Studies on Transition Temperature of the Superconducting Materials Related to Elastic Constants

Md. Abdus Salam,[a] Bikiran Prasad Barua,[a] and Md. Minhaj Uddin[b]

*[a]BCSIR Laboratories, Chittagong and [b]Department of Physics,
University of Chittagong, Bangladesh*

Abstract

For a face-centered-cubic structure crystal the parameters like atomic mass M, atomic number Z, lattice spacing are the important factors in the determination of a many body Hamiltonian H. Instead of using fcc lattice spacing we can also utilize atomic volume Ω. Using the superconducting transition temperature expressed as $T_c = T_c^{(M)}(Z, \Omega)$, a well defined region in superconducting elements is possible. T_c may also be related to BCS theory through Debye temperature. This Debye temperature is related to elastic constants C_{11}, C_{12} and C_{44}, atomic weight and atomic volume. Also T_c for five fcc transitions metals is linear in the Cauchy deviation $C^* = (C_{12} - C_{44})/(C_{12} + C_{44})$, such linearity is also seen in bcc transition elements. Finally *via* elastic constants mass density and atomic volume, a correlation between C^* and the Debye Ω temperature has been established for the five fcc transition elements. This correlation indirectly sets up a relation between transition temperature and elastic constant.

Introduction

For heavy fermions superconductor, the superconducting transition temperatures are shown T_c to correlate with a characteristic energy $h^2/(m^* \xi^2)$, m^* being the effective mass and $\hat{\imath}$ the coherence length. It is very difficult to identify the correlations between superconducting properties and elastic properties of fcc elements due to their complex crystallographic structure. These correlations would be helpful to study the new classes of superconductors with relevant variables (Angilella, *et al.,* 2000; Angilella, *et al.,* 2002 and Angilella, *et al.* 2004).

According to the BCS theory (Schrieffer, 1964) the attraction caused by even a weak lattice distortion can overcome $h^2/(m^* \xi^2)$, m^* strong Coulomb's repulsion. Thus the net effect is the attraction of two electrons via a lattice distortion to form a pair of electron known as the cooper pair, questions have come up regarding the role of strong electron-electron interactions in both the high T_c cuprites and heavy fermions materials.

If we were able to solve the many-body Schrödinger equation for the superconduct-

ing elements, then by treating the motion of nuclei and T_c electrons on the same basement, plus full inclusion of electron-electron interactions. These interactions, such uncertainties engaged in separating electron lattice and Coulomb repulsions between electrons would be bypassed.

Let us consider some superconducting metallic elements. We treat these elements by the following procedure: Firstly we single-out the face-centered-cubic (fcc) lattice. We would need the atomic volume Ω (of course, essentially equivalently the lattice parameter a) to specify the structure. Again atomic number Z is required to signify the external potential which created by the nuclei. Any element that has a many-body Hamiltonian containing both electron and nuclear kinetic energy also need nuclear mass M. We also take here some fundamental constants such as nuclear mass *h, e* and electronic mass *m*.

For our structure which we have taken fcc, the superconducting transition temperature T_c depends on *M, Z* and Ω. This is apart from the many-body partition function; once the Schrödinger equation has been solved from the fundamental constants such as Plank's constant *h, e* the charge of electron and electronic mass *m*.

$$T_c = T_c^{(M)} (Z,\Omega) \qquad (1)$$

We have more than one atomic number for all other types of superconductors.

Materials and Methods

As described in the introduction in the beginning, the methodology of the work is given below. In section 1 described below we have represented $T_c = T_c^{(M)} (Z,\Omega)$ to lead our present work. This is the work of testing that T_c depends on atomic number *Z* and atomic volume Ω in fcc transition elements. Our chosen five fcc elements are *Al, Pb, La, Ir* and *Th*. This elements are considered in the (Z,Ω) plane with respect to their transition temperature. There is weak but relatively unimportant dependence of T_c on nuclear isotopic mass. In section 2 we have introduced new quantity, Cauchy discrepancy which is related to T_c *i.e.* the departure of C_{12} from C_{44} where these are two of the elastic constants (C_{11} being the other) required to characterize a cubic crystal. In section 3 using the essential ingredient of BCS theory the Cauchy deviation relates to the Debye temperature. In section 4 we have summarized and designed some clue for advance research both theoretical and experimental. At last we have shown in the Appendix for that a particular critical field H_c *(0)* and energy gap E_g (0) can be des-cribed as function of the Cauchy discrepancy. This function considers zero temperature properties.

Evidence of correlation between transition temperatures T_c and atomic number (z) or atomic volume (Ω) in fcc transition elements.

For graphical view we have made a plot for the five fcc elements in the (Ω,Z) plane and

attached every experimental values of T_c to the recognized coordinates.

The functional form $T_c(\Omega, Z)$ comments us that (1) transition temperature significantly decreases with increasing atomic number for constant volume (2) For constant Z, there is plainly substantial variation of T_c with atomic volume, which is proportional to the reciprocal of the concentration, It may be mentioned here that atomic volume Ω and atomic number Z are important variables in characterizing T_c for a definite element. It is also observed that high pressure can turn many elements into superconductors *via* an insulator-metal transition.
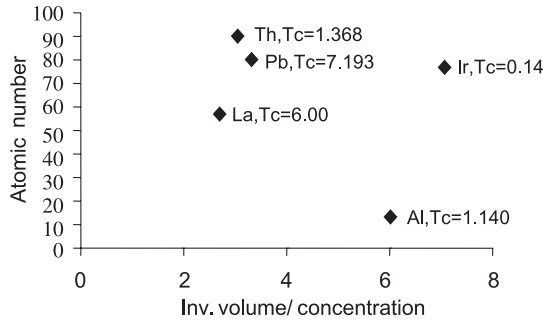

Fig.1.   Shows five superconducting fcc transition elements in the (Ω, Z) plane. Actual abscissa is the reciprocal of the atomic volume Ω^{-1}. To each point the value of the critical temperature T_c is shown.

Transition T_c temperature usually increases with increasing pressure for most super - - conducting elements at ambient pressure (See Table I). Within BCS theory [see also Eq. below] or its extension by McMillan,

this is usually justified in terms of a pressure-induced lattice stiffening which reduces the electron-phonon constant at a more rapid rate than the electron density of states at the Fermi level is increased (Hochheimer, *et al.* 2001).

Table I. Presssure derivatives of T_c[5],experimental bulk moduli [6], and inferred partial derivatives of T_c with respect to Ω at constant Z, Eq.(2), of the fcc superconducting transition metals at $P = 0$.

Elements	Al	Th	Pb	Ir	La
$\frac{\partial T_c}{\partial P}[K/GPa]$	1.15	7.09	276.42	-39.65	445.19
$B[GPa]$	72.2	54.3	43.00	355.00	24.30
$\frac{\partial T_c}{\partial \Omega}[10^{31}K.m^{-3}]$	-0.50	-1.17	-39.22	0.99	-29.21

Pressure derivatives of T_c can then are straightforwardly related to volume derivatives at constant Z from the relation.

$$\frac{\partial \log T_c}{\partial \log \Omega} = -B\frac{\partial \log T_c}{\partial P} \qquad (2)$$

Where B is the bulk modulus (See Table I)

However, this partial derivative indicates us that T_c depend apparently in a sensitive way on these two variables. Because, chosen fcc structure allows the detailed form of the function $T_c(\Omega, Z)$ for this structure. We know that there is a correlation between T_c and the Cauchydiscrepancy $C^* = (C_{12} - C_{44})/(C_{12} + C_{44})$ between elastic constants. By applying this clue we can characterize T_c by a single variable, rather than the pair (Ω, Z) used in fig. 1.
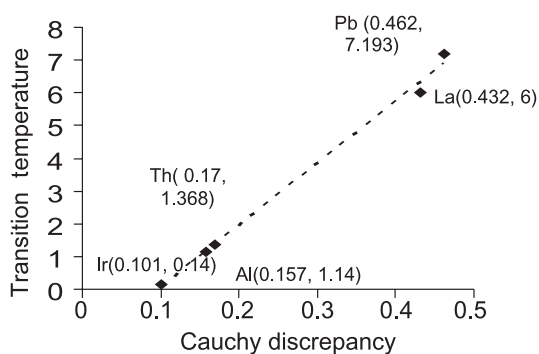
Fig.2. **Superconducting transition tempera-tures for fcc transition elements corre-lated with Cauchy discrepancy, Eq(3). Solid line is best fit to the point [see text for discursion, in particular eq.(4)]. Redrawn from ref [8] see also[6] for an update on elastic constants data.**

Correlation between superconducting transi-tion temperature T_c and the cauchy discrepan-cy C^* in face-centered-cubic transition metals

For face-centered-cubic transition metals, an empirical relationship exists between the superconducting transition temperature and Cauchy discrepancy. This correlation may arise from many-atom effects.

We have drawn a pot of verses Cauchy dis-crepancy for five fcc elements by following the previous work of H.M Ledbetter (Myers, 1997) carried out almost a quarter of Century ago. The quantity defined by

$$C^* = \frac{C_{12} - C_{44}}{C_{12} + C_{44}} \quad (3)$$

Ledbetter (Myers, 1997) also included some

alloys, namely $Nb_{0.9}Zr_{0.1}, Nb_{0.4}Ti_{0.6}$ and $Ti_{0.7}v_{0.3}$ but we have omitted these from redrawn fig. 2. It should be mentioned, that a high pressure, nonmagnetic, but also a non bcc phase of iron has been recently reported to display superconductivity with $T_c < 2k$ between 15 and 30 GPa. (Shimizu, *et al.,* 2001) The equation of the straight line drawn in fig. 2 is

$$T_c[K] = AC^* - B \quad (4)$$

Here A= 17.7K and B=1.65K ,we have no relevant theory to evaluate A&B. Several previous studies relate elastic constants to superconductivity. The physical meaning of equation (4) indicates us to think the relation with C^* to a basic ingredient of BCS theory, the Debye temperature θ_D.

Correlation between cauchy discrepancy C^* and debye temperature, θ_D which give the scale of T_c in the bcs theory

The criterion for the transition temperature of an element or alloy involves the density of states $N(E_F)$ at the Fermi level and the elec-tron-phonon coupling constant V which can be estimated from the electrical resistivity. For $N(E_F) << 1$ the BCS theory predicts (Allen and Mitrov, 1982; Myers, 1997)

$$T_c = 1.30\theta_D \exp\left(\frac{1}{N(E_F)V}\right) \quad (5)$$

This is not a successful way of correlating values of T_c for the metallic elements. Nevertheless, it suggests that one should re-open empirically the question of a correlation

between T_c and θ_D. There is an interesting apparent paradox: the higher the resistivity at room temperature the more likely it is that a metal will be a superconductor when cooled.
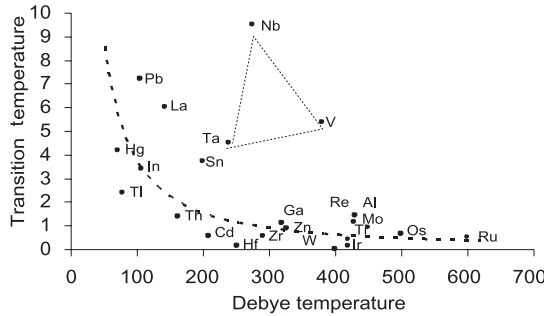

Fig.3(a). **Superconducting critical tempera-tures versus debye temperatures for numerous elements. Redrawn after (Launay and Dolecek, 1947). Solid and dashed lines are guides to the eye. See text for discussion.**

De Launay and Dolecek (Launay and Dolecek, 1947) considered the variation of the superconducting transition temperature T_c with the Debye characteristic temperature θ_D. We have redrawn data by De Launay and Dolecek in fig. 3.

While for mainly non-transition elements the continuous line drawn in fig. 3(a) already given by De Launay and Dolecek (1947) a decade before BCS theory, shows a relation between T_c and θ_D is far from simple. And the triangle involving Ta, V. and Nb modified from the 1947 figure of De Launay and Dolecek (1947) shows no relation to the con-tinuous curve.
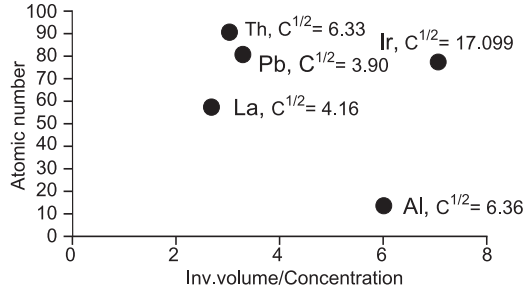

Fig.3(b). **Shows five superconducting fcc tran-sition elements in the (Ω, Z) plane. To each point the values of square root $C^{\frac{1}{2}}$ of the 'average' elastic constant as defined by equation (7) in $GPa^{\frac{1}{2}}$**

Debye temperature θ_D can be related with Cauchy deviation C^* by obeying the first principles theory. On the other hand T_c is much more related to C^* is shown in previous section.

To make a correlation between T_c and Cauchy discrepancy, many earlier workers have calculated the Debye temperature for cubic crystals by using the elastic constants C_{11}, C_{12} and C_{44}, the mass density ρ and atomic volume Ω. While Houston's method (Houstan, 1948) is favoured and has been developed by (Betts *et al.* 1956; Betts *et al.* 1956) we have found the semi-empirical relation of Blackman (Blackman, 1951), quoted in Huntington's review article (Huntington, 1958), an important introducto-ry point which is

$$\theta_D{}^3 = \frac{3.15}{8\pi}\left(\frac{h}{k_B}\right)^3 \frac{s}{\rho^{\frac{3}{2}}\Omega} \times \left(C_{11} - C_{12}\right)^{\frac{1}{2}}\left(C_{11} + C_{12} + \right.$$

$$2C_{44}\left.\right)^{\frac{1}{2}}\left(C_{44}\right)^{\frac{1}{2}} \qquad (6)$$

Here s is the number of atoms in the unit cell of volume Ω and ρ is the mass density. Equation (6) can be true into the definition of an 'average' elastic constant, C or C^* by approximation.

$$C^* = \left(\frac{8\pi}{3.15}\right)^{\frac{2}{3}} \left(\frac{k_B}{h}\right)^2 \frac{\rho\Omega^{\frac{2}{3}}}{s^{\frac{2}{3}}} \theta_D{}^2 \tag{7}$$

So our final correlation between transition temperature T_c and Cauchy discrepancy C^* is

$$T_c[K] = A\left(\frac{8\pi}{3.15}\right)^{\frac{2}{3}} \left(\frac{k_B}{h}\right)^2 \frac{\rho\Omega^{\frac{2}{3}}}{s^{\frac{2}{3}}} \theta_D{}^2 - B \tag{8}$$

Fig. 3(b) same as fig. 1, but coordinates in the (Ω,Z) plane are now labeled by the values of square root $C^{\frac{1}{2}}$ of the average elastic constant. It is clear from this fig. at constant volume Ω . $C^{\frac{1}{2}}$ related to θ_D through equation (7). Again $C^{\frac{1}{2}}$ increases with increasing Z in contrast to the behavior of T_c in fig. 1.

At constant $Z, C^{\frac{1}{2}}$ increases with decreasing atomic volume also. According to BCS theory, we are interested to correlate with but now via the Cauchy discrepancy. In fig. 4 the functional form obtained empirically being recorded in the caption and represent a remarkable correlation for the five fcc elements.

Results and Discussion

By considering fig. 3, we can draw our conclusion that there is no simple relation between Debye temperature θ_D and the superconducting transition temperature T_C. Fig. 1 and fig. 3 (b) have been led us to take step to correlate C having dimension of an elastic constant and defined in equation (7). This average elastic constant can be expressed with θ_D and with the Cauchy discrepancy C^* in equation (3) .We have focused on these quantities for five fcc elements and got an clear interrelation, as fig. 4 demon
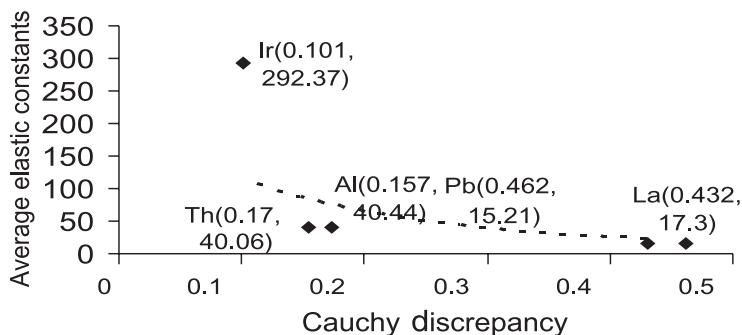
Fig. 4.   Shows 'average' elastic constant C, Eq.(7), as a function of Cauchy discrepancy C^*, Eq.(3), for the five fcc transition metals. Dashed line is a guide for the eye, which actually employs an exponential form, of the *kind C = α+βexp (-γC^*), with α = 20.5 Gpa, β = 300.5 Gpa, γ= 10.5 Gpa*

strates and the functional form has been extracted. Since as Ledbetter (1980) already pointed out in 1980, T_C relates linearly to C^* as in fig. 2. Equation (Ledbetter, (1980) made a clear correlation between T_C and θ_D with mass density and atomic volume entering through the definition of the average elastic constant. Again we thought the BCS theory in another eye sight for zero temperature quantities which is critical field H_C (0) and energy gap E_g (0). Here we make a correlation simply with the Cauchy discrepancy for five fcc superconducting transition elements by plotting a graph.

discrepancy C^*. Our main objectives to make a Appendix is to display a remarkable correlation between experimentally estimated values of the critical field $H_C(0)$ and the energy gap E_g (0), as extracted from tunneling experiments, and the Cauchy discrepancy C^* (Eqn.-3). Fig. 5, shows H_C (0) plotted against C^* for five fcc transition elements on which attention was focused in the body of the text. The data for $H_C(0)$ have been taken from Kittel's book (Kittel, 1991; Myers, 1997). Evidently, as for T_C in fig. 2, a marked correlation again exists, the dashed line
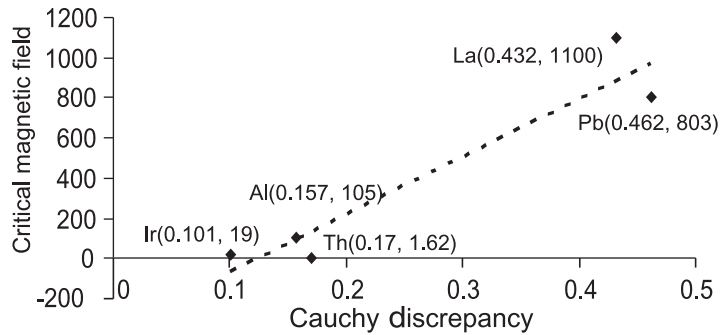

Fig. 5.   Experimental results for critical field $H_C(0)$, as extracted from tunneling measurements, Vs Cauchy discrepancy C^*, as defined in Equation (3)

Our present studies stimulates advance researcher concerning generalization of basic approach set out here to other group of superconductors.

Appendix

Here, we have Introduced zero temperature properties that are functions of Cauchy

having the equation

$$H_C(0) = b_1 C^* - b_2 \qquad (9)$$

Here, b_1= 0.41 Tesla and b_2 = 0.04 Tesla.

Again we have collected data for the energy gap $E_g(0)$ given by Kittel (1991) (see also Poole, *et al.* 1995), and fig. 6 is shown the same set of five fcc transition elements. The
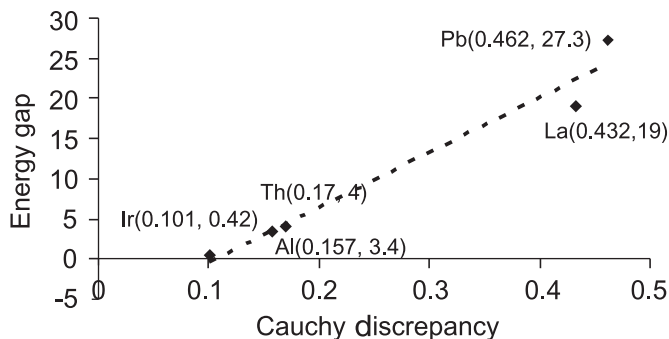
Fig. 6. **Experimental results for energy gap $E_g(0)$, as extracted from tunneling measurement, *Vs* Cauchy discrepancy C^*, as defined in Equation (3)**

dashed line, but now with more substantial scatter of the experimental points than for either T_C or $H_C(0)$, have the equation.

$$E_g(0) = e_1 C^* - e_2 \qquad (10)$$

With $e_1 = 55.8 \times 10^{-4} eV$ and $e_2 = 5.16 \times 10^{-4} eV.$

BCS theory predicts a constant value for the ratio $E_g(0)/K_B T_C$. On the basis of our present study equation (4) and (10) very nearly fit for the five fcc transition elements. Finally we have plotted the 'average' ratio $E_g(0)/K_B T_C$ from equation (4) and (10) as a function of C^* in fig. 7 where using parameter A, B, e_1 and e_2 are given.
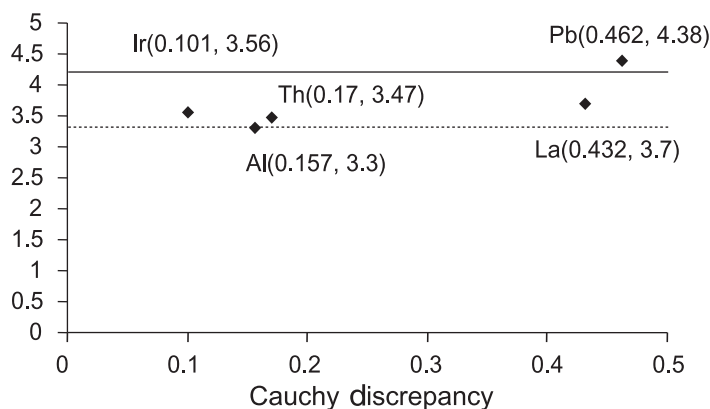

Fig. 7. **EBCS ratio $E_g(0)/k_B T_c$ for fcc transition elements. Solid line is ratio of Eqs (4) and (10), While dashed line is BCS theoretical value**

References

Allen, P.B. and Mitrov, B. (1982) Solid state physics, edited by H. Ehrenreich, F. Seitz, and Turnbull (Academic Press by New york, 1982), **37** : 220-248.

Angilella, G.G.N. Leys, F.E. March, N.H. and Pucci, R. (2004) Correlation between Character-istics energies in non-s-wave Superconductors *Phy. Lett.* A322, 475-480

Angilella, G.G.N. March, N.H. and Pucci, R. (2000) for non-s-wave pairing Superconductors correlated with coherence length and effective mass. *Phys. Rev* B **62** : 13919-13921

Angilella, G.G.N. March, N.H. and Pucci, R. (2002) Superconducting Transition Temperatures and coherence length in non-s-wave pairing materials correlated with spin fluctuation meditated interaction. *Phys. Rev.* B **65** : 092509(1-4)

Betts, D.D. Bhatia, A.B. and Horton, G. K. (1956) Debye Characteristic Temperature of Certain Non-cubic Crystals, *Phys. Rev.*104, 43-47

Betts, D.D. Bhatia, A.B. and Wyman, M. (1956) Houston Method and its application to the calculation of Characteristic Temperature of cubic Crystals, *Phys. Rev.* **104** : 37-42

Blackman, M. (1951) On the calculation of characteristic temperatures from the Elastic constants, Phil. Mag. **42** : 1441-1442

Hochheimer, H.D. Kuchta, B. Dorhout, P. K. and Yarger, J.L. (Kluwer, Dordrecht, 2001) Schilling, J.S. in frontiers of high pressure research P : Application of high pressure to low dimensional novel electronic materials, **48** of NATO science series.

Houstan, W.V. (1948) Normal Vibration of a Crystal Lattice. *Rev.Mod. Phys* **20** :161-166

Huntington, H.B. (1958) Solid State Physics, edited by F. Seitz and D. Turnbull (Academic Press, New York,), **7** : pp-214-300

Kittel, C. (1991) Introduction to Solid State Physics (J. Wiley and Sons, New York) pp 367, 396

Launay, J. De. and Dolecek, R.L. (1947) Superconductivity and the Debye character-istic temperature, *Phys. Rev.* **72** : 141-143

Ledbetter, H.M. (1980) Correlation between superconducting transition temperature and the Cauchy discrepancy in a body-centered-cubic transition metals. *Phys. Lett.* **77** A, 359-361

Mehl, M.J. and Papaconstantopoulos, D.A (1996) Application of a tight-binding total-energy method for transition and noble metals: elastic constant, vacancies, and surfaces of monatomic metals, *Phys. Rev*. B **54** : 4519 - 4530.

Myers, H. P. (1997) Introductory Solid State Physics (Taylor and Francis, London,) pp 182-190.

Poole, Ch.P. Farach, H A. and Creswick, R. J. (1995) Superconductivity (Academic press, San Diego), pp (320-340)

Schrieffer, J.R. (1964) Theory of Superconductivity (W.A .Benjamin, New York) pp (24-57)

Shimizu, K. Kimura, T. Furomoto, S. Takeda, K. Kontani, K. Onuki, Y. and Amaya, K. (2001) Superconductivity in the non-magnetic state of iron under pressure. *Nature* **412** : 316-318