

THE PENETRATION DEPTH OF H₃S SUPERCONDUCTOR BY SEMICLASSICAL APPROACH

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Abstract

The penetration depth is a magnetic field mechanism by which an external magnetic field penetrates into superconductors' surfaces and is related to the Meissner effect. The penetration depth property was studied by the semiclassical approach to identify other properties of superconductors. In this study, we investigated the penetration depth of the H₃S superconductor under external pressure. The H₃S superconductor is high T_c , s-wave isotropic, and high pressure prepared superconductors. We derive an analytical equation for the near-zero temperature penetration depth with pressure effect parameters. The derived equations were then numerically calculated and predicted the experimental data on H₃S superconductor penetration depth. We discovered that the temperature dependent penetration depth under pressure of H₃S superconductor is reasonable at $T_c(\chi = 473, \varepsilon_0 = 91, Qp = 0.1) = 200.832$ K, as well as is the influence of the directly χ parameter on $T_c(\chi, \varepsilon_0, Qp)$, $\Delta(0, \chi, \varepsilon_0, Qp)$, and $\lambda(T, \chi, \varepsilon_0, Qp)/\lambda(0, \chi, \varepsilon_0, Qp)$, with $Qp > 0.1$ does not corresponding theory

Keywords: Penetration depth, Semiclassical approach, Meissner effect, BCS theory, H₃S superconductor

Introduction

The metallic hydrogen (MH) is phase of hydrogen when exposed to high pressure was predicted by Wigner and Huntington with a basic phase diagram of MH density and a transition pressure of roughly 25 GPa, after which it was proposed by Ashcroft as a high-temperature superconductor with critical temperatures (T_c) probably higher than room temperature around 50-235 K (Wigner and

Huntington, 1935; Ashcroft, 1968). Before the discovery of high T_c MH, Eremets *et al.* reported hydrogen-dominant materials' superconductivity on silane, T_c is 17 K at 96 and 120 GPa and becomes to metal phase at 50 GPa, after then Li *et al.* predicted H₂S structure at 10-200 GPa by computational method, with the transition temperature at 80 K at 160 GPa, (Eremets *et al.*,

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2008; Li *et al.*, 2014), until Drozdov *et al.* discovered H₃S superconductor, the materials of which transforms to a metal at 90 GPa on a diamond anvil cell (DAC) and reports a T_c at 203 K by magnetic susceptibility investigations (Drozdov *et al.*, 2015). In 2017, Dias and Silvera produced a MH experiment to confirm that hydrogen forms metallic at 495 GPa of pressure, with reflectance as high as 0.91 (Dias and Silvera, 2017). Theoretical physics involves calculating thermodynamic properties under pressure in order to explain and predict the discovery of an experiment. Krzysosiak *et al.* proposed the dispersion relation $\varepsilon_k(p)$, the all-carrier energy depend on external pressure (p) and density of state depend on the magnitude of the local fluctuation (χ) for T_c and thermodynamic properties under high pressure developed by BCS-theory such as the ratio of zero-temperature gap and critical temperature ($2\Delta(0, \chi, x_0, p) / T_c(\chi, x_0, p)$) and the ratio of the heat capacity jump between the superconducting state and the normal state ($\Delta C(T_c) / C_N(T_c)$). They reported that H₃S superconductor parameters are $T_c(1) > T_c(0)$, and $x_0 < 0$, $\chi > 0$, where $T_c(1)$ is the critical temperature under pressure, $T_c(0)$ is critical temperature normal condition, and x_0 is a distance from the Fermi level (Krzysosiak *et al.*, 2018) and was confirmed by Chanpoom *et al.* that the dispersion relation of the carriers is reasonable at $Qp \approx 0.1$ and calculated the isotope effect under pressure within the weak-coupling limit (Chanpoom *et al.*, 2022). In other theory, Kim applied the BCS-theory to Brinkman-Rice theory (BR) for explained superconductivity at room temperature by electron pairs; he then derived the $T_{c,BCS-BR}$ equation and effective mass, ($m^*/m = 1/(1 - (U/U_c)^2)$) of superconductors and reported that $\hbar\omega_D = 1560$ K, $\Delta_0 = 179.29$ K, $T_c = 200.8$ K, $T_{c, BRBCS} = 201.4$ K, $\lambda_{BCS} = 0.03$ and $\lambda^* = 0.461$ of H₃S superconductor (Kim, 2021).

The mechanism through which an external magnetic field penetrates the surfaces of superconductors is known as the penetration depth. It was proposed by London *et al.* (London *et al.*, 1935) and Chandrasekhar and Einzel developed as the semiclassical approach. The semiclassical approach explains the fermi surface and energy gap of superconductors (Chandrasekhar and Einzel, 1993). After that, Prozorov and Giannetta measured the penetration depth in unconventional superconductors. Examples are semiclassical approach to the penetration depth for an isotropic s-wave gap, a 2D cylindrical Fermi surface, an anisotropic gap and a 3D spherical Fermi surface (Prozorov and Giannetta, 2006) and the superconducting gap function (Gross *et al.*, 1968). Finally, Changjan *et al.* calculated the London penetration depth in single band anisotropic s-wave

superconductors' ab-components and c-component (Changjan *et al.*, 2021).

In this study, we estimate the temperature dependent penetration depth of H₃S superconductor using semiclassical approach. Under external pressure the weak-coupling limits BCS theory determined the critical temperature ($T_c(\chi, \varepsilon_0, Qp)$) and zero energy gap ($\Delta(0, \chi, \varepsilon_0, Qp)$) (Bardeen *et al.*, 1957). The density of states (DOS) χ and ε_0 parameters (Gonczarek and Mulak, 1999), and also the pressure system dispersion relation ($\varepsilon_k(p)$) are the external pressure conditions. Subsequently, all temperature dependent penetration depth calculations of H₃S superconductors were compared to BCS-theory.

Materials and Methods

Semiclassical approach

The penetration depth, λ in superconducting state with the symmetric tensor, R_{ii} as (Chandrasekhar and Einzel, 1993)

$$\lambda_{ii} = \left(\frac{c}{4\pi R_{ii}} \right)^{1/2}, i = x, y, z \quad (1)$$

Where $R_{ii} = R_{iiD} + R_{iiP}$, R_{iiD} is diamagnetic term, and R_{iiP} is paramagnetic term, then

$$R_{ii}(T) = \frac{e^2}{4\pi^3 \hbar c} \oint dS_F \frac{\vec{v}_F^i \vec{v}_F^i}{|\vec{v}_F|} \left(1 + 2 \int_{\Delta(k)}^{\infty} dE_k \left(\frac{\partial f(E_k)}{\partial E_k} \right) \frac{N(E_k)}{N(0)} \right) \quad (2)$$

where dS_F is the Fermi surface, $\vec{v}_F^i$ is the components of Fermi velocity, $E_k = \sqrt{\varepsilon_k^2 + \Delta^2(T, k)}$ is the energy of quasiparticles with ε_k is the Fermi energy and $\Delta(T, k)$ is the energy gap depend on k-space, $N(E_k)/N(0) = E_k / \sqrt{E_k^2 - \Delta^2(T, k)}$ is DOS at Fermi level, and $f(E_k) = 1 / e^{E_k/k_B T} + 1$ is the Fermi function. For the effective mass, m_{ii} as $m_{ii} \equiv \frac{ne^2}{cR_{ii}}$, where n is the density of conduction electrons and, then $\lambda_{ii} = (m_{ii} c^2 / 4\pi n e^2)^{1/2}$ like London equations.

The penetration depth, $\lambda_{ii}(0)/\lambda_{ii}(T)$, for an isotropic gap described as $\Delta(T, k) = \Delta(T)$, can be calculated using the relations of $R_{ii}(T)/R_{ii}(0)$ in Equation (2).

$$\left(\frac{\lambda_{ii}(0)}{\lambda_{ii}(T)} \right)^2 = \frac{R_{ii}(T)}{R_{ii}(0)} = 1 - \frac{1}{2k_B T} \int_0^{\infty} \text{sech}^2 \left(\frac{\sqrt{\varepsilon_k^2 + \Delta^2(T)}}{2k_B T} \right) d\varepsilon_k. \quad (3)$$

External pressure

A p parameter, which is imposed on the new superconducting state equilibrium, represents external pressure relative to atmospheric pressure. For new conditions, we use the energy allocated to each unit cell of the dispersion relation by Taylor's series expansion as (Krzysosiak *et al.*, 2018; Chanpom *et al.*, 2022; Ruangrungrrote *et al.*, 2023)

$$\varepsilon_k(p) = \varepsilon_k(0) + p \left(\frac{d\varepsilon_k(p)}{dp} \right)_{p=0} + \frac{p^2}{2} \left(\frac{d^2\varepsilon_k(p)}{dp^2} \right)_{p=0} \quad (4)$$

We simply consider 2 terms of Equation (4) as

$$\varepsilon_k(p) = \varepsilon_k(0) + Qp \quad (5)$$

Here $\varepsilon_k(0)$ is carrier energy at Fermi surface, $Q = (d\varepsilon_k(p)/dp)_{p=0}$, and Qp is assumed to be constant with unit of energy. The energy Qp is proportional to the product of the effective mass of carriers (m^*) and the volume per unit cell (VP), divided by the total mass of the unit cell (M). Therefore, for a pressure of $P \approx 10^9$ Pa, we can estimate Qp to be approximately 0.0086 meV.

Substituting Equation (5) into Equation (3), we get the near zero-temperature approximation of penetration depth under external pressure as (Burns, 1992)

$$\frac{\lambda_{ii}(T)}{\lambda_{ii}(0)} \approx 1 + \frac{\sqrt{\pi\Delta(0)}}{2k_B T} \left(1 - \frac{2}{\sqrt{\pi}} \tanh(Qp) \right) \cdot \exp\left(-\frac{\Delta(0)}{k_B T}\right) \quad (6)$$

After that, for new condition of BCS -like model, $\Delta(T)$ we consider self-consistent equation as (Bardeen *et al.*, 1957)

$$\Delta_k = -\frac{1}{2} \sum_{k'} \frac{V_{kk'}}{\sqrt{\varepsilon_k^2 + \Delta_k^2}} \tanh\left(\frac{\sqrt{\varepsilon_{k'}^2 + \Delta_{k'}^2}}{2T}\right) \quad (7)$$

where $V_{kk'} = -V_0 f(k)f(k')$ is coefficient of electron interaction.

For the isotropic s-wave, the gap equation is

$$\frac{1}{N_0 V} = \int_0^{\hbar\omega_D} \frac{N(\varepsilon)}{\sqrt{\varepsilon_k^2(p) + \Delta^2(T)}} \tanh\left(\frac{\sqrt{\varepsilon_k^2(p) + \Delta^2(T)}}{2k_B T}\right) d\varepsilon_k \quad (8)$$

where $N_0 V$ is coupling constant, ω_D is Debye cut off frequency.

Under external pressure, the DOS of these superconductors has been modified to occur at a narrow fluctuation below the Fermi level as (Gonzczarek and Mulak, 1999)

$$N(\varepsilon) = N_0(1 + \chi\delta(\varepsilon_k(0) - \varepsilon_0)) \quad (9)$$

where χ is the magnitude of the local fluctuation function and ε_0 is the position away the Fermi level.

Substituting equations (5) and (9) into equation (8), we get the BCS-gap equation under external pressure as

$$\frac{1}{N_0 V} = \int_0^{\hbar\omega_D} \frac{1 + \chi\delta(\varepsilon_k(0) - \varepsilon_0)}{\sqrt{(\varepsilon_k(0) + Qp)^2 + \Delta^2(T, \chi, \varepsilon_0, Qp)}} \tanh\left(\frac{\sqrt{(\varepsilon_k(0) + Qp)^2 + \Delta^2(T, \chi, \varepsilon_0, Qp)}}{2k_B T(\chi, \varepsilon_0, Qp)}\right) d\varepsilon_k(0). \quad (10)$$

This equation can be reduced to BCS gap equation for $\chi=0$, $\varepsilon_0=0$, and $Qp=0$.

For $T = 0$, $\Delta(T, \chi, \varepsilon_0, Qp) = \Delta(0, \chi, \varepsilon_0, Qp)$ and neglecting terms higher order term, equation (10) became

$$\frac{1}{N_0 V} = \int_0^{\hbar\omega_D} \frac{1 + \chi\delta(\varepsilon_k(0) - \varepsilon_0)}{\sqrt{(\varepsilon_k(0) + Qp)^2 + \Delta^2(0, \chi, \varepsilon_0, Qp)}} d\varepsilon_k(0). \quad (11)$$

$$\frac{1}{N_0 V} = \ln\left(2 \frac{\hbar\omega_D + Qp}{\Delta(0, \chi, \varepsilon_0, Qp)}\right) + \frac{\chi}{\sqrt{(\varepsilon_0 + Qp)^2 + \Delta^2(0, \chi, \varepsilon_0, Qp)}}. \quad (12)$$

We obtained the relation equation of $\Delta(0, \chi, \varepsilon_0, Qp)$ and $\Delta(0, 0, 0, 0)$ as

$$\frac{\Delta(0, \chi, \varepsilon_0, Qp)}{\Delta(0, 0, 0, 0)} = \left(\frac{\hbar\omega_D + Qp}{\hbar\omega_D} \right) \times \exp\left(\frac{\chi}{\sqrt{(\varepsilon_0 + Qp)^2 + \Delta^2(0, \chi, \varepsilon_0, Qp)}}\right). \quad (13)$$

For $T = T_c(\chi, \varepsilon_0, Qp)$, $\Delta(T, \chi, \varepsilon_0, Qp) = 0$ and neglecting terms higher order term, equation (10) became

$$\frac{1}{N_0 V} = \int_0^{\hbar\omega_D} \frac{\tanh\left(\frac{\varepsilon_k(0) + Qp}{2T_c(\chi, \varepsilon_0, Qp)}\right) d\varepsilon_k(p)}{\varepsilon_k(0) + Qp} + \chi \frac{\tanh((\varepsilon_0 + Qp)/2T_c(\chi, \varepsilon_0, Qp))}{\varepsilon_0 + Qp}. \quad (14)$$

$$\frac{1}{N_0 V} = \ln\left(\frac{\hbar\omega_D + Qp}{2T_c(\chi, \varepsilon_0, Qp)}\right) - \ln\left(\frac{\pi}{4\gamma}\right) + \chi \frac{\tanh\left(\frac{\varepsilon_0 + Qp}{2T_c(\chi, \varepsilon_0, Qp)}\right)}{(\varepsilon_0 + Qp)} \quad (15)$$

We obtained the relation equation of $T_c(\chi, \varepsilon_0, Qp)$ and $T_c(0, 0, 0)$ as

$$\frac{T_c(\chi, \varepsilon_0, Qp)}{T_c(0, 0, 0)} = \left(\frac{\hbar\omega_D + Qp}{\hbar\omega_D} \right) \times \exp\left[\frac{\chi}{(\varepsilon_0 + Qp)} \tanh\left(\frac{\varepsilon_0 + Qp}{2T_c(\chi, \varepsilon_0, Qp)}\right)\right]. \quad (16)$$

Results and Discussion

The experimental data of H₃S, specifically T_c at 203 K, was analyzed using Brinkman-Rice picture and BCS-theory to perform numerical calculations. This analysis led to the determination of several parameters, namely $\hbar\omega_D$, Δ_0 , T_c , and N_0V , which were found to be 1560 K, 179.29 K, 200.8 K, and 0.30, respectively (Kim, 2021). The equation (10) was used with pressure parameters, and the resulting values of χ and ε_0 , which were found to be 473 and 91, respectively, with a Qp value of 0.1. Based on these values, we were able to determine that the values of T_c and Δ_0 for H₃S were 200.832 K and 379.432 K, respectively. Pressure parameters related to this study were presented in Table 1.

Table 1. Shows pressure parameters, $T_c(\chi, \varepsilon_0, 0.1)$ and $\Delta(0, \chi, \varepsilon_0, 0.1)$

χ	ε_0	$T_c(\text{K})$	$\Delta(0)(\text{K})$
32	0	77.521	140.062
100	100	100.085	181.012
473	91	200.832	379.432
573	200	216.886	403.589
673	200	238.958	447.774
673	100	244.840	466.305
1000	200	306.155	582.888
1000	100	311.131	598.640

To further analyze the data, we employed equation (3) to compute the penetration depth versus temperature with variations of χ and ε_0 , while keeping $Qp = 0.1$, as shown in Figure 1(a). The solid curve is $\chi = 473$ and $\varepsilon_0 = 91$, whereas each dashed curve represents a different pressure parameter. In Figure 1(b), we observed that the onset of each line on the penetration depth chart was different for $\chi = 32$, $\varepsilon_0 = 0$ and $\chi = 100$, $\varepsilon_0 = 100$. The pressure parameters were considered with $\chi = 473$ and $\chi = 91$ while varying Qp , as presented in Table 2. Following, the penetration depth was then calculated with variations of Qp , as shown in Figure 2(a). The solid curve represents $\chi = 473$, $\varepsilon_0 = 91$, and $Qp = 0.1$, while each dashed curve represents a different Qp value between 50 to -1 under London equation. In Figure 2(b), show that the onset of each line on the penetration depth chart was different for Qp values. In our numerical calculations, we determined that the ratio of the energy gap to the critical temperature (gap-to- T_c) was 3.786 for $T_c = 203$ K and $\Delta_0 = 384.263$ K. This value is close to the prediction of the BCS-theory, and previous research by Tanlansev *et al.*

(Tanlansev *et al.*, 2017; Tanlansev, 2019) found that the H₃S superconductor exhibits weak-coupling behavior with $3.3 < 2\Delta_0/T_c < 4.0$. The energy gap, Δ_0 was determined to be within the range of 290.113 - 324.927 K, while the T_c was approximately 203 K.

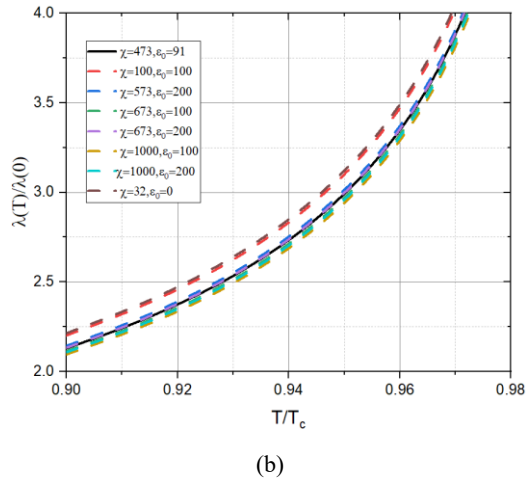
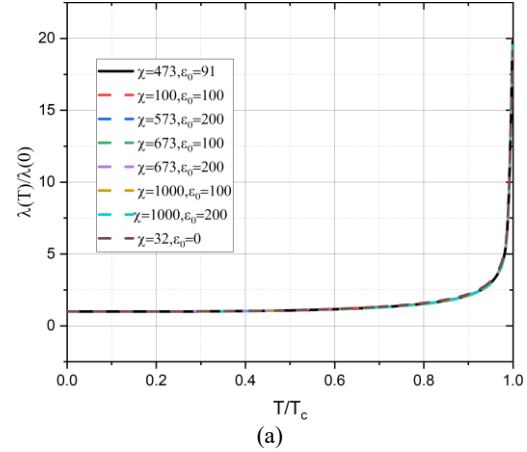


Figure 1. Shows (a) The temperature dependent penetration depth with χ and ε_0 variations. (b) The onset of each line of H₃S superconductor

Table 2. Shows pressure parameters, $T_c(473, 91, Qp)$ and $\Delta(0, 473, 91, Qp)$

Qp	$T_c(\text{K})$	$\Delta(0)(\text{K})$
-50	210.635	401.125
-10	202.967	384.263
-0.1	200.875	379.530
0.1	200.832	379.432
10	198.654	374.452
50	188.895	351.584

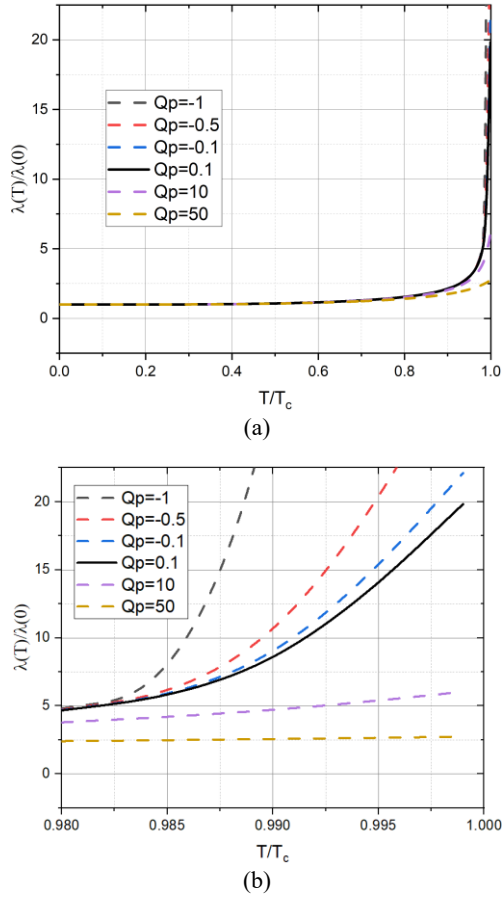


Figure 2. Shows (a) The temperature dependent penetration depth with Q_p variations. (b) The onset of each line of H_3S superconductor

Our model, which considers weak coupling in the superconducting gap function and uses both s-wave and d-wave models for pairing states, was compared to the equations (3) and (6) proposed by Gross et al., which is:

$$\Delta(T, \vec{k}) = \Delta_0(T)g(\vec{k}). \quad (17)$$

Here $g(\vec{k})$ is a dimensionless function for the directional variation of gap at Fermi surface and the temperature dependent gap equation as

$$\Delta_0(T) = \Delta_0(0) \tanh\left(\frac{\pi T_c}{\Delta_0(0)} \sqrt{a\left(\frac{T_c}{T} - 1\right)}\right). \quad (18)$$

Where a is a parameter that depends on the state of pairing. In each case, s-wave parameters are $g = 1$, $\Delta_0 = 1.76T_c$, $a = 1$; d-wave parameter are $g = \cos(2\phi)$, $\Delta_0 = 2.14T_c$, $a = 4/3$.

In Figures 3(a) and 3(b) indicate that the solid curve obtained from numerical calculations fits the s-wave model well. In contrast, the dashed line from analytical calculations only approximates the penetration depth value, which ranges from approximately 0 to 0.4 T/T_c .

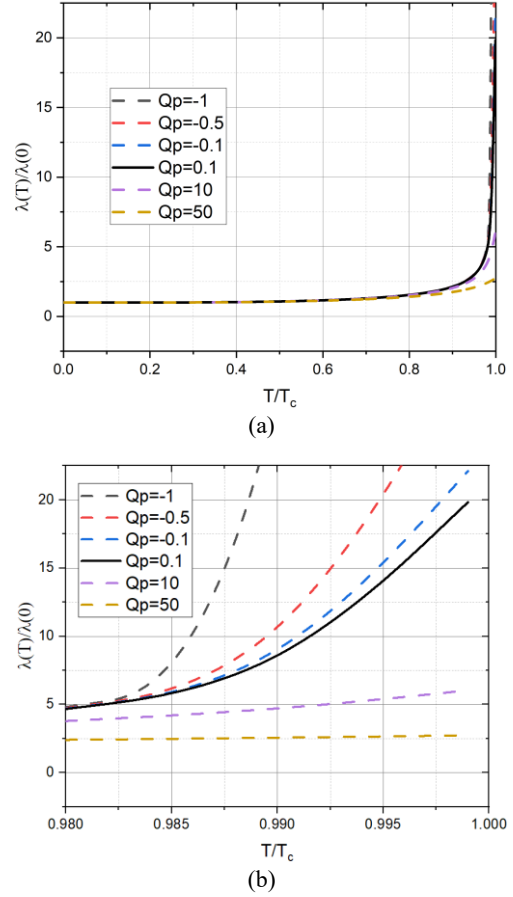


Figure 3. Shows (a) The temperature dependent penetration depth at $\chi = 473$, $\varepsilon_0 = 91$, and $Q_p = 0.1$ of our models is compared to Gross model. (b) The onset of each line of H_3S superconductor

Conclusions

In this research, the critical temperature formula, the energy gap at zero temperature formula, and the penetration depth at near-zero temperature formula were all derived under pressure. Following that, the temperature dependent penetration depth is reasonable, as well as the effect of the directly χ parameter on T_c (χ , ε_0 , Q_p), $\Delta(0, \chi, \varepsilon_0, Q_p)$, and $\lambda(T, \chi, \varepsilon_0, Q_p)/\lambda(0, \chi, \varepsilon_0, Q_p)$, whereas $Q_p > 0.1$ is

unreasonable. We discovered that the H₃S superconductor penetration depth fits well with the s-wave BCS theory via Gross model. The gap-to- T_c ratios is approximately 3.78 near 3.52 of BCS theory. Therefore, the penetration depth under pressure of s-wave isotropic superconductor can be investigated using the BCS theory, semiclassical approach and external pressure equation.

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