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# London Penetration Depth Study of Nb<sub>2</sub>InC Nanolaminate

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Using the approach of strong coupling Eliashberg theory the London penetration depth ( $\lambda_L$ ) function of strained Nb<sub>2</sub>InC compound has been obtained. Studied system belongs to the large family of MAX phases which share good thermal, electrical, and mechanical properties. This is the result of layered structure ensuring both good metallic and ceramic characteristics. Such combination could be of great use as long superconducting ribbons or planes composed with other flexible material. This paper examines the effect of magnetic field penetration inside superconducting material under applied current. Applied biaxial strain with values between  $-10\%$  and  $10\%$  was taken into consideration. Obtained results indicate the possible amendment of the magnetic penetration depth ( $\lambda_L$ ) with the use of strain applied to the material. Highest value of the London penetration depth is reported in case of strains maintaining the highest critical temperature. Reduction of  $\lambda_L(0)$  value to the least in the region of lowest  $T_c$  can be observed. This implies greater protection against supercurrent vortices breaking superconducting state.

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## 1. Introduction

Nanolaminates occupy the center of interest due to their outstanding features since their first synthesis in 1960 [1]. General formula of  $M_{n+1}AX_n$  can be used to describe this chemical group with M being the transition metal element, A — a  $p$ -block element, X — either carbon or nitrogen and  $n$  is integer of 1, 2, or 3. Base of the crystal structure is made of  $M_2X$  hexagonal layers intercalated with A element between the planes. This configuration supports great electrical and thermal conductance raised from the presence of many free electrons inside the overlapping layers [2]. In fact, many of this group leave behind metallic elements as regards to the electric conductance [3]. Layered structure provides the resistance to thermal shock and allows to maintain high temperatures [4]. Furthermore, the excellent machinability of such materials together with creep and fatigue resistance leads to their replacement of steel and other alloys in the industry [5]. Therefore, there is no surprise on constantly increasing number of research on nanolaminates.

The  $P6_3/mmc$  space group in which MAX phases and similar structures crystallize are often seen in materials that reveal superconducting state. In particular, MgB<sub>2</sub> compound, borocarbides, oxides and cuprates exhibit high critical temperature complemented with other features which make them good candidates for industrial use. On the top of the foregoing properties, some compounds of MAX phases group also does

maintain superconducting state. Although, for over 70 known nanolaminates only 8 appear to manifest the Meissner–Ochsenfeld effect under the transition temperature [6, 7]. These are as follows: Ti<sub>2</sub>InC, Ti<sub>2</sub>GeC, Mo<sub>2</sub>GaC, Nb<sub>2</sub>AsC, Nb<sub>2</sub>SC, Nb<sub>2</sub>SnC, Nb<sub>2</sub>AlC, Nb<sub>2</sub>InC ( $T_c = 3, 7.5, 4, 2, 5, 7.8, 0.44, 7.5$  K, respectively) [8–15]. Despite the increasing interest over this group, the genesis of superconductivity was examined *in situ* only for the case of Nb<sub>2</sub>AlC by Xiang et al. in 2013 [16]. Authors indicate that the superconductivity in this material emerges from the coupling of electrons on  $4d$  orbital of Nb with  $E_{2g}$  and  $A_{1g}$  phonons. The origin of superconducting state has not been clarified for the rest of MAX phase superconductors.

Phase of zero resistance in such versatile material leads to the idea of cables in form of tapes or ribbons that can handle high currents. There are couple of problems that need to be addressed in order to realize this project. In particular, superconducting state breaks when vortices of supercurrent happen to overlap in the mixed state. Hence, it is important to decrease their penetration depth ( $\lambda_L$ ).

Few experimental data on the structural and electronic characteristics have been obtained for similar nanolaminate Nb<sub>2</sub>InC [17–19]. Furthermore, the *ab initio* studies done by Li et al. [20] announce the possibility of transition temperature modification using the biaxial stress on the material. Their calculations show that  $T_c$  can vary by over 20 K during the change of applied strain from  $-4\%$  to  $-10\%$  together with corresponding change of logarithmic average phonon frequency  $\omega_{ln}$ . Main trend of  $T_c$  appear to rise with the change of both compressive and decompressive strain applied. Those results are in contrast to conclusions brought by Romeo and Escamilla on the basis of BCS theory [21]. Their work states the

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reduction of transition temperature value with pressure increase [22]. Noteworthy, the research on the possibility of  $T_c$  enhancement within the material should be considered to have the most importance. In the light of above, further studies are highly recommended to ascertain the exact origin of superconducting state in this compound.

In present paper the London penetration depth functions of superconducting state in the strained Nb<sub>2</sub>InC are reported. Relatively high electron–phonon constant values obtained by Li et al. [20] were the reason to use the approach of the strong coupling Eliashberg theory. Main input of the Eliashberg spectral functions which model the interaction between the electrons and phonons have been derived from the above work.

## 2. The theoretical model

The Eliashberg formalism assumes the equations for the function of the order parameter  $\phi(\omega)$  and the wave function renormalization factor  $Z(\omega)$  [23]. The imaginary part of both functions  $\phi_n \equiv \phi(i\omega_n)$  and  $Z_n \equiv Z(i\omega_n)$  assume the shape of [24, 25]:

$$\phi_m = \frac{\pi}{\beta} \sum_{n=-M}^M \frac{\lambda(i\omega_m - i\omega_n) - \mu^* \theta(\omega_c - |\omega_n|)}{\sqrt{\omega_n^2 Z_n^2 + \phi_n^2}} \phi_n, \quad (1)$$

and

$$Z_m = 1 + \frac{1}{\omega_m} \frac{\pi}{\beta} \sum_{n=-M}^M \frac{\lambda(i\omega_m - i\omega_n)}{\sqrt{\omega_n^2 Z_n^2 + \phi_n^2}} \omega_n Z_n. \quad (2)$$

The  $\omega_m$  part, also called the Matsubara frequency is defined as:  $\omega_m \equiv (\pi/\beta)(2m-1)$ , where  $m = 0, \pm 1, \pm 2, \dots, \pm M$  up to value of 1100 with  $\beta \equiv (k_B T)^{-1}$ . The term  $\mu^* \theta(\omega_c - |\omega_n|)$  involves the Coulomb interactions responsible for depairing effects. The Coulomb pseudopotential is represented by  $\mu^*$  part [26]. Pairing kernel takes the following form:

$$\lambda(z) \equiv 2 \int_0^{\Omega_{\max}} d\Omega \frac{\Omega}{\Omega^2 - z^2} \alpha^2 F(\Omega). \quad (3)$$

As mentioned in previous section, the main input of the Eliashberg spectral function  $\alpha^2 F(\Omega)$  has been taken from this work [20]. Maximum phonon frequency  $\Omega_{\max}$  varies with the applied strain between values of 72 and 80 meV. This is caused by the changes in the lattice parameters under the pressure in the crystal structure. The Heaviside step function describes the  $\theta$  term. Cessation frequency  $\omega_c$  has been evaluated as  $\omega_c = 10\Omega_{\max}$ .

## 3. The numerical results

In order to compute the critical temperatures for strained Nb<sub>2</sub>InC compound the Coulomb pseudopotential value is needed. Commonly accepted figure of  $\mu^* = 0.13$  has been considered in this paper. Transition temperatures have been calculated using the Combescot formula with the use of  $\omega_{\ln}$  and the electron–phonon constant  $\lambda$  values given by Li et al. The Combescot formula can be defined as:

$$T_c^C = \frac{2}{\pi} e^{c-1/2} \omega_{\ln} \times \exp\left(\frac{-(1+\lambda)}{\lambda - \mu^*} - \frac{\lambda \mu^*}{(\lambda - \mu^*)^2} - \frac{\lambda^2}{(\lambda - \mu^*)^2} R\right),$$

where coefficient  $2e^c \simeq 1.13$  is one of the BCS constants and  $R = \frac{\pi}{8} - 1$  [27]. Results have been collated with the outcome of the Allen–Dynes formula [28] used by Li et al. together with the results of the non-generalized, strong coupling Eliashberg formalism approach from our work on Nb<sub>2</sub>InC thermodynamic properties  $T_c^{NG}$  [29] in Table I.

TABLE I

Collected values of the critical temperatures obtained with the use of the Combescot  $T_c^C$ , the Allen–Dynes  $T_c^{AD}$  formula and non-generalized  $T_c^{NG}$  [29] approach together with the experimental value [15].

Strain	$T_c^C$	$T_c^{AD}$	$T_c^{NG}$	Exp.
10%	35.18	18.18	20.85	–
8%	35.40	16.93	19.95	–
6%	31.06	14.43	16.9	–
4%	11.75	4.64	6.13	–
2%	16.98	6.94	8.98	–
0%	19.30	7.81	9.83	7.5
–2%	3.02	0.92	1.73	–
–4%	0.93	0.24	0.62	–
–6%	7.15	2.42	3.78	–
–8%	52.58	25.01	34.76	–
–10%	49.07	25.98	33.34	–

Great discrepancy between the experimental and attained value by the Combescot formula can be noted. This can be the clue to adjust the estimation of depairing effects strength as the Combescot formula is more advanced in terms of the Coulomb pseudopotential parameter than the equation of the Allen–Dynes approach. Similar conclusion can be derived from our recent calculations of  $T_c^{NG}$  for which we have taken into consideration the value of  $\mu^* = 0.13$ . Thus, the depairing effects should have more weight in the analysis of the Nb<sub>2</sub>InC nanolaminate.

Following with the choice of the Coulomb pseudopotential values the wave function renormalization factor can be computed which renormalizes electron effective mass ( $m_e^*$ ) by the relationship of  $m_e^* = Z_{m=1} m_e$ , where the electron band mass is described by the  $m_e$  term. Subsequently, the order parameter function models with good approximation the influence of temperature on the energy gap located on the Fermi surface. Those functions act as input into final calculation on the London penetration depth

$$\frac{1}{e^2 \nu_F^2 N(\varepsilon_F) \lambda_L^2(T)} = \frac{4\pi}{3\beta} \sum_{m=1}^M \frac{\Delta_m^2}{Z_m^S (\omega_m^2 + \Delta_m^2)^{3/2}}, \quad (4)$$

where  $e$  describes the electric charge of an electron and  $\nu_F^2$  is the Fermi velocity [30] and  $\Delta_m = \phi_m/Z_m$ .

Zeroth temperature London penetration depth is defined as  $\lambda_L(0) = ev_F \sqrt{N(\varepsilon_F)} \lambda_L(T=0 \text{ K})$ .

Values of  $(\lambda_L(T)/\lambda_L(0))^{-2}$  are plotted as a function of normalized temperature in Fig. 1 together with the BCS predictions for range of studied strain. It can be noted that the course of those functions can vary between given strain with the trend to fall under the BCS curve in case of lower critical temperatures, although the shape for highest  $T_c$  arc over the predicted curve.

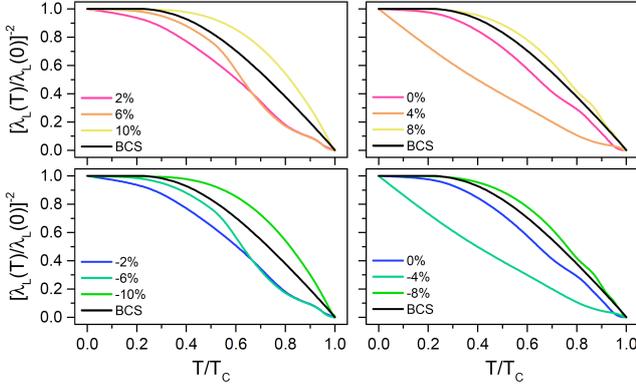


Fig. 1. Course of the normalized London penetration depth functions plotted for  $\text{Nb}_2\text{InC}$  nanolaminate together with the BCS theory predictions.

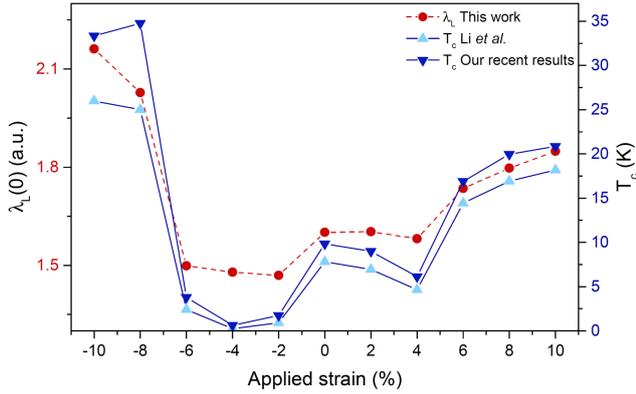


Fig. 2. Values of the  $\lambda_L(0)$  for  $\text{Nb}_2\text{InC}$  nanolaminate plotted with the anticipated transition temperatures.

Complicated courses for lowest transition temperatures above the value of  $0.5 T/T_c$  can be noted. This may be caused by large intervals between computations of  $\phi_m$  and  $Z_m$  function. The exact origin of this effect is not certain, especially in the case of strains maintaining higher  $T_c$ . For the better view,  $\lambda_L(0)$  values have been plotted against anticipated transition temperatures in Fig. 2. There, strong dependence on critical temperature can be observed. Significant change of penetration depth by the value of  $\Delta\lambda_L(0) = 0.53$  a.u. can be seen with the change of strain between  $-6\%$  and  $-8\%$ . This lead to the conclusion of magnetic reluctance decrease in the volume close to the supercurrent vortex core, with the increment

of  $T_c$ . In other words, the magnetic field will be less attenuated which at the first glance is in contrary to the fact of better electromagnetic (i.e. diamagnetism) properties of compounds having higher transition temperature. Similar results were observed for doped, iron based superconductors [31]. Although, for overdoped material (yet for highest critical temperature) the fall of  $\lambda_L(0)$  can be noticed in the case of  $\text{Ca}_{10}(\text{Pt}_3\text{As}_8)((\text{Fe}_{1-x}\text{Pt}_x)_2\text{As}_2)_5$  proving not exact mechanism lying behind this effect.

#### 4. Conclusions

This paper shed light on the influence of strain applied to the material on the superconducting state properties of critical temperature and the London penetration depth. Numerical computations performed within the framework of strong-coupling Eliashberg formalism demonstrate that  $\lambda_L(0)$  value can vary widely with the change of transition temperature. Also, results prove the inability of BCS theory to accurately determine the London penetration depth behavior in strong coupling systems such as studied  $\text{Nb}_2\text{InC}$ . The ability to amend the London penetration depth can have great importance in the superconducting ribbons and planes use. In view of the above results it is highly recommended to study this compound in the experimental way.

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