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On the Magnetic Penetration Depth in Superconducting Ultrathin Lead Films

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In the present paper, we report a theoretical study of the magnetic London penetration depth in ultrathin Pb films consisting of five to ten monolayers. Our calculations were performed within the framework of the strong-coupling approach. We observed that for thin films, the thermodynamic parameter exhibits an oscillatory behaviour connected with a quantum size effect. Moreover, we proved that the London penetration depth of Pb films cannot be correctly described using the Bardeen–Cooper–Schrieffer theory of superconductivity due to the strong-coupling and retardation effects. The Eliashberg theory, used in this paper, goes beyond the BCS theory to include these effects which allows to describe the superconducting state on the quantitative level.

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1. Introduction

Relationships between size effects and thermodynamic properties in the superconducting thin films are crucial for the potential applications of these materials in nanotechnology as well as other fields of science and engineering. Recent theoretical studies and experimental measurements show that the quantum size effects in a two-dimensional ultrathin metal films appear as oscillations in many physical properties upon variation of film thickness [1–6]. For instance, in photoemission experiments combined with transport measurements reported by Guo et al. [3] and in scanning tunneling spectroscopy measurements reported by Eom et al. [1] the oscillations of critical temperature and superconducting order parameter as a function of the number of atomic monolayers have been found for ultrathin Pb films grown on Si(111) substrate. This phenomenon is directly related to the quantization of the electron wave vector resulting from the confinement of its motion in the direction perpendicular to the film [7]. According to the Bardeen–Cooper–Schrieffer (BCS) theory of superconductivity [8, 9], T_c depends exponentially on the density of states at the Fermi surface

$$k_B T_c = 1.14 \hbar \omega_D \exp(-1/N(\varepsilon_F)V), \quad (1)$$

where the density of states per spin oscillates with the film thickness L in the following way: $N(\varepsilon_F) = (m_e^*/\pi \hbar^2 L) [2L/\lambda_F]$. Moreover, k_B is the Boltzmann constant, ω_D is the Debye frequency, V is the phonon-mediated attractive interaction at the Fermi surface, m_e^* is the electron effective mass, \hbar is the Planck constant divided by 2π , λ_F denotes the Fermi electron wavelength, and $[2L/\lambda_F]$ is the integer part of $2L/\lambda_F$ [10]. In the case of Pb, the λ_F is nearly 4 monolayers (4 ML), so the oscillating period is 2 ML [3, 11].

It was also shown that superconductivity remains surprisingly robust, even for films as thin as 5 ML where $T_c = 6.1$ K [1]. Next, together with the film thickness increase, the decrease of the quantum oscillations of T_c is observed. This result was confirmed by Qin et al. in paper [6]. Moreover, we can notice that for Pb films in the ultrathin regime (5–50 ML) the values of T_c of around 6.2 K are about 15% lower than the bulk value of 7.2 K. The growth of film thickness up to 500 ML leads to the bulk value of T_c and the superconducting energy gap which suggest the existence of a 2D to 3D transition thickness somewhere between 50 and 500 ML [1].

Motivated by the mentioned results, in our previous paper [4], we studied the thermodynamic properties of superconducting Pb films within the framework of the Eliashberg formalism. In particular, the energy gap, free energy difference between the superconducting and normal state, thermodynamic critical field and the specific heat were determined for an ultrathin regime (5–10 ML). We found an oscillatory behaviour of the above thermodynamic properties modulated by quantum size effects. Similar oscillations can also be observed in other physical systems [12–16]. Moreover, we proved that the thermodynamic properties of Pb films cannot be correctly described using the BCS theory of superconductivity due to the strong coupling and retardation effects.

In this paper, we investigate the temperature dependence of the London penetration depth in Pb films in a thickness range from 5 ML to 10 ML. By comparison of our theoretical results with experimental measurements, we show that the numerical calculations conducted in the framework of Eliashberg formalism provide a qualitative description of the Pb ultrathin films.

2. Theoretical model and computational methods

In the framework of the Eliashberg formalism, the London penetration depth (λ_L) can be calculated in the following way:

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$$\frac{1}{e^2 v_F^2 N(\varepsilon_F) \lambda_L^2(T)} = \frac{4\pi}{3\beta} \sum_{n=1}^M \frac{\Delta_n^2}{Z_n [\omega_n^2 + \Delta_n^2]^{3/2}}, \quad (2)$$

where e is the electron charge, v_F is the Fermi velocity and $\beta = 1/k_B T$ [17]. The superconducting order parameter is defined as: $\Delta_n = \phi_n/Z_n$, where the imaginary axis Eliashberg functions $\phi_n \equiv \phi(i\omega_n)$ and $Z_n \equiv Z(i\omega_n)$ can be written as follows [18]:

$$\phi_n = \frac{\pi}{\beta} \sum_{m=-M}^M \frac{\lambda(i\omega_n - i\omega_m) - \mu^* \theta(\omega_c - |\omega_m|)}{\sqrt{\omega_m^2 Z_m^2 + \phi_m^2}} \phi_m \quad (3)$$

and

$$Z_n = 1 + \frac{1}{\omega_n} \frac{\pi}{\beta} \sum_{m=-M}^M \frac{\lambda(i\omega_n - i\omega_m)}{\sqrt{\omega_m^2 Z_m^2 + \phi_m^2}} \omega_m Z_m. \quad (4)$$

The Matsubara frequency is defined as $\omega_n \equiv (\pi/\beta)(2n-1)$ where $n = 0, \pm 1, \pm 2, \dots, \pm M$, and $M = 1100$. The pairing kernel for the electron-phonon interaction is given by

$$\lambda(i\omega_n - i\omega_m) \equiv 2 \int_0^{\Omega_{\max}} d\omega \frac{\omega}{\omega^2 + (\omega_n - \omega_m)^2} \alpha^2 F(\omega). \quad (5)$$

In the framework of the Eliashberg formalism, the depairing interactions between the electrons are described by the Coulomb pseudopotential μ^* . Symbol θ denotes the Heaviside unit function and ω_c is the cut-off frequency set to ten times the maximum phonon frequency $\omega_c = 10\Omega_{\max} = 100$ meV.

We solved the Eliashberg equations in a numerical way using the self-consistent iteration methods [19], which have been extensively examined and successfully used in our previous study [20–23].

3. Results and discussion

The computed zeroth temperature London penetration depth and measured critical temperature [1] for Pb as a function of film thickness are presented in Fig. 1A. The rough oscillations of $\lambda_L(0)$ caused by the quantum size effect can be readily observed. Moreover, we can note the saturation effect of oscillations for higher values of thickness. Similar situation is also observed for superconducting critical temperature [4] although the oscillations of $\lambda_L(0)$ are out of phase to that of T_c for low values of thickness ($L \in \{5, 6, 7\}$ ML).

The normalized λ_L^{-2} as a function of temperature is presented and compared with the BCS theory prediction in Fig. 1B. The differences observed between the BCS and the Eliashberg theory in a middle region of temperature are connected with the fact that the BCS approach, in contrast to the Eliashberg theory, does not include the strong coupling corrections and retardation effects of electron-phonon interactions. It should be noted that in the case of investigated Pb films consisting of five to ten atomic layers the electron-phonon coupling constant (λ_{ep}) is above 1.5 [5] (BCS gives fairly good approxima-

tion for $\lambda_{ep} \leq 0.5$). Due to the absence of appropriate experimental reports about the London penetration depth in ultrathin lead films, we compared our prediction with available data for superconducting lead nanowires [24] and for thicker lead films (150–400 Å) [25]. As expected, the experimental results are more compatible with our calculations for thin films than with the predictions of BCS theory.

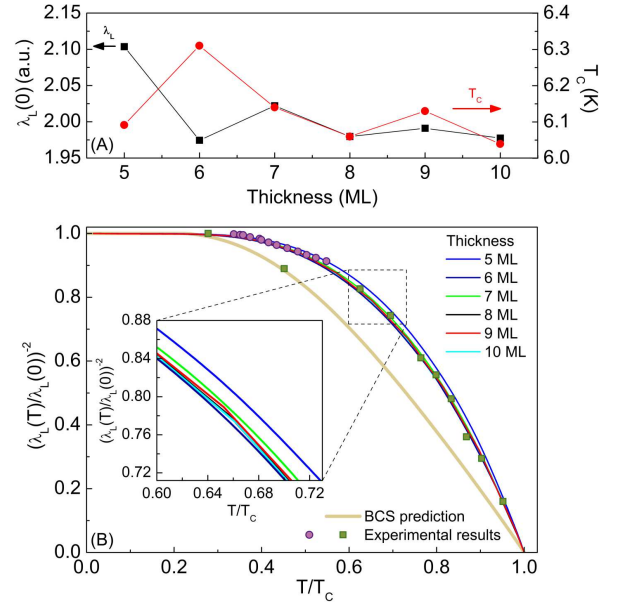


Fig. 1. (A) The zeroth temperature London penetration depth (black squares) defined as $\lambda_L(0) = ev_F \sqrt{N(\varepsilon_F)} \lambda_L(T=0 \text{ K})$ and critical temperature (red circles) [1] as a function of film thickness. (B) The normalized London penetration depth as a function of temperature compared with BCS prediction. The experimental results for lead nanowires (squares) and for films in the range of 150–400 Å (circles) are taken from [24] and [25].

4. Conclusions

We investigated the effects of thickness on the London penetration depth in ultrathin lead films. Calculations conducted within the framework of the strong coupling Eliashberg theory of superconductivity proves that $\lambda_L(0)$ oscillate with film thickness. This behaviour is caused by the quantum size effects existing in the investigated range of thickness. Moreover, our study shows that the London penetration depth for strong coupling systems cannot be correctly described using the BCS theory.

We expect that the results presented in this paper can be reproduced in future measurements which can confirm our calculations. Therefore, we strongly encourage experimentalists to carry out appropriate experiments.

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