Effects of pressure on the superconducting properties of magnesium diboride

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We discuss the effects of hydrostatic pressure on the superconducting properties of MgB_2 within the framework of the Eliashberg theory. By considering the pressure dependences of all parameters appearing in the McMillan formula, we show that the calculated pressure derivative of T_c as well as the variation of T_c with pressure are in good agreement with recent measurements. The pressure dependences of the energy gap Δ_0, the effective interaction strength $N(E_F)v$, the critical magnetic field $H_c(0)$, and the electronic specific-heat coefficient γ are also predicted for this system. A comparison of the pressure effects in nontransition elements clearly suggests that MgB_2 is an electron-phonon-mediated superconductor.

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I. INTRODUCTION

The recent discovery of superconductivity in MgB_2 (Ref. 1) has attracted considerable interest in the study of this material, both to understand the mechanism of superconductivity and to explore other properties of MgB_2 and related materials. The high transition temperature $T_c \approx 40$ K in this material offers another possibility for finding high-T_c superconductivity in some binary intermetallic compounds besides cuprates and C_{60}-based compounds. Meanwhile, the high critical currents observed in MgB_2 thin films[2] and wires[3] reveal that MgB_2 belongs to a class of low-cost, high-performance superconducting materials for magnets and electronic applications.

Measurements of the isotope effect and of the influence of pressure on the transition temperature and critical field of superconductors yield information on the interaction causing the superconductivity. Indeed, the pressure (or volume) and the mass number would seem to be the only variables whose effects might be capable of immediate theoretical interpretation. By observing how pressure changes the parameters of the lattice in the normal state and in the superconducting state, and comparing the measurements with the theoretical predictions, one can test the validity of some theoretical models. Olsen *et al.*[4] shaved that the volume (V) dependence of effective interaction $N(E_F)v$, $d\ln N(E_F)v/d\ln V$, can be scaled well with the deviation ξ from the full isotope effect, where ξ is defined by $T_c \propto M^{-0.5(1-\xi)}$ in superconducting metals. Bud'ko *et al.*[5] and Hinks *et al.*[6] reported a sizable isotope effect for B [$\alpha_B = 0.26(3)$ or $0.30(1)$] in the newly discovered superconductor MgB_2. Although the total isotope coefficient $\alpha = 0.32(1)$ (Ref. 6) is smaller than the canonical BCS value of 0.5, it is the same as that in Cd (Ref. 7). The isotope effect along with other measurements such as inelastic neutron scattering,[8,9] tunneling,[10] NMR (Ref. 11), and specific heat,[12–14] confirmed that MgB_2 is an electron-phonon mediated s-wave superconductor.

Soon after the discovery of superconductivity in MgB_2, the effect of pressure on T_c was studied by two groups[15,16] by resistivity or ac susceptibility measurements. Both groups observed a decrease of T_c with increasing pressure, with an initial pressure derivative dT_c/dP of -0.8 K/GPa (Ref. 15) or -1.6 K/GPa (Ref. 16), respectively. Moreover, Monteverde *et al.*[15] found that the superconductivity is not destroyed by applying high pressure up to 25 GPa, at which point T_c is as high as 21 K. A somewhat larger dT_c/dP of -2.0 K/GPa was recently reported by Saito *et al.*[17] from high-pressure resistivity measurements. Using a He-gas apparatus, Tomita *et al.*[18] determined a dT_c/dP of -1.11 K/GPa under pure hydrostatic pressure conditions. In order to find the reason why the reported values of dT_c/dP are different among different groups, Lorenz *et al.*[19] carried out high-pressure experiments on MgB_2 samples with different T_c's at ambient pressure and different pressure media. T_c was found to decrease linearly over the whole pressure range (0–1 GPa). In the He environment, the two samples with the initial $T_c = 39.2$ and 37.4 K yield the pressure derivatives of -1.07 and -1.45 K/GPa, respectively. The former is obviously very close to that of Tomita *et al.*[18] The latter approaches their previous data,[16] which was obtained by using the Fluorinert FC77 as pressure medium. They therefore concluded that the variation in the value of dT_c/dP by various groups results from the differences in sample preparation conditions. The value of $dT_c/dP \simeq -1.1$ K/GPa is then confirmed to give the true hydrostatic pressure dependence of T_c in MgB_2.

Two theoretical models have been tried to describe the systematics of the behavior of T_c under pressure in MgB_2. Based on the theory of hole superconductivity, Hirsch[20] predicted an increased T_c with the decrease of B-B intraplane distance under the application of in-plane biaxial pressure. However, this prediction has not yet been confirmed experimentally. No uniaxial pressure measurement was reported due to the extreme difficulty in growing a MgB_2 single crystal. The experiments of hydrostatic pressure effect on T_c do not particularly support this theory, provided that no charge transfer between the Mg and B layers occurs. Alternatively, the experimental results were analyzed[16,18,21,22] by using the McMillan formula[23] derived from Eliashberg theory,[24] supporting electron-phonon mediated superconductivity. Interestingly, Loa and Syassen[21] analyzed the pressure effect on T_c from the McMillan formula on the basis of their calculated elastic and electronic structure data. Assuming that the electron-ion matrix element I is pressure independent, they

found that the pressure effect on T_c is in good agreement with experimental data by using a lattice Grüneisen parameter $\gamma_G=1$. These assumptions, however, deserve some refinements. Recent band-structure calculations suggested that MgB_2 is a traditional sp metal superconductor.[25–27] The pressure dependence of I has long been an interesting issue in the research of pressure effects in simple sp metals.[28–32] Ziman's calculation of the electron-phonon interaction led to $\langle I^2\rangle \propto N(E_F)^{-2}$, at least in the limit of long wavelengths.[33] This then indicated that the consideration of the pressure dependence of I would be important for better understanding the superconducting properties of MgB_2 under pressure. On the other hand, it was found[18] that the choice of the lattice Grüneisen parameter γ_G is crucially important in explaining both the magnitude and sign of the pressure derivative of T_c when using the McMillan formula. The value of $\gamma_G=1$ in the calculation of Loa and Syassen is obviously lower than those reported recently.[34,35] The pressure dependence of the effective electron-electron Coulomb repulsion μ^* appearing in the McMillan formula was usually neglected in previous studies due to the assumption of the small change of μ^* compared with that of the electron-phonon coupling parameter λ (Ref. 36). However, the magnitude of μ^* is also of interest in connection with the possibility that superconductivity may be destroyed by pressure.[36,37] It was argued that the pressure dependence of μ^* makes a significant contribution to the behavior of T_c under very high pressures, and must be handled carefully.[32,38,39]

In this paper we discuss the pressure dependences of some interested superconducting properties in MgB_2. The outline of this paper is as follows: In Sec. II we present a theoretical approach for pressure effects on the superconducting properties in the simple sp metal superconductors. Section III contains the theoretical results obtained and a comparison with experiments for MgB_2. We draw conclusions in Sec. IV.

II. THEORETICAL FORMULATION

For our purposes, the relation between T_c and microscopic parameters is given adequately by the McMillan equation[23]

$$T_c=\frac{\Theta_D}{1.45}\exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right], \tag{1}$$

which relates T_c to the electron-phonon coupling parameter λ, the Coulomb repulsion strength μ^*, and a temperature Θ_D characteristic of the phonons.

Considering the variations of Θ_D, λ, and μ^* with pressure or volume, and introducing parameters $\varphi=\partial\ln\lambda/\partial\ln V$ and $\phi=\partial\ln\mu^*/\partial\ln V$, we can obtain the pressure coefficient of T_c,

$$\frac{d\ln T_c}{dP}=\frac{\gamma_G}{B_0}-\frac{1.04\lambda(1+0.38\mu^*)}{[\lambda-\mu^*(1+0.62\lambda)]^2}\frac{\varphi}{B_0}+\frac{1.04\mu^*(1+\lambda)(1+0.62\lambda)}{[\lambda-\mu^*(1+0.62\lambda)]^2}\frac{\phi}{B_0}, \tag{2}$$

where $B_0\equiv 1/\kappa_V=-\partial P/\partial\ln V$ is the bulk modulus, and Θ_D is assumed to be proportional to $\langle\omega^2\rangle^{1/2}$ and $\gamma_G=-\partial\ln\langle\omega^2\rangle^{1/2}/\partial\ln V$ being the effective Grüneisen parameter.

It is well known that the usual BCS result for the energy gap can be expressed by[40]

$$\Delta_0=2\Theta_D\exp\left[-\frac{1}{N(E_F)v}\right], \tag{3}$$

where $N(E_F)$ is the electronic density of states at the Fermi energy E_F and v is the pairing potential arising from the electron-phonon interaction. If we renormalize the Morel-Anderson result[41] by introducing the renormalization parameter $Z_n(0)\equiv 1+\lambda$ into their analysis, the effective interaction strength $N(E_F)v$ can be rewritten as[42]

$$N(E_F)v=\frac{\lambda-\mu^*}{1+\lambda}. \tag{4}$$

The logarithmic volume derivative of $N(E_F)v$ is then given by

$$\frac{d\ln N(E_F)v}{d\ln V}=\frac{\lambda(1+\mu^*)}{(\lambda-\mu^*)(1+\lambda)}\varphi-\frac{\mu^*}{\lambda-\mu^*}\phi. \tag{5}$$

Considering the experimental observations of the pressure dependence of the energy gap of the superconductor,[43] we differentiate Eq. (3) with respect to pressure

$$\frac{d\ln\Delta_0}{dP}=\frac{\gamma_G}{B_0}-\frac{1}{B_0}\left[\frac{\lambda(1+\mu^*)}{(\lambda-\mu^*)^2}\varphi-\frac{\mu^*(1+\lambda)}{(\lambda-\mu^*)^2}\phi\right]. \tag{6}$$

The BCS expression for the critical field H_c at absolute zero temperature is[40]

$$\frac{H_c(0)^2}{8\pi}=2N(E_F)\omega^2\exp\left[-\frac{2}{N(E_F)v}\right]. \tag{7}$$

Differentiating Eq. (7) with respect to pressure, one obtains an expression of the pressure coefficient of $H_c(0)$,

$$\frac{d\ln H_c(0)}{dP}=\frac{d\ln\Delta_0}{dP}-\frac{\gamma_N}{2B_0}+\frac{1}{2B_0}, \tag{8}$$

where $\gamma_N=\partial\ln N(E_F)/\partial\ln V$.

The expressions for γ_G, φ, and ϕ can be integrated to give

$$\Theta_D(V)=\Theta_D(0)[V/V_0]^{-\gamma_G}, \tag{9}$$

$$\lambda(V)=\lambda(0)[V/V_0]^{\varphi},$$

$$\mu^*(V)=\mu^*(0)[V/V_0]^{\phi}.$$

Here V and V_0 are the unit-cell volumes under the applied pressure and at ambient pressure, respectively. These two volumes can be related according to the first-order Murnaghan equation of state $V(P)=V(0)(1+B_0'P/B_0)^{-1/B_0'}$. Equation (9) is then rewritten as

$$\Theta_D(P)=\Theta_D(0)\left[1+\frac{B_0'P}{B_0}\right]^{\gamma_G/B_0'}, \tag{10}$$

$$\lambda(P)=\lambda(0)\left[1+\frac{B_0'P}{B_0}\right]^{-\varphi/B_0'},$$

$$\mu^*(P)=\mu^*(0)\left[1+\frac{B_0'P}{B_0}\right]^{-\phi/B_0'}.$$

From Eqs. (1) and (10) we arrive at the expression for the pressure dependence of T_c:

$$T_c(P)=T_c[\Theta_D(P),\lambda(P),\mu^*(P)]. \tag{11}$$

Knowing B_0, B_0', γ_G, γ_N, ϕ, and φ, one can evaluate the pressure effects on the superconducting properties, especially the behavior of T_c under pressure. B_0 and B_0' can be obtained from the compressibility data determined by neutron or synchrotron x-ray diffractions. A direct experimental determination of γ_G can be made by measuring electron tunneling[44–46] or inelastic neutron scattering[47] under high pressure. In general, for metals in which different techniques yield similar Grüneisen constants, a good approximation of γ_G is provided by the room-temperature value determined from the Grüneisen equation

$$\gamma_G=\frac{\alpha_V V_m}{\kappa_V C_p}, \tag{12}$$

where α_V is the volume coefficient of thermal expansion, V_m is the molar volume, and C_p is the molar heat capacity at constant pressure. The approximation for γ_G of Slater is derived from the pressure derivative of the bulk modulus[48]:

$$\gamma_G^S\equiv\frac{B_0'}{2}-\frac{1}{6}=-\frac{2}{3}-\frac{1}{2}\frac{V\partial^2P/\partial V^2}{\partial P/\partial V}. \tag{13}$$

The formula for μ^*, due to Morel and Anderson,[41] used here is

$$\mu^*=\frac{\mu}{1+\mu\ln(E_F/\omega_{ph})}, \tag{14}$$

with $\mu=0.5\ln[(1+a^2)/a^2]$ and $a^2=\pi e^2N(E_F)/k_F^2$, from which we evaluate the volume dependence of μ^* as

$$\phi=\mu^*\left[\frac{2}{3}-\gamma_G-\frac{1-e^{-2\mu}}{2\mu^2}\left(\gamma_N+\frac{2}{3}\right)\right]. \tag{15}$$

Here the variation of k_F with volume has been calculated from the fundamental definition $k_F=(3\pi^2Z/V)^{1/3}$, with Z the valency. Unfortunately, to the best of our knowledge γ_N has never been measured directly for any superconductor; in the case of a free-electron gas it would have a value of 2/3. Using the expression given by Migdal[49] for the electronic specific-heat coefficient γ, for the electronic Grüneisen parameter one obtains

$$\gamma_e=\frac{\partial\ln\gamma}{\partial\ln V}=\gamma_N+\frac{\lambda}{1+\lambda}\varphi. \tag{16}$$

The electronic Grüneisen parameter γ_e is usually deduced from measurements through the simple relation[50]

$$\gamma_e=\frac{\alpha_e V_m}{\kappa_V C_e}. \tag{17}$$

Here α_e is the contribution to the expansion coefficient from the electrons at lower temperatures, and C_e is the electronic heat capacity. A theoretical estimate of γ_e can also be given from the measurement of the volume dependence of the orbital susceptibility[51] or from band-structure considerations.[52]

The electron-phonon coupling parameter λ can be expressed as

$$\lambda=\frac{N(E_F)\langle I^2\rangle}{M\langle\omega^2\rangle}\equiv\frac{\eta}{M\langle\omega^2\rangle}, \tag{18}$$

where $\langle I^2\rangle$ is the mean-square electron-ion matrix element, and M is the ionic mass. The McMillan-Hopfield parameter η [or $N(E_F)\langle I^2\rangle$] has been regarded as a local ''chemical'' property of an atom in a crystal. Allen and Dynes[53] pointed out that η is the most significant single parameter in understanding the origin of the high T_c of conventional superconductors. For strong-coupling systems, the variation in η is more important than the variation of $\langle\omega^2\rangle$ in causing T_c to change. Softening $\langle\omega^2\rangle$ often does enhance T_c, but a very high T_c should be caused more by a large η than by a small $\langle\omega^2\rangle$.

The logarithmic volume derivative of λ, and φ is then obtained

$$\varphi=\frac{\partial\ln\eta}{\partial\ln V}+2\gamma_G\equiv S+2\gamma_G. \tag{19}$$

In order to understand how the electronic contribution $\eta=N(E_F)\langle I^2\rangle$ varies with volume, we use the Gaspari-Gyoriffy theory[54] for η, i.e.,

$$\eta=\frac{k_F^2}{\pi^2N(E_F)}\sum_l\frac{2(l+1)\sin^2(\delta_{l+1}-\delta_l)N_lN_{l+1}}{N_l^1N_{l+1}^1}, \tag{20}$$

where N_l is the lth angular momentum component of the density of states, N_l^1 is the lth component of the single scatterer density of states evaluated at E_F, and δ_l the phase shift.

For simple metals, the scatterers are assumed to be weak. We can take $N_l=N_l^1$, and approximate $\sin^2(\delta_{l+1}-\delta_l)$ by $(\delta_{l+1}-\delta_l)^2$. Equation (20) is rewritten as

$$\eta=\frac{k_F^2}{\pi^2N(E_F)}\sum_l 2(l+1)(\delta_{l+1}-\delta_l)^2. \tag{21}$$

This expression is identical to the pseudopotential formula of McMillan.[23,55] Assuming that the phase shift δ_l does not vary very much under pressure for simple sp superconductors, we then obtain

$$S = -\gamma_N - \frac{2}{3}. \tag{22}$$

The form in Eq. (22) is the same as that of Baryakhtar and Makarov,[56] who used the constant of the electron-phonon interaction of Fröhlich and Mitra.[57] The expression is an improvement over the expressions of $S=0$ and $-4/3$ obtained by Olsen *et al.*[58] and Seiden,[36] respectively. It is interesting to notice that substitution of $\gamma_N=2/3$ into Eq. (22) yields $S=-4/3$. Equation (22) reduces to the expression of Seiden,[36] who modified McMillan's expression for λ somewhat by considering the effects of a real lattice spectrum as opposed to the jellium model. Since the electronic Grüneisen parameter γ_e usually varies among different metals even in the simple non-transition elements,[7,50,52] we believe that Eq. (22) should provide a more reasonable value of S compared with Seiden's formula.

III. RESULTS AND DISCUSSION

Using the experimental value of $T_c=39.25$ K (Refs. 18 and 19), and the theoretical estimates of $\lambda=0.87$ and $\mu^*=0.10$ (Ref. 27), we obtained $\Theta_D=860$ K from Eq. (1) for MgB_2. We believe that all these parameters, which will enter our calculations, are reliable. For example, the inelastic neutron-scattering measurements[9] provide an estimate of $\lambda \sim 0.9$, which is close to that we used. The calculated value of $\Theta_D=860$ K is in the range from 746 to 1050 K determined from the specific-heat measurements.[12–14]

We took the structural parameters $B_0=147.2$ GPa and $B_0'=4$ from the measurements under the pure hydrostatic pressures up to 0.62 GPa (Ref. 59), and under high pressures up to 15 GPa (Refs. 22 and 35), respectively. To our knowledge no inelastic neutron-scattering or tunneling data exist for MgB_2 under hydrostatic pressure. We have to use Eq. (12) or (13) for estimating the lattice Grüneisen parameter γ_G. The measurements of heat capacity[60] give a C_p of 47.80 J/(K mol) at $T=298.16$ K. $V_m=1.75\times10^{-5}$ m^3/mol, $\kappa_V=6.79\times10^{-12}$ Pa^{-1}, and $\alpha_V=2.22\times10^{-5}$ K^{-1} can be drawn from the neutron-diffraction data.[59] We therefore obtained $\gamma_G=1.2$ by using Eq. (12). Based on the first-order Murnaghan equation for $V(P)$ and the Slater expression of Eq. (13), we obtained a somewhat larger value of γ_G of 1.83 compared to that from Eq. (12). For most simple metals, there is not much difference between the room-temperature lattice Grüneisen parameter given through Eq. (12) and the Slater relation.[36,61] It was found that the Slater expression can usually yield reasonable values of γ_G for most metals.[62] The only uncertainty entering Eq. (12) in our calculation comes from the indirect measurements of the linear coefficients of thermal expansion.[59] Roundy *et al.*[34] reported a value of $\gamma_G \approx 2.3$ from *ab initio* calculations, which is close to our calculated γ_G^S according to Eq. (13). Meanwhile, Goncharov *et al.*[35] determined a large E_{2g} mode Grüneisen parameter of 2.9 ± 0.3 from the measurements of Raman spectra under pressure. This value is obviously larger than those derived from Eqs. (12) and (13).

In the calculations of electronic density of states, Loa and Syassan[21] found that $N(E_F)$ decreases with pressure at a rate of $d\ln N(E_F)/dP=-3.1\times10^{-3}$ GPa^{-1}. Combining this calculated value and experimental value of B_0, we obtained $\gamma_N=0.46$. The volume dependence of μ^* is then derived from Eq. (15), once having the values of γ_G and μ. For simple sp metals, a^2 has a typical value of 0.4 (Ref. 41), which yields $\mu=0.63$. The volume dependence of λ, φ, is therefore determined from Eqs. (19) and (22). Using $\gamma_N=0.46$, we have $S=-1.13$ for MgB_2, which is smaller in magnitude than $-4/3$ in Seiden's formula for simple metals.[36] For the transition metals, Hopfield[63] commented that S is a relatively constant quantity with a value of about -3.5. The values of $S=-3.5$–-3.1, obtained by inverting the measured dT_c/dP for $YNi_{2-x}M_xB_2C$ (M=Co and Cu) (Ref. 64), are comparable to that of the transition metals, but are larger in magnitude compared to that of MgB_2.

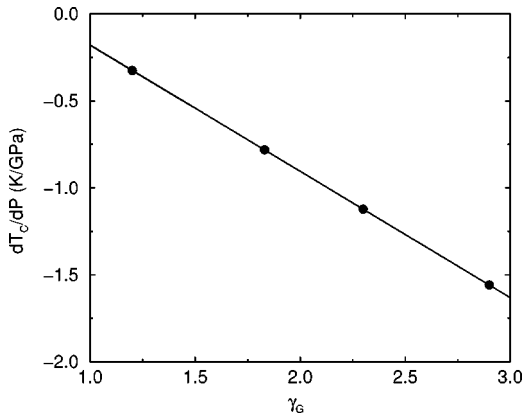

FIG. 1. Pressure derivative of T_c as a function of the lattice Grüneisen parameter γ_G in MgB_2. The circles show the calculation from the four different values of $\gamma_G=1.2$, 1.83, 2.3, and 2.9.

With the parameters determined above, we have calculated the pressure derivatives of T_c for MgB_2 by using Eq. (2). In Fig. 1 we plotted dT_c/dP as a function of γ_G in the interested range. It is interesting to note that γ_G plays a predominant role for the pressure effect of T_c. For the four different γ_G's considered here dT_c/dP are negative. The values obtained from $\gamma_G=1.83$ and 2.3 are -0.78 and -1.12 K/GPa, respectively. These are close to the hydrostatic pressure value of -1.1 K/GPa (Refs. 18 and 19). Thus the hydrostatic pressure results can be reproduced in terms of our present model by using the values of γ_G obtained from either the Slater relation or *ab initio* calculation. It is difficult to obtain the measured results by using $\gamma_G=1$, as suggested by Loa and Syassen.[21] We noted that a value for γ_G of 2.27 is necessary so as to account for the pressure effect on T_c for MgB_2. As emphasized above, all quantities entering Eq. (12) are experimental values, and only α_V was taken from indirect measurements. Thus it is highly expected to operate the thermal expansion measurement to yield a direct α_V. The present results indicate that the range from $\gamma_G=1.83$ to 2.3 should cover the reasonable choices for the lattice Grüneisen parameters.

To verify these results, and also to study the behavior of T_c as a function of pressure, we have performed explicit

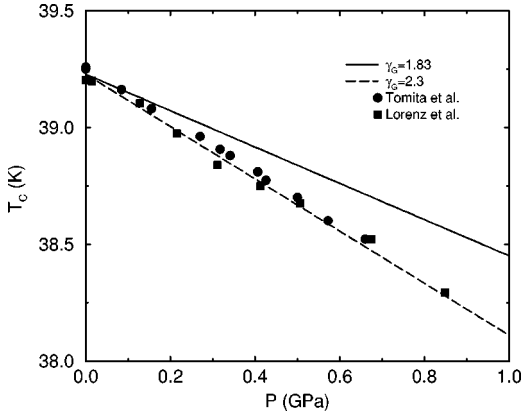

FIG. 2. Variation of T_c with pressure in the region of 0 to 1.0 GPa of MgB_2 for $\gamma_G=1.83$ and 2.3, respectively. The circles and squares represent the hydrostatic pressure experimental data taken from the works of Tomita *et al.* (Ref. 18) and Lorenz *et al.* (Ref. 19), respectively.

calculation based on Eq. (11). The theoretical results in the pressure range from 0 to 1.0 GPa, are shown in Fig. 2. The experimental data points of Tomita *et al.*[18] and Lorenz *et al.*[19] measured under hydrostatic pressure conditions are also plotted for comparison. It is clearly seen that our calculations agree well with the experiments.

In Fig. 3 we presented the calculated results as well as the experimental data points of Monteverde *et al.*[15] and Deemyad *et al.*[65] measured in the relatively high-pressure region. Here we assume that phase transitions of all kinds do not occur under pressure range that we consider. We note that the experimental data points of Deemyad *et al.*[65] are well situated in our theoretical curve calculated by using $\gamma_G=2.3$. Interestingly, the agreement between our theoretical curve calculated by using $\gamma_G=1.83$ and the experimental data points of Monteverde *et al.*[15] is seen to be reasonable, although there are some scatters among different samples and the reason is not clear. Furthermore, although the pressure

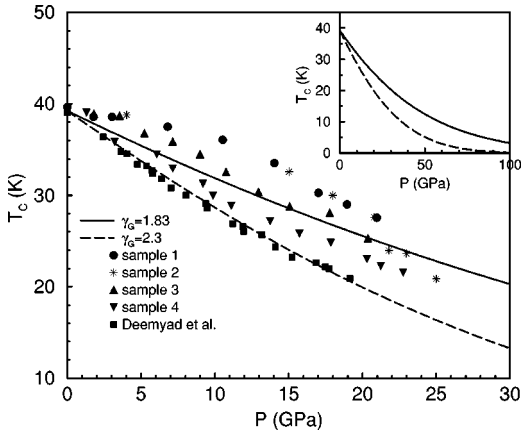

FIG. 3. Pressure dependence of the transition temperature in MgB_2 up to 30 GPa. Experimental data are from the works of Monteverde *et al.* (Ref. 15) for samples 1–4 and Deemyad *et al.* (Ref. 65). The inset is a calculation of T_c under pressure up to 100 GPa.

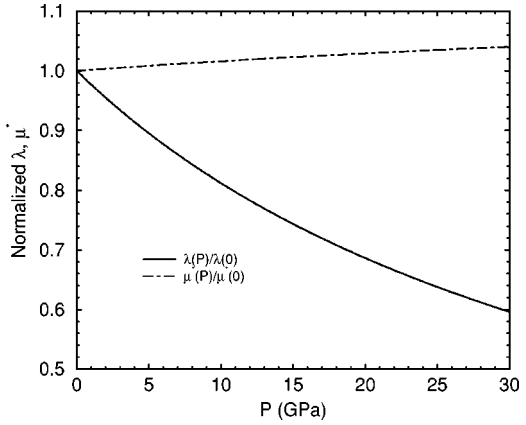

FIG. 4. Pressure dependence of normalized Coulomb (μ^*) and electron-phonon coupling (λ) coupling strengths in MgB_2 calculated by using $\gamma_G=2.3$.

measurements are limited to the region below 25 GPa, it is seen from the inset of Fig. 3 that Eq. (11) continues to describe the pressure dependence of T_c as high as 100 GPa. Even at this point, the superconductivity is not destroyed by pressure in newly discovered superconductor MgB_2. There was a discrepancy on whether pressure can destroy superconductivity.[36,37,66,67] However, our results support the conclusion of Olsen and collaborators[37,66] that the possibility of destruction of superconductivity by the application of sufficiently high pressure most likely does not exist. It follows from the comparison of Figs. 2 and 3 that the pressure effect on T_c indeed provides a support to the electron-phonon mediated superconductivity in MgB_2.

In Fig. 4 we present the normalized λ and μ^* as functions of pressure up to 30 GPa, calculated from Eq. (10) by using $\gamma_G=2.3$. The Coulomb pseudopotential μ^* increases slightly with pressure. Whereas λ changes significantly with pressure. The contribution from $\mu^*(\mathrm{P})$ to the variation of T_c with pressure is much less important than that of $\lambda(P)$. Thus in the range from 0 to 30 GPa the pressure effect of T_c for MgB_2 is dominated by the competition of λ and Θ_D (or $\langle\omega^2\rangle^{1/2}$).

Table I contains the calculated values of pressure dependences of superconducting parameters for MgB_2 from Eqs. (5), (6), (8), and (16) by using $\gamma_G=1.83$ and 2.3, respectively. The reliable values of γ_e is readily determined using Eqs. (16), (19), and (22). We obtained $\gamma_e=1.64$ and 2.07 for MgB_2, which are close to $\gamma_e=1.7$ for Pb and for Sn, $\gamma_e=2.0$ for Al (Ref. 67). The negative sign for $d\ln H_c(0)/dP$ predicted for MgB_2 is in agreement with the measurements

TABLE I. Pressure dependences of superconducting state parameters in MgB_2. The units of $d\ln X/dP$ [$X=T_c$, Δ_0, are $H_c(0)$] are in 10^{-2} GPa^{-1}.

γ_G	γ_e	$\frac{d\ln N(E_F)v}{d\ln V}$	$\frac{d\ln T_c}{dP}$	$\frac{d\ln\Delta_0}{dP}$	$\frac{d\ln H_c(0)}{dP}$
1.83	1.64	1.71	−1.99	−1.58	−1.39
2.3	2.07	2.34	−2.86	−2.30	−2.11

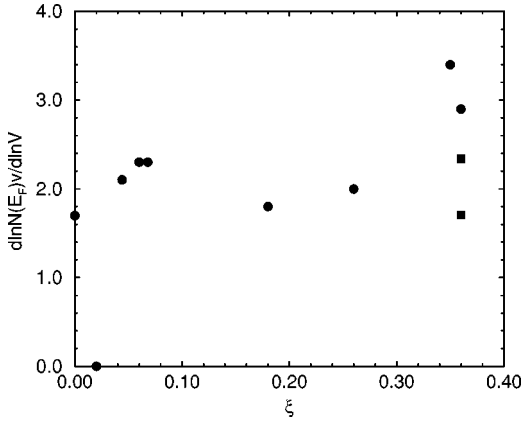

FIG. 5. Relation between the logarithmic volume derivative of $N(E_F)v$ and the deviation ξ from the full isotope effect exponent $\alpha=0.5(1-\xi)$ in nine simple sp metal superconductors and MgB_2. The two squares are the values for MgB_2.

for all simple element superconductors with the exception of thallium.[68] For simple sp metal superconductors, Rohrer[69] demonstrated that $d\ln N(E_F)v/d\ln V$ must have approximately a value of 2.0. However, it was realized[68] that transition metals fail to show such a simple behavior. Our estimated $d\ln N(E_F)v/d\ln V=1.71$ and 2.34 for MgB_2 are comparable to those obtained for simple sp metal superconductors.[68,69] Early measurements for most simple metals[29,43,46] showed that there is difference between the quantities in $d\ln\Delta_0/dP$ and $d\ln T_c/dP$. This can be understood with the aid of the results by Geĭlikman and Kresin,[70] that is, $2\Delta_0/k_BT_c=3.52[1+5.3(T_c/\omega_{ph})^2\ln\omega_{ph}/T_c]$. The calculated data of MgB_2 listed in Table I make it possible to support this theory. Since the phonon spectrum shifts under pressure, it follows that for all superconductors with $2\Delta_0/k_BT_c>3.52$ a change of $2\Delta_0/k_BT_c$ under pressure can be expected. It is interesting from the viewpoint of experiment to investigate the tunneling characteristics of MgB_2 under hydrostatic pressure.

Figure 5 is a plot of $d\ln N(E_F)v/d\ln V$ versus the deviation ξ from the full isotope effect for nine simple sp metal superconductors as well as MgB_2. The experimental values of $d\ln N(E_F)v/d\ln V$ for simple metals are chosen from the work of Olsen, Andres, and Geballe.[58] The experimental results for isotope effect exponent α and its deviation ξ are taken from the works in Refs. 7 and 71–75. There are no experimental data available for Al and In now, we took the calculated results from Leavens and Carbotte.[42] We summarize these results for simple sp metals in Table II. Olsen *et al.*[4] suggested that $d\ln N(E_F)v/d\ln V$ is related to the isotope effect exponent α in metal superconductors. As seen from Fig. 5, the relation between $d\ln N(E_F)v/d\ln V$ and ξ is not very clear when more data included. An isotope effect $\alpha=0.32(1)$ (Ref. 6) in MgB_2 is consistent with what appears to be a systematic variation of α across nontransition elements. It is well known that deviations of the isotope effect exponent from 1/2 are a measure of the relative strengths of the Coulomb and phonon-mediated electron-electron interactions. It is indicated, from the compared values of ξ for MgB_2 (Ref. 6) with Zn (Ref. 73), Cd (Ref. 7), and Al (Ref. 42), that MgB_2 should be a medium coupling superconductor.

TABLE II. Experimental values of $d\ln N(E_F)v/d\ln V$, the isotope effect exponent α, and its derivative $\xi=1-2\alpha$ in nine simple sp metal superconductors.

Element	Z	$\frac{d\ln N(E_F)v}{d\ln V}$	α	ξ
Zn	2	2.0	0.37	0.26
Cd	2	2.9	0.32	0.36
Hg(α)	2	1.7	0.50	0
Al	3	3.4	0.325	0.35
Ga	3	1.8	0.41	0.18
In	3	2.3	0.466	0.068
Tl	3	0	0.49	0.02
Sn	4	2.3	0.47	0.06
Pb	4	2.1	0.478	0.044

IV. SUMMARY AND CONCLUSIONS

The major conclusions given by present investigation can be summarized as follows.

(i) A simple expression was derived for the pressure dependences of superconducting properties in a simple sp superconductor on the basis of McMillan equation. The logarithmic volume derivatives of λ, μ^*, and Θ_D can be self-consistently determined from experiments and theories. We gave an expression for φ from the theory of Gaspari and Gyorffy.[54] The theory of Morel and Anderson[41] was used to obtain ϕ, which makes it possible to investigate the pressure dependence of μ^*. Neglecting the pressure dependence of μ^*, the present theoretical model can be reduced to the two popular models of Seiden[36] and Baryakhtar and Makarov[56] when taking $\gamma_N=2/3$ and neglecting the direct electron-electron interaction, respectively. Furthermore, we obtained an explicit expression for the change of T_c as a function of pressure with the help of Murnaghan equation. The present model enables us to study the pressure behaviors of some interested superconducting parameters such as the zero-temperature energy gap Δ_0, the critical field at absolute zero temperature $H_c(0)$, the effective interaction strength $N(E_F)v$, and the electronic specific-heat coefficient γ.

(ii) We investigated the pressure effects on superconducting properties in the newly discovered superconductor MgB_2 using our simple approach. It was found that the hydrostatic pressure derivative of T_c can be reproduced by using the values of γ_G obtained from either the Slater relation or *ab initio* calculation. The calculated $d\ln N(E_F)v/d\ln V\approx 2.0$ in MgB_2 is close to those obtained in simple sp superconductors. The quantitative agreement for the variation of T_c with pressure in the low-pressure region as well as high-pressure region is very good when comparing our theoretical results with experimental data measured by three groups. The predicted values of $d\ln H_c(0)/dP$, $d\ln\Delta_0/dP$, and γ_e are also comparable to those in simple sp metal superconductors. All these characteristic pressure behaviors allow us to conclude

that MgB_2 should be a simple electron-phonon-mediated sp superconductor, and the mechanism in simple sp metal superconductors is also responsible for the superconductivity in MgB_2.

Note added. Recently, the authors have learned that the superconductivity is not destroyed up to 44 GPa where T_c is still as high as 12 K.[76] The intrinsic $dT_c/dP \approx -1.1$ K/GPa under hydrostatic pressure conditions was recently reported by other three groups.[76–78] We have also learned a possible explanation given by Tissen *et al.*[79] for the large $-dT_c/dP$ observed in the low-$T_c = 37.4 \pm 0.1$ samples.

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[1] J. Nagamatsu, N. Nakagawa, T. Muranaka, Y. Zenitanl, and J. Akimitsu, Nature (London) **410**, 63 (2001).
[2] C.B. Eom, M.K. Lee, J.H. Choi, L.J. Belenky, X. Song, L.D. Cooley, M.T. Naus, S. Patnaik, J. Jiang, M. Rikel, A. Polyanskii, A. Gurevich, X.Y. Cai, S.D. Bu, S.E. Babcock, E.E. Hellstrom, D.C. Larbalestier, N. Rogado, K.A. Regan, M.A. Hayward, T. He, J.S. Slusky, K. Inumaru, M.K. Haas, and R.J. Cava, Nature (London) **411**, 558 (2001).
[3] S. Jin, H. Mavoori, C. Bower, and R.B. van Dover, Nature (London) **411**, 563 (2001).
[4] J.L. Olsen, E. Bucher, M. Levy, J. Muller, E. Corenzwit, and T. Geballe, Rev. Mod. Phys. **36**, 168 (1964).
[5] S.L. Bud'ko, G. Lapertot, C. Petrovic, C.E. Cunningham, N. Anderson, and P.C. Canfield, Phys. Rev. Lett. **86**, 1877 (2001).
[6] D.G. Hinks, H. Claus, and J.D. Jorgensen, Nature (London) **411**, 457 (2001).
[7] C. Palmy, Phys. Lett. A **29**, 373 (1969).
[8] T.J. Sato, K. Shibata, and Y. Takano, cond-mat/0102468 (unpublished).
[9] R. Osborn, E.A. Goremychkin, A.I. Kolesnikov, and D.G. Hinks, Phys. Rev. Lett. **87**, 017005 (2001).
[10] G. Karapetrov, M. Iavarone, W.K. Kwok, G.W. Crabtree, and D.G. Hinks, Phys. Rev. Lett. **86**, 4374 (2001).
[11] H. Kotegawa, K. Ishida, Y. Kitaoka, T. Muranaka, and J. Akimitsu, Phys. Rev. Lett. **87**, 0127001 (2001).
[12] R.K. Kremer, B.J. Gibson, and K. Ahn, cond-mat/0102432 (unpublished).
[13] Ch. Wälti, E. Felder, C. Degen, G. Wigger, R. Monnier, B. Delley, and H.R. Ott, Phys. Rev. B **64**, 172515 (2001).
[14] F. Bouquet, R.A. Fisher, N.E. Phillips, D.G. Hinks, and J.D. Jorgensen, Phys. Rev. Lett. **87**, 047001 (2001).
[15] M. Monteverde, M. Núñez-Regueiro, N. Rogado, K.A. Regan, M.A. Hayward, T. He, S.M. Loureiro, and R.J. Cava, Science **292**, 75 (2001).
[16] B. Lorenz, R.L. Meng, and C.W. Chu, Phys. Rev. B **64**, 012507 (2001).
[17] E. Saito, T. Taknenobu, T. Ito, Y. Iwasa, K. Prassides, and T. Arima, J. Phys.: Condens. Matter **13**, L267 (2001).
[18] T. Tomita, J.J. Hamlin, J.S. Schilling, D.G. Hinks, and J.D. Jorgensen, Phys. Rev. B **64**, 092505 (2001).
[19] B. Lorenz, R.L. Meng, and C.W. Chu, cond-mat/0104303 (unpublished).
[20] J.E. Hirsch, Phys. Lett. A **282**, 392 (2001).
[21] I. Loa and K. Syassen, Solid State Commun. **118**, 279 (2001).
[22] T. Vogt, G. Schneider, J.A. Hriljac, G. Yang, and J.S. Abell, Phys. Rev. B **63**, 220505 (2001).
[23] W.L. McMillan, Phys. Rev. **167**, 331 (1968).
[24] G.M. Eliashberg, Zh. Éksp. Teor. Fiz. **38**, 966 (1960) [Sov. Phys. JETP **11**, 696 (1960)].
[25] J. Kortus, I.I. Mazin, K.D. Belashchenko, V.P. Antropov, and L.L. Boyer, Phys. Rev. Lett. **86**, 4656 (2001).
[26] J.M. An and W.E. Pickett, Phys. Rev. Lett. **86**, 4366 (2001).
[27] Y. Kong, O.V. Dolgov, O. Jepsen, and O.K. Andersen, Phys. Rev. B **64**, 020501 (2001).
[28] R. Hodd, Phys. Rev. **180**, 530 (1969).
[29] P.N. Trofimenkoff and J.P. Carbotte, Phys. Rev. B **1**, 1136 (1970).
[30] M.A. Coulthard, J. Phys. F: Met. Phys. **1**, 195 (1971).
[31] H.R. Ott and R.S. Sorbello, J. Low Temp. Phys. **14**, 73 (1974).
[32] M.M. Dacorogna, M.L. Cohen, and P.K. Lam, Phys. Rev. B **34**, 4865 (1986).
[33] J. M. Ziman, *Electrons and Phonons* (Clarendon Press, Oxford, 1960).
[34] D. Roundy, H. J. Choi, H. Sun, S. G. Louie, and M. L. Cohen (unpublished).
[35] A.F. Goncharov, V.V. Struzhkin, E. Gregoryanz, J. Hu, R.J. Hemley, H.-K. Mao, G. Lapertot, S.L. Bun'ko, and P.C. Canfield, Phys. Rev. B **64**, 100509 (2001).
[36] P.E. Seiden, Phys. Rev. **179**, 458 (1969).
[37] R.I. Boughton, G. Brändli, J.L. Olsen, and C. Palmy, Helv. Phys. Acta **42**, 587 (1969).
[38] D.U. Gubser and A.W. Webb, Phys. Rev. Lett. **35**, 104 (1975).
[39] D.A. Papaconstantopoulos and B.M. Klein, Physica B **107**, 725 (1981).
[40] J. Bardeen, L.N. Cooper, and J.R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
[41] P. Morel and P.W. Anderson, Phys. Rev. **125**, 1263 (1962).
[42] C.R. Leavens and J.P. Carbotte, Can. J. Phys. **49**, 724 (1971).
[43] J.P. Franck and W.J. Keeler, Phys. Rev. Lett. **20**, 379 (1968).
[44] J.P. Franck and W.J. Keeler, Phys. Lett. A **25**, 624 (1967).
[45] J. Yamashita and S. Asano, J. Phys. Soc. Jpn. **29**, 264 (1970).
[46] N.V. Zavaritskiĭ, E.S. Itskevich, and A.N. Voronovskiĭ, Zh. Éksp. Teor. Fiz. **60**, 1408 (1971) [Sov. Phys. JETP **33**, 762 (1971)].
[47] R. Lechner and G. Quittner, Phys. Rev. Lett. **17**, 1259 (1966).
[48] J. C. Slater, *Introduction to Chemical Physics* (McGraw-Hill, New York, 1939).
[49] A.B. Migdal, Zh. Éksp. Teor. Fiz. **34**, 1438 (1958) [Sov. Phys. JETP **7**, 996 (1958)].
[50] T.H.K. Barron, J.G. Collins, and G.K. White, Adv. Phys. **29**, 609 (1980).
[51] E. Fawcett and G.K. White, J. Appl. Phys. **39**, 576 (1968).

[52] G.C. Fletcher and M. Yahaya, J. Phys. F: Met. Phys. **9**, 1529 (1979).
[53] P.B. Allen and R.C. Dynes, Phys. Rev. B **12**, 905 (1975).
[54] G.D. Gaspari and B.L. Gyorffy, Phys. Rev. Lett. **28**, 801 (1972).
[55] R. Evans, G.O. Gaspari, and B.L. Gyorffy, J. Phys. F: Met. Phys. **3**, 39 (1973).
[56] V.G. Baryakhtar and V.I. Makarov, Zh. Éksp. Teor. Fiz. **49**, 1934 (1965) [Sov. Phys. JETP **22**, 1320 (1966)].
[57] H. Fröhlich and T.K. Mitra, Proc. Phys. Soc. Jpn. **1**, 544 (1968).
[58] J.L. Olsen, K. Andres, and T.H. Gebelle, Phys. Lett. A **26**, 239 (1968).
[59] J.D. Jorgensen, D.G. Hinks, and S. Short, Phys. Rev. B **63**, 224522 (2001).
[60] R.M. Swift and D. White, J. Am. Chem. Soc. **79**, 3641 (1957).
[61] K. A. Gschneidner, Jr., in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, New York, 1964), Vol. 16.
[62] V.L. Moruzzi, J.F. Janak, and K. Schwarz, Phys. Rev. B **37**, 790 (1988).
[63] J.J. Hopfield, Physica (Amsterdam) **55**, 41 (1971).
[64] C. Looney, A.K. Gangopadhyay, A.-K. Klehe, and J.S. Schilling, Physica C **252**, 199 (1995).
[65] S. Deemyad, J.S. Schilling, J.D. Jorgensen, and D.G. Hinks, Physica C **361**, 227 (2001).
[66] J.L. Olsen and H. Rohrer, Helv. Phys. Acta **33**, 872 (1960); M. Levy and J.L. Olsen, Solid State Commun. **2**, 137 (1964).
[67] T.F. Smith and C.W. Chu, Phys. Rev. **159**, 353 (1967).
[68] M. Levy and J. S. Olsen, in *Physics of High Pressures and the Condensed Phase*, edited by A. Van Itterbeek (North-Holland, Amsterdam, 1965).
[69] H. Rohrer, Helv. Phys. Acta **33**, 675 (1960).
[70] B.T. Geĭlikman and V.Z. Kresin, Fiz. Tverd. Tela (Leningrad) **7**, 3294 (1965) [Sov. Phys. Solid State **7**, 2659 (1966)].
[71] E. Maxwell, Phys. Today **12**, 14 (1952).
[72] R.R. Hake, D.E. Mapother, and D.L. Decker, Phys. Rev. **112**, 1522 (1958).
[73] R.E. Fassnacht and J.R. Dillinger, Phys. Rev. **164**, 565 (1967).
[74] R. E. Fassnacht and J.R. Dillinger, Phys. Lett. A **28**, 741 (1969).
[75] R. Meservey and B. B. Schwartz, in *Superconductivity*, edited by R. D. Parks (Dekker, New York, 1969).
[76] V.V. Struzhkin, A.F. Goncharov, R.J. Hemley, H.-K. Mao, G. Lapertot, S.L. Bud'ko, and P.C. Canfield, cond-mat/0106576 (unpublished).
[77] S.I. Schlachter, W.H. Fietz, K. Grube, and W. Goldacker, cond-mat/0107205 (unpublished).
[78] J. Tang, L.C. Qin, A. Matsushita, Y. Takano, K. Togano, H. Kito, and H. Ihara, Phys. Rev. B **64**, 132509 (2001).
[79] V.G. Tissen, M.V. Nefedova, M.N. Kolesnikov, and M.P. Kulakov, Physica C **363**, 194 (2001).