupation numbers, the creation and annihilation operators for electron in the Wannier state at the lattice site  $R_i$  with spin  $\sigma$ , respectively.  $\varepsilon_i$  is the atomic potential,  $t_{ij}$  denotes the hopping integral and  $I_i$  is the intraatomic Coulomb interaction. These parameters may assume different values according to which sort of atoms occupy the site  $i$  and  $j$ . We start, as in paper [1], from an exact expression for the stiffness constant  $D$  (Edwards and Fisher [9])

$$D = \frac{1}{3m} \left[ \frac{1}{2} \sum_k \langle n_{k+} + n_{k-} \rangle \nabla_k^2 \varepsilon_k - \sum_k \sum_{k'} \langle \langle a_{k-}^+ a_{k+}; a_{k'+}^+ a_{k'-} \rangle \rangle_{\omega=0} \nabla_k \varepsilon_k \cdot \nabla_{k'} \varepsilon_{k'} \right], \quad (2)$$

here  $m$  is the alloy magnetization, and  $\varepsilon_k$  the single band dispersion relation.

In this formula essential role plays the two-particle Green function  $\langle \langle a_{k-}^+ a_{k+}; a_{k'+}^+ a_{k'-} \rangle \rangle_{\omega=0}$  and the electron energy  $\varepsilon_k$ . The electron energy  $\varepsilon_k$  of b. c. c. structure was assumed in the tight binding approximation:

$$\varepsilon_k = 8t \left[ 1 - \cos\left(\frac{1}{2} ak_x\right) \cos\left(\frac{1}{2} ak_y\right) \cos\left(\frac{1}{2} ak_z\right) \right], \quad (3)$$

here  $a$  is the lattice constant and  $t$  is a parameter proportional to the bandwidth  $W$  of pure metals.

The value of the two-particle Green function was calculated similarly as in Ref. [1]. We transform  $\langle \langle a_{k-}^+ a_{k+}; a_{k'+}^+ a_{k'-} \rangle \rangle_{\omega=0}$  into the Wannier representation and then we resolve by iteration the equation of motion. The Green function  $\langle \langle a_{i-}^+ a_{j+}; a_{m+}^+ a_{p-} \rangle \rangle_{\omega}$  in the Wannier representation satisfies the following equation

$$\begin{aligned} G_0(l^\alpha j^\beta; m^\gamma p^\delta) &= [\omega - \varepsilon_j^\beta + \varepsilon_i^\alpha]^{-1} \{ \langle [a_{i-}^+ a_{j+}; a_{m+}^+ a_{p-}]_+ \rangle_{\alpha\beta\gamma\delta} \\ &+ \sum_{r \neq i \neq j} \sum_{\varepsilon=A,B} [t_{jr}^{\beta\varepsilon} G_0(l^\alpha r^\varepsilon; m^\gamma p^\delta) - t_{ri}^{\varepsilon\alpha} G_0(r^\varepsilon j^\beta; m^\gamma p^\delta)] \\ &+ t_{ij}^{\alpha\beta} [G_0(l^\alpha l^\alpha; m^\gamma p^\delta) - G_0(j^\beta j^\beta; m^\gamma p^\delta)] \\ &- I_i^\alpha G_0(l^\alpha l^\alpha; m^\gamma p^\delta) \delta_{ij} \delta_{\alpha\beta} + I_j^\beta G_2(j^\beta j^\beta l^\alpha j^\beta; m^\gamma p^\delta) \\ &- I_i^\alpha G_1(l^\alpha l^\alpha l^\alpha j^\beta; m^\gamma p^\delta) \}, \end{aligned} \quad (4)$$

where

$$\begin{aligned} G_0(l^\alpha j^\beta; m^\gamma p^\delta) &= \langle \langle a_{i-}^+ a_{j+}; a_{m+}^+ a_{p-} \rangle \rangle_{\omega}^{\alpha\beta\gamma\delta}, \\ G_1(l^\alpha l^\alpha l^\alpha j^\beta; m^\gamma p^\delta) &= \langle \langle n_{i+} a_{i-}^+ a_{j+}; a_{m+}^+ a_{p-} \rangle \rangle_{\omega}^{\alpha\alpha\alpha\beta\gamma\delta}, \\ G_2(j^\beta j^\beta l^\alpha j^\beta; m^\gamma p^\delta) &= \langle \langle n_{j-} a_{i-}^+ a_{j+}; a_{m+}^+ a_{p-} \rangle \rangle_{\omega}^{\beta\beta\alpha\beta\alpha\delta}. \end{aligned} \quad (4a)$$

The Greek superscripts denote the type of atoms ( $A$  or  $B$ ) at the given site. The higher-order Green function we take in the Random Phase Approximation

$$\begin{aligned} \langle \langle n_{i+} a_{i-}^+ a_{j+}; a_{m+}^+ a_{p-} \rangle \rangle_{\omega} &\approx \langle n_{i+} \rangle (1 - \delta_{ij}) \langle \langle a_{i-}^+ a_{j+}; a_{m+}^+ a_{p-} \rangle \rangle_{\omega}, \\ \langle \langle n_{j-} a_{i-}^+ a_{j+}; a_{m+}^+ a_{p-} \rangle \rangle_{\omega} &\approx \langle n_{j-} \rangle (1 - \delta_{ij}) \langle \langle a_{i-}^+ a_{j+}; a_{m+}^+ a_{p-} \rangle \rangle_{\omega}. \end{aligned} \quad (5)$$

Then, substituting (5) into (4) we get the system of equations which were solved by iteration. The small parameter of iteration was  $\xi = t/\Delta$ , ( $\Delta = Im$ ). The final expression of two-particle Green function has the form

$$G_0(I^{\alpha}j^{\beta}; m^{\gamma}p^{\delta}) \approx \delta_{lp}\delta_{jm}[W_1 + c_lW_2 + c_jW_3 + c_l c_j W_4 + W_5(1 - c_l - c_j) \sum_{r \neq l \neq j} c_r + W_6 c_l c_j \sum_{r \neq l \neq j} c_r], \quad (6)$$

where

$$c_i \begin{cases} 1 & \text{if the site } i \text{ is occupied by an atom } B \\ 0 & \text{otherwise} \end{cases}$$

$$W_1 = x(A, A) + \kappa y(A, A), \quad W_2 = p(B, A) + \kappa u(B, A) - W_1,$$

$$W_3 = -W_1 + p(A, B) + \kappa u(A, B), \quad W_4 = -W_1 - W_2 - W_3 + x(B, B) + \kappa r(A, B),$$

$$W_5 = -r(B, A), \quad W_6 = -r(A, B) - r(B, A) + y(B, B),$$

$$u(\alpha\beta) = d^2(\alpha\beta) [t^2(\beta\beta)d(\alpha\beta) + t^2(\alpha\beta)d(\beta\beta) + 2t^2(\alpha\beta)t(\beta\beta) [f(\alpha)d(\alpha\beta) - f(\beta)d(\beta\beta)]],$$

$$r(\alpha\beta) = d^2(\beta\beta) \{t^2(\alpha\beta) [d(\alpha\beta) + d(\beta\alpha)] + 2t(\beta\beta)t^2(\alpha\beta)f(\beta) [d(\beta\alpha) - d(\alpha\beta)]\},$$

$$p(\alpha\beta) = d(\alpha\beta) [1 + 2t^2(\alpha\beta)d(\alpha\beta) \{f(\alpha) + f(\beta)\}],$$

$$x(\alpha\beta) = d(\alpha\beta) [1 + 4t^2(\alpha\alpha)d(\alpha\alpha)f(\alpha)],$$

$$y(\alpha\alpha) = 2d^3(\alpha\alpha)t^2(\alpha\alpha),$$

$$d(\alpha\beta) = [\omega - \varepsilon_{\beta} + \varepsilon_{\alpha} + I^{\alpha} \langle n_{+}^{\alpha} \rangle - I^{\beta} \langle n_{-}^{\beta} \rangle]^{-1},$$

$$f(\alpha) = [\omega + I^{\alpha}]^{-1}, \quad t(\alpha\beta) = t^{\alpha\beta}, \quad \Delta_{\alpha} = m^{\alpha} I^{\alpha}, \quad \kappa = \sum_{r \neq l \neq j} 1. \quad (7)$$

The two-particle Green function was calculated in the previous paper [2] in the pair approximation. Now we take into consideration the interactions between the first and second neighbours. In this case the configurational average of the two-particle-Green function has the form

$$\begin{aligned} \overline{\langle\langle a_{k-}^{+} a_{k+}^{-}; a_{k'}^{+} a_{k'-}^{-} \rangle\rangle}_{\omega=0} &= \frac{1}{Nz} \sum'_{ij} [W_1 + \langle c_i \rangle W_2 + \langle c_j \rangle W_3 \\ &+ \langle c_i c_j \rangle W_4 + W_5 \sum_{r \neq l \neq j} \langle (1 - c_l - c_j) c_r \rangle + W_6 \sum_{r \neq l \neq j} \langle c_l c_j c_r \rangle] \delta_{kk'}. \end{aligned} \quad (8)$$

If we denote the right-hand side of expression (8) by  $\frac{1}{Nz} \sum'_{ij} G_{ij}(c, \alpha) \delta_{kk'}$  where  $\alpha$  is the short-range order parameter, we get the following expression for  $D$

$$D = \frac{1}{3m} \left[ \frac{1}{2} \sum_k \langle n_{k+} + n_{k-} \rangle \nabla_k^2 \varepsilon_k - \sum_k |\nabla_k \varepsilon_k|^2 \frac{1}{Nz} \sum'_{ij} G_{ij}(c, \alpha) \right]. \quad (9)$$

In paper [2] we considered the influence of local ordering on the stiffness constant  $D$  in term of short-range order parameter  $\lambda^B$ . Now we used the following relations for the configurational average of  $c_l$  operators [10].

(i) Disordered system (DO)

The configurational average of  $c_l$  operator has a standard form (see Edwards and Jones [11])

$$\begin{aligned}\langle c_l^A \rangle &= 1 - c \\ \langle c_l^B \rangle &= c \\ \langle c_l^\alpha c_j^\beta \rangle &= \langle c_l^\alpha \rangle \langle c_j^\beta \rangle \quad \text{if } l \neq j \\ &= \langle c_l^\alpha \rangle \delta_{\alpha\beta} \quad \text{if } l = j.\end{aligned}\quad (10)$$

(ii) Long-range order (LRO)

We used the definitions from Ref. [10]:

$$\langle c_l^\alpha \rangle = p_l^\alpha, \quad \langle c_l^\alpha c_j^\beta \rangle = p_l^\alpha p_j^\beta \quad \text{if } l \neq j, \quad (11)$$

where  $p_l$  is a local concentration in the  $l$ -site. In the case of a binary alloy, Ducastelle and Gautier [10] defined a local value  $\delta p_l$  by:

$$p_l^A = 1 - c - \delta p_l, \quad p_l^B = c + \delta p_l. \quad (12)$$

(iii) Short-range order (SRO)

In the case of a short-range order we only take into consideration the pair correlation functions  $g_{ij}^{\alpha\beta}$  [10]

$$\begin{aligned}\langle c_i^\alpha c_j^\beta \rangle &= c^\alpha \delta_{\alpha\beta} \delta_{ij} \quad \text{if } i = j \\ &= c^\alpha c^\beta g_{ij}^{\alpha\beta} \quad \text{if } l \neq j, \\ \langle c_i^\alpha c_j^\beta c_k^\gamma \rangle &= c^\alpha c^\beta c^\gamma g_{ijk}^{\alpha\beta\gamma},\end{aligned}\quad (13)$$

where

$$g_{ijk}^{\alpha\beta\gamma} \approx g_{ij}^{\alpha\beta} g_{jk}^{\beta\gamma} g_{ki}^{\gamma\alpha}.$$

The correlation functions  $g_{ij}^{\alpha\beta}$  can be expressed in terms of the short-range order parameter  $\alpha_{ij}$

$$g_{ij}^{AB} = 1 - \alpha_{ij}, \quad g_{ij}^{AA} = 1 + \frac{c}{(1-c)} \alpha_{ij}, \quad g_{ij}^{BB} = 1 + \frac{(1-c)}{c} \alpha_{ij}. \quad (14)$$

The short-range order parameter  $\alpha$  is connected with the parameter  $\lambda^B$  (Ref. [2]) by a simple relation

$$\alpha_{ij} = 1 - \frac{(1 - \lambda_{ij}^B)}{2(1 - c)}. \quad (15)$$

Using the relations (10)–(13) we can write the configurational average of two-particle Green function for order alloys. At the beginning we denote by  $G^{\text{DO}}$  the Green function for disordered system. It has the form

$$G^{\text{DO}} = W_1 + c(W_2 + W_3 + W_5\kappa) + c^2(W_4 - 2W_5\kappa) + c^3W_6\kappa. \quad (16)$$

The Green function for SRO alloys may be written as follows:

$$G_{ij}^{\text{SRO}}(c, \alpha) = G^{\text{DO}} + c(1-c) [W_4\alpha_{ij} - W_5 \sum_{r \neq i \neq j} (\alpha_{ir} + \alpha_{jr})] \\ + W_6(1-c) \sum_{r \neq i \neq j} [c^2(\alpha_{ir} + \alpha_{jr} + \alpha_{ij}) + c(1-c)(\alpha_{ij}\alpha_{ir} + \alpha_{jr}\alpha_{ir} + \alpha_{ij}\alpha_{jr})]. \quad (17)$$

Then for LRO system we have

$$G_{ij}^{\text{LRO}}(c) = G^{\text{DO}} + W_2\delta p_i + W_3\delta p_j + W_4[c(\delta p_i + \delta p_j) + \delta p_i\delta p_j] \\ + W_5[(1-2c) \sum_{r \neq i \neq j} \delta p_r - (\delta p_i + \delta p_j) \sum_{r \neq i \neq j} (c + \delta p_r)] \\ + W_6[\{\delta p_i\delta p_j + c(\delta p_i + \delta p_j)\} \sum_{r \neq i \neq j} (c + \delta p_r)]. \quad (18)$$

Substituting expressions (17)–(19) into (9) we get the general formula for the spin wave stiffness constant for the ordering systems. In the case when  $\alpha_{ij} = \alpha$  we can replace the parameter  $\alpha$  by  $\lambda$  and we get the similar expression as in paper [2].

The electron energy  $\epsilon_k$  was taken in this paper in the tight binding approximation (3), and the value of the sums  $\frac{1}{N} \sum_{k\sigma} n_{k\sigma} f(k)$ , where  $f(k) = |\nabla_k \epsilon_k|^2$  or  $\nabla_k^2 \epsilon_k$  were obtained by integration over 1/8 at the first Brillouine Zone for the b. c. c. lattice. We used the mesh of 216000 points. The Fermi energy  $\epsilon_F$  was determined from the condition

$$\frac{1}{N} \sum_{k\sigma} n_{k\sigma} = n, \quad (19)$$

where  $n$  is the number of holes.

In the calculations we used the notation

$$P(A) = \left(\frac{16}{Wa}\right)^2 \frac{1}{N} \sum_k \langle n_{k+} - n_{k-} \rangle |\nabla_k \epsilon_k|^2, \quad (20)$$

and

$$L(A) = \frac{16}{Wa^2} \frac{1}{N} \sum_k \langle n_{k+} + n_{k-} \rangle \nabla_k^2 \epsilon_k, \quad (21)$$

where

$$A = \frac{2\epsilon_F}{W}. \quad (22)$$

The plots of the function  $n$ ,  $P$  and  $L$  versus  $A$  are presented in Figs 1 and 2.

Then substituting (20) and (21) into (9) we get the following expression for the spin wave stiffness constant  $D$  in the ferromagnetic alloys.

$$D(c, \alpha) = \frac{Wa^2}{96m} \left[ L(A) - \frac{W}{8} P(A) \frac{1}{Nz} \sum_{ij}' G_{ij}(c, \alpha) \right]. \quad (23)$$

For the comparison of our and other theoretical and experimental results we computed  $D(c, \alpha)/D(0, 0)$ . The numerical results are presented in the next Sections.

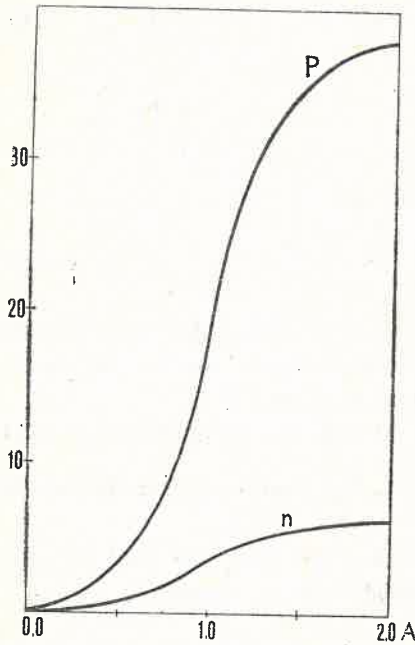


Fig. 1

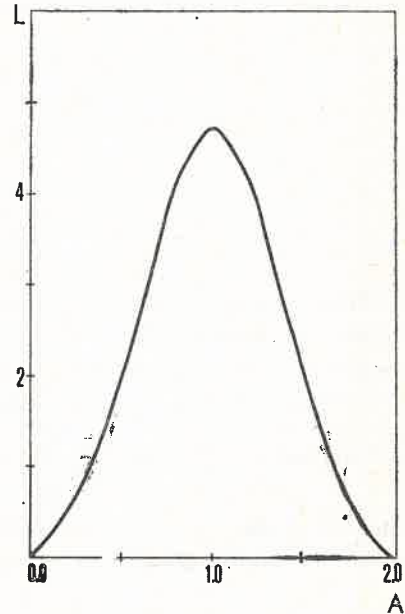


Fig. 2

Fig. 1. Plots of the functions  $P$  and  $n$  versus  $A = \frac{2}{W} \varepsilon_F$

Fig. 2. Plot of the function  $L$  versus  $A = \frac{2}{W} \varepsilon_F$

### 3. The spin wave stiffness constant in f. c. c. NiFe alloys in the generalized model

In Ref. [1] the stiffness constant  $D$  was calculated for a simple model in which the magnetic moment of the alloy was constant at the whole region of concentration. At low concentration this model gives good agreement with the experimental data, but when the concentration increases, the value of  $D(c)/D_{Ni}$  deviates from the experimental points (see: Ref. [1], Fig. 6).

Now we consider a more general model of NiFe alloys. Iron is treated as a weak ferromagnet as in Ref. [12] and the magnetic moment of the alloy changes linearly with the

concentration of impurity in the region from 0–60% Fe [13]. In numerical calculations we examined the role of interactions between the first and second neighbours (the second shell). The calculations of the spin wave stiffness constant were made for the following values of parameters:  $I_{\text{Fe}} = I_{\text{Ni}} = 0.95$  eV,  $\varepsilon_{\text{Fe}} - \varepsilon_{\text{Ni}} = 0.0$  eV,  $W_{\text{Ni}} = 3.3$  eV and  $W_{\text{Fe}} = 5.4$  eV. We have considered three models:

Model A. The magnetic moment of the alloy was constant and the values of the functions  $L$  and  $P$  were taken as those for a pure metal. This model corresponds to the calculations in Ref. [1] in which only the interactions between central atom and nearest neighbours were considered. The result is presented by a curve  $A$  in Fig. 3.

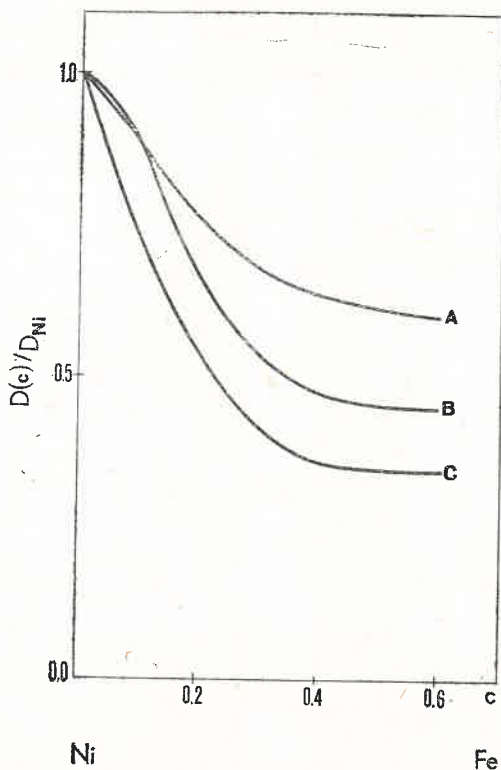


Fig. 3. Stiffness constant  $D(c)/D_{\text{Ni}}$  for the f. c. c. NiFe alloys. The curves  $A$ ,  $B$ ,  $C$  correspond to the model described in text

Model B. The magnetic moment was assumed to change linearly with the concentration of impurity up to 60% Fe. In this way the values of  $L$  and  $P$  changed too. The curve  $B$  in Fig. 3 shows this result.

Model C. In this case we consider the B model, including the interaction between the first and second neighbours. The result is labeled by letter  $C$  in Fig. 3.

In these three cases we assumed the hopping integral  $t_{AB}$  between different sites to

be of the form:  $t_{AB} = \sqrt{t_A t_B}$  and  $t_{AB} = \frac{1}{2}(t_A + t_B)$ . The values of  $D(c)/D_{\text{Ni(Fe)}}$  for these hopping integrals differ about 1% Ni(Fe) from each other. The numerical analysis showed that the slope of  $D(c)/D_{\text{Ni(Fe)}}$  increases when the model becomes more realistic.

#### 4. Nickel-iron and iron-nickel ferromagnetic alloys

In this Section we consider the face-centered-cubic NiFe and the body centered-cubic FeNi alloys. The properties of these alloys are very interesting because for about 70% Fe at the NiFe alloy the stiffness constant goes to zero. In our calculations we examined the dependence of  $D$  on the concentration from 0 to 60% Fe at NiFe alloy and from 0 to 25% Ni at FeNi alloy. We have taken the same values of parameters for these alloys. The intraatomic Coulomb interaction  $I$  was put  $I_{\text{Ni}} = I_{\text{Fe}} = 0.95$  eV and  $\delta = \epsilon_{\text{Fe}} - \epsilon_{\text{Ni}}$  was taken to be  $-0.2$  and  $0.0$  eV, the bandwidths of pure components are  $W_{\text{Ni}}^{\text{fcc}} = 3.3$  eV

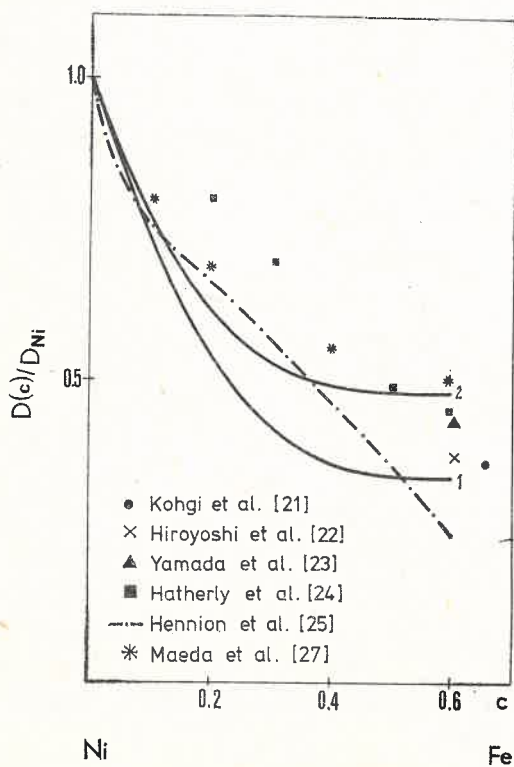


Fig. 4

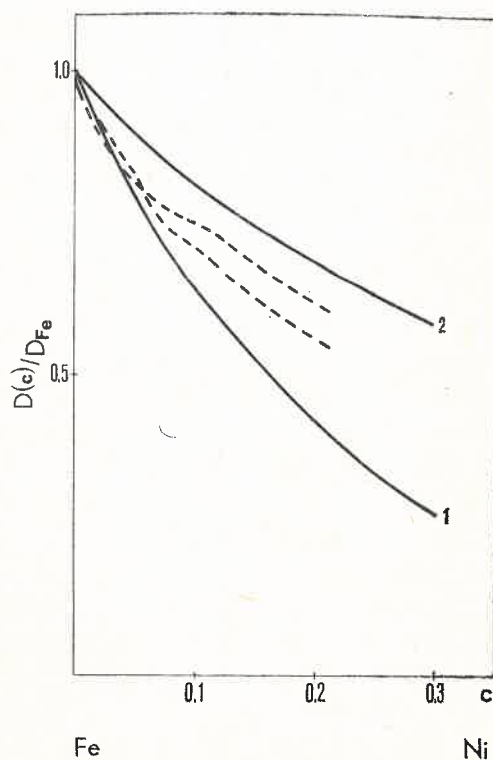


Fig. 5

Fig. 4. Values of  $D$  as a function of impurity concentration  $c$  for the f. c. c. NiFe alloys. The full curves 1 and 2 correspond to  $\delta = 0.0$  and  $-0.2$  eV, respectively. The points and broken curve denote experimental data

Fig. 5. Stiffness constant  $D(c)/D_{\text{Fe}}$  for the b. c. c. FeNi alloys. The full curves 1 and 2 correspond to  $\delta = 0.0$  and  $0.2$  eV, respectively. The broken curve denotes Edwards and Hill [6] CPA-RPA results for the different models



and  $W_{\text{Fe}}^{\text{fcc}} = 5.4$  eV for NiFe alloy. In the case of the b. c. c. FeNi alloy  $\delta$  has the opposite sign, and  $W_{\text{Fe}}^{\text{bcc}} = 5.9$  eV. The small difference between the intraatomic Coulomb interaction of the components only slightly changes the slope of the curves  $D(c)/D_{\text{pure}}$ .

The numerical results are presented in Figs 4 and 5. The points denote the experimental data and the dashed curve — the theoretical results. The solid curve presents our results.

### 5. The stiffness constant in b. c. c. alloys

#### a. FeCo alloy

Using the method presented in Section 2 we computed the stiffness constant in FeCo alloys. The calculations were made for the different concentration in the region from 0 to 60% Co. The bandwidths of Fe and Co were taken as in Ref. [14] and the alloy magnetic moment changed as reported by Hasagawa and Kanamori [13]. The numerical analysis was made for the different values of intraatomic Coulomb interaction and atomic potentials. Our aim was to show how the change of the parameters modifies the character of curves  $D(c)/D_{\text{Fe}}$ . The results are presented in Fig. 6(a-c). The dashed curve denotes Edwards' and Hill's [6] RPA-CPA result. Curves 1-4 correspond to  $\delta = -1.0, -0.8, -0.6$  and  $1.0$  eV, respectively.

#### b. FeMn alloy

Yamauchi et al. [5] estimated the stiffness constant  $D$  from measurements of magnetization of  $\alpha$ -phase Fe-Mn alloys at low temperatures. The  $\alpha$ -phase FeMn alloy is stable only up to about 5 at % Mn, but it can be extended up to more than 10 at % Mn by cold working. The magnetic moment of FeMn alloys decreases linearly while increasing Mn concentration up to about 11 at % Mn and then decreases very rapidly [5]. Because the change of magnetic moment in this region of concentration is very small (about  $0.15 \mu_{\text{B}}$ ) therefore in the numerical computation we assumed a value of magnetic moment in the alloy to be constant. The bandwidths of Fe and Mn are very similar and we take  $W_{\text{Fe}} = W_{\text{Mn}} = 5.9$  eV [14]. The values of intraatomic Coulomb interaction were estimated from Ref. [13] to be  $I_{\text{Fe}} = 0.97$  eV and  $I_{\text{Mn}} = 0.72$  eV.

In the case of low concentration the average two-particle Green function (formula (9)) for disordered alloys has a simple form

$$G(c, 0) = W_1 + c(W_2 + W_3 + \kappa W_5). \quad (24)$$

The numerical calculations of the spin wave stiffness constant  $D$  were made up to 10 at % Mn. The results are shown in Fig. 7. The points present the experimental data [5], and the full curve gives theoretical results for  $\delta = -0.5$  eV.

#### c. FeCr alloy

The magnetic properties of FeCr alloys in the composition range 0-70 at % Cr were studied recently by Aldred et al. [3, 4]. The iron-chromium system has a critical concentration at which the ferromagnetism disappears as a function of concentration.

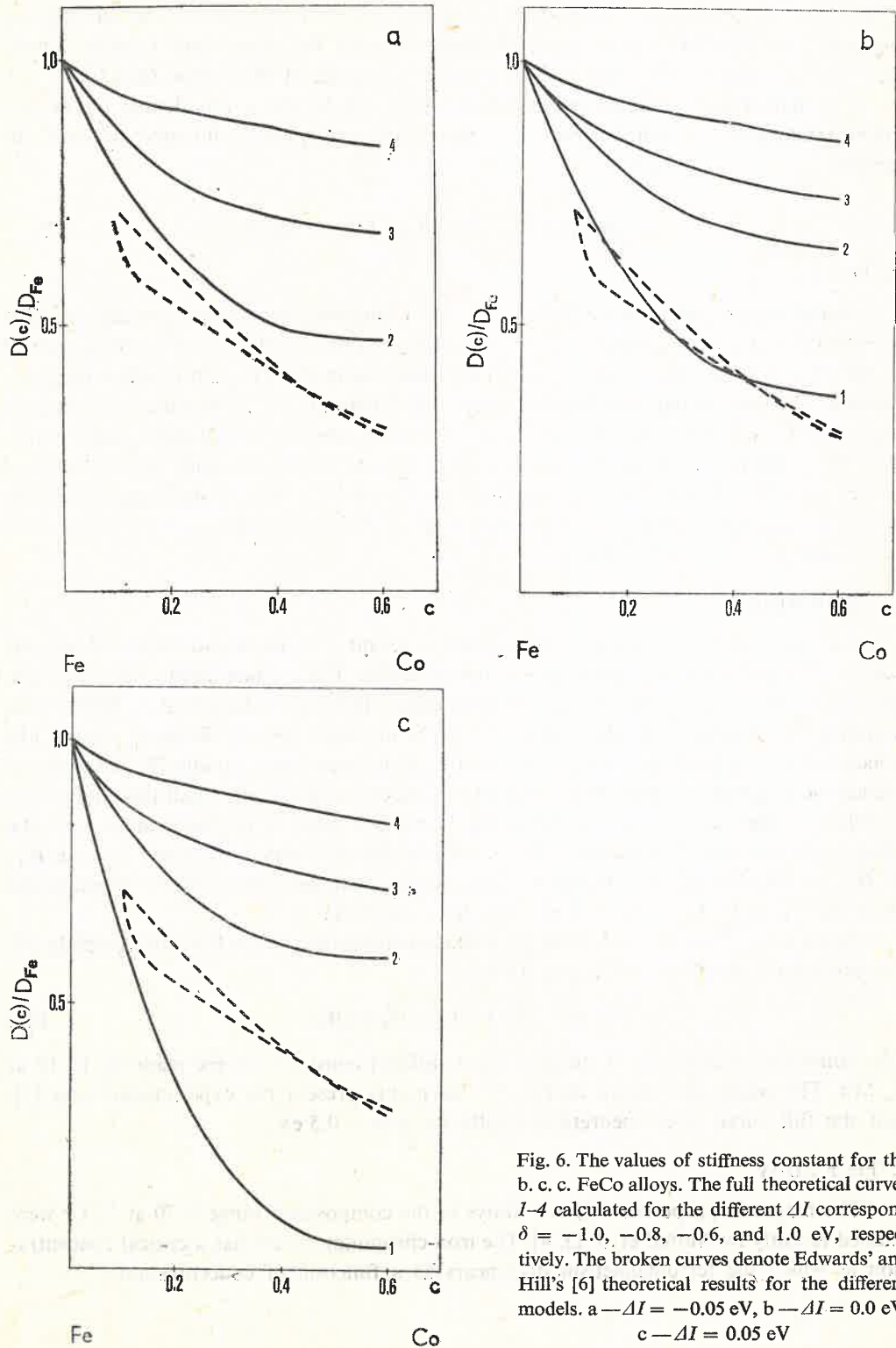


Fig. 6. The values of stiffness constant for the b. c. c. FeCo alloys. The full theoretical curves 1-4 calculated for the different  $\Delta I$  correspond  $\delta = -1.0, -0.8, -0.6,$  and  $1.0$  eV, respectively. The broken curves denote Edwards' and Hill's [6] theoretical results for the different models. a  $-\Delta I = -0.05$  eV, b  $-\Delta I = 0.0$  eV, c  $-\Delta I = 0.05$  eV

The bulk magnetic moment in FeCr alloys decreases linearly with increasing the chromium concentration. Aldred [3] calculated the stiffness coefficients from the temperature dependence of the magnetization. These results are compared with those obtained directly by inelastic-neutron-scattering experiments (Lowde et al. [15]) and with our theoretical results. The theoretical values of  $D$  in the composition range 0–20% Cr were computed using the model presented in Section 2. The bandwidths of Fe and Cr were assumed to be 5.9 eV and 6.2 eV, respectively.

The difference between atomic potentials  $\delta = \varepsilon_{\text{Cr}} - \varepsilon_{\text{Fe}}$  was taken as 1.0 eV. The theoretical results for the different values of  $\Delta I = I_{\text{Cr}} - I_{\text{Fe}}$  are presented in Fig. 8. Curves 1, 2, 3

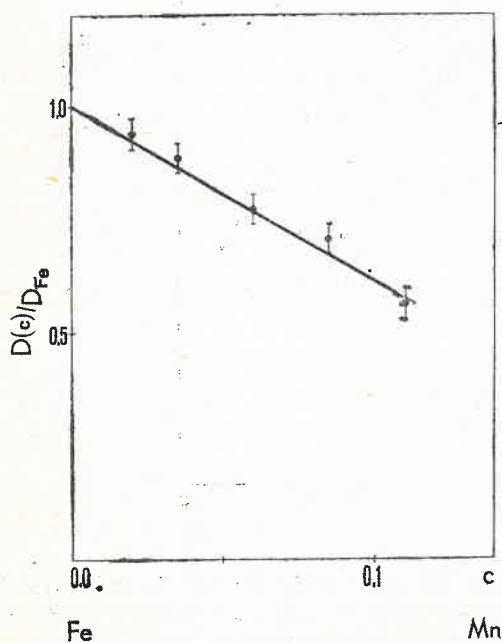


Fig. 7

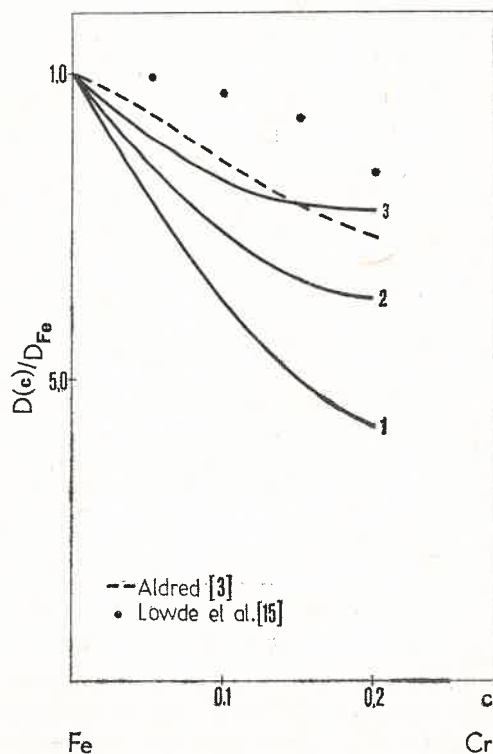


Fig. 8

Fig. 7. Stiffness constant  $D$  versus composition for b. c. c. FeMn alloy. The points are the experimental data [5]. The full curve presents theoretical results for  $\Delta I = -0.25$  eV and  $\delta = -0.5$  eV

Fig. 8. Values of  $D$  for the b. c. c. FeCr alloys, as a function of Cr concentration. The broken curve presents Aldred [3] experimental data. The points denote Lowde et al. [15] data. The full curves 1–3 correspond to the present theoretical calculations for  $\delta = 1.0$  eV and  $\Delta I = -0.30, -0.35, -0.40$ , respectively

correspond to  $\Delta I = -0.30, -0.35$  and  $-0.40$  eV, respectively. The broken curve presents the experimental results obtained by Aldred [3], and the points present the inelastic-neutron-scattering data (Lowde et al. [15]).

### 6. Spin wave stiffness coefficient in FePd f. c. c. alloys

The ferromagnetic FePd alloy has the face-centered-cubic lattice above 50 at % Pd in the system. Recently Yamauchi et al. [16] estimated the values of stiffness constant  $D$  in disordered f. c. c. PdFe alloys from the temperature dependence of the magnetization. Their results are shown in figure 9 (broken curve).

In order to calculate the theoretical dependence of stiffness constant on the concentration in PdFe alloys we assumed the following model:

We start with the  $\text{Fe}_{0.5}\text{Pd}_{0.5}$  f. c. c. alloy. The experimental value of  $D$  for such a system is about  $0.200 \text{ eV \AA}^2$ . The parameters of theory were chosen in such a way,

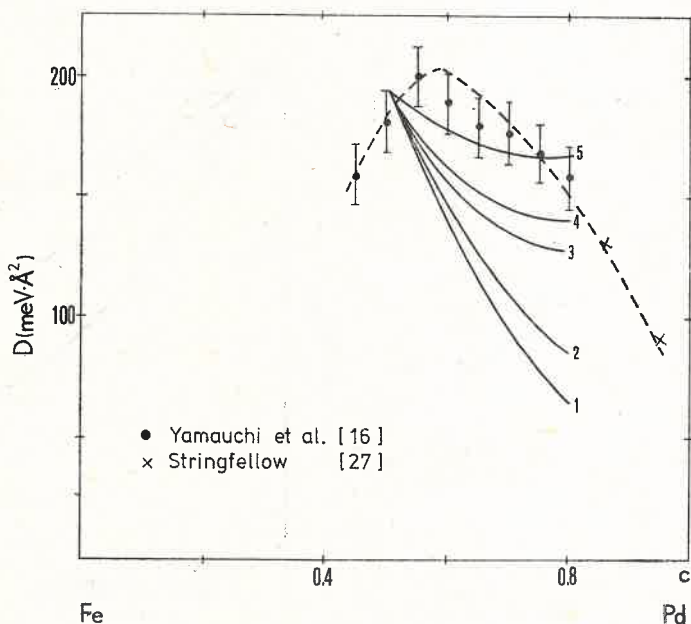


Fig. 9. Value of  $D(c)/D_{\text{Fe}}$  as a function of impurity concentration for FePd f. c. c. alloys. The points denote experimental data. The broken curve presents the smoothed version of Yamauchi et al. [16] experimental results. The full curves are the present theoretical results for the different values of  $\Delta I$  and  $\delta$  (the number in brackets denotes the curve).  $\Delta I = 0$ ,  $\delta = 0.3 \text{ eV}$  (1),  $\Delta I = 0$ ,  $\delta = 0.4 \text{ eV}$  (2),  $\Delta I = -0.05$ ,  $\delta = 0.3 \text{ eV}$  (3),  $\Delta I = -0.05$ ,  $\delta = 0.4 \text{ eV}$  (4),  $\Delta I = -0.10$ ,  $\delta = 0.4 \text{ eV}$  (5)

in order to get similar value of  $D$ . The magnetic moment of the  $\text{Fe}_{0.5}\text{Pd}_{0.5}$  alloy was estimated to be  $1.6 \mu_{\text{B}}$  and found to change linearly with the increasing Pd concentration. The FePd alloy in the region 50–80 at % Pd was considered as a strong ferromagnet. The bandwidths of iron and palladium were taken as 5.4 and 3.75 eV, respectively. The value of the intraatomic Coulomb interaction of Fe was estimated to be 0.65 eV. We computed the stiffness constant for the different value of  $\delta$  and  $\Delta I = I_{\text{Pd}} - I_{\text{Fe}}$ . The results (curves 1–5) are presented in figure 9. The points denote the

experimental data and the broken curve was fitted by Yamauchi et al. [16] Although our theoretical results do not agree with the experimental data the character of the curves is similar. The theoretical value of  $D$  decreases with an increase of palladium concentration.

### 7. Conclusions

Up to 1977 various expressions were derived for the spin wave stiffness constant  $D$  in ferromagnetic alloys. The spin wave spectrum can be obtained from the poles of the dynamical transverse susceptibility (Yamada and Shimizu [20], Edwards and Hill [6], Riedinger and Nauciel-Bloch [24], Jezierski [1]), or using the method of effective magnon Hamiltonian (Morkowski [8]). The both methods give the final result in the RPA-CPA.

Edwards and Hill [6] showed that the most important parameter for determining  $D$  in NiFe alloys, within the RPA, is the exchange splitting  $\Delta I$  for pure Ni. Jezierski [1] has shown, for NiFe alloys, that the change of parameter  $\Delta I$  (where  $\Delta I = I_{\text{Fe}} - I_{\text{Ni}}$ ) gives the change of the slope of the coefficient  $D$  (see Ref. [1], Fig. 5). In present and previous papers we considered the magnon energy in the ferromagnetic f. c. c. and b. c. c. transition metal alloys. The binary alloys were described in terms of a single-band model of an itinerant electron ferromagnet. A simple Hamiltonian (1) was used in which the change of the hopping integral, atomic potential, and intra-atomic Coulomb interaction was considered. The values of spin wave stiffness constant  $D$  as a function of concentration for the different alloys were computed using the expression derived by Edwards and Fisher [9]. The two-particle Green function  $\langle\langle a_{k-}^+ a_{k+}; a_{k'}^+ a_{k'-} \rangle\rangle_{\omega=0}$  which appeared in the expression (2) was calculated directly from the equation of motion. The equation (4) was solved for a full Hamiltonian (1) without using the Hartree-Fock Approximation. The higher-order Green functions in the equation of motion were calculated in the Random Phase Approximation. Then, using the iterative method, the two-particle Green function was found as a function of  $c_i$  operators. Finally, the configurational average of the two particle Green function depended on the concentration and short range order parameters.

Those approximations and the method of calculations allowed us to consider the effects of interaction between the first and second neighbours and the effects of local ordering. The second important magnitude was the electron energy  $\varepsilon_k$ . In our papers we took  $\varepsilon_k$  in the tight binding approximation. In the TBA we have only one parameter  $W$  (bandwidth) which characterized the band structure of pure metal. The bandwidths of transition metals were taken according to McAlister et al. [14]. Besides the bandwidth in our theory there are two other parameters: atomic potential and intraatomic Coulomb interaction. The values of those parameters were assumed similarly as in other theoretical papers. In the computations we established that the magnetic moments of considered alloys changed with the concentration.

In paper [2] the influence of local ordering on the stiffness constant was examined. In the case of NiFe alloy our results indicated that the stiffness constant  $D$  for ordered alloys is greater than for disordered systems. Although our results for ordered f. c. c. Ni<sub>3</sub>Fe alloy are less than experimental data (Mikke et al. [17, 18] and Jankowska et al. [19])

the qualitative character is similar. The theoretical results presented in this paper for the b. c. c. Fe-base alloys indicated that the simple single band model with the change of hopping integral may be adequate to describe the magnon energy in the ferromagnetic transition metal alloys.

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#### REFERENCES

- [1] A. Jezierski, *Acta Phys. Pol.* **A51**, 839 (1977).
- [2] A. Jezierski, *Acta Phys. Pol.* **A52**, 413 (1977).
- [3] A. T. Aldred, *Phys. Rev.* **B14**, 219 (1976).
- [4] A. T. Aldred, B. D. Rainford, J. S. Kouvel, T. J. Hicks, *Phys. Rev.* **B14**, 228 (1976).
- [5] H. Yamauchi, H. Watanabe, Y. Suzuki, H. Saito, *J. Phys. Soc. Jap.* **36**, 971 (1974).
- [6] D. M. Edwards, D. J. Hill, *J. Phys. F* **6**, 607 (1976).
- [7] J. Morkowski, A. Jezierski, (to be published).
- [8] J. Morkowski, *Solid State Commun.* **19**, 787 (1976); *Physica* **86-88B**, 343 (1977).
- [9] D. M. Edwards, B. Fischer, *J. Phys. (France)* **32**, C1 697 (1971).
- [10] F. Ducastelle, F. Gautier, *J. Phys. F* **6**, 2039 (1976).
- [11] S. F. Edwards, R. C. Jones, *J. Phys. C* **4**, 2109 (1971).
- [12] M. Sakoh, D. M. Edwards, *Phys. Status Solidi (b)* **70**, 611 (1975).
- [13] H. Hasegawa, J. Kanamori, *J. Phys. Soc. Jap.* **33**, 1607 (1972).
- [14] A. J. McAlister, J. R. Cuthill, R. C. Dobbyn, M. L. Williams, R. E. Watson, *Phys. Rev.* **B12**, 2973 (1975).
- [15] R. D. Lowde, M. Shimizu, M. W. Stringfellow, B. H. Torrie, *Phys. Rev. Lett.* **14**, 698 (1965).
- [16] H. Yamauchi, E. Saito, H. Watanabe, *Physica* **86-88B**, 347 (1977).
- [17] K. Mikke, J. Jankowska, A. Modrzejewski, *J. Phys. F* **6**, 631 (1976).
- [18] K. Mikke, J. Jankowska, Z. Osetek, A. Modrzejewski, *J. Phys. F* **7**, L211 (1977).
- [19] J. Jankowska, Z. Osetek, K. Mikke, (to be published).
- [20] H. Yamada, M. Shimizu, *J. Phys. Soc. Jap.* **28**, 327 (1970).
- [21] M. Kohgi, Y. Ishikawa, N. Wakabayashi, *Solid State Commun.* **18**, 509 (1976).
- [22] H. Hiroyoshi, H. Fujimori, H. Saito, *J. Phys. Soc. Jap.* **31**, 1278 (1971).
- [23] O. Yamada, F. Ono, I. Nakai, *Physica* **86-88B**, 311 (1977).
- [24] M. Hatherly, K. Hirikawa, R. D. Lowde, J. F. Mallett, M. W. Stringfellow, B. H. Torrie, *Proc. Phys. Soc.* **84**, 55 (1964).
- [25] H. Hennion, B. Hennion, A. Castets, D. Tocchetti, *Solid State Commun.* **17**, 899 (1975).
- [26] T. Maeda, H. Yamauchi, H. Watanabe, *J. Phys. Soc. Jap.* **35**, 1635 (1973).
- [27] M. W. Stringfellow, *J. Phys. C* **1**, 1699 (1968).