Physica B 475 (2015) 66–72

Contents lists available at ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Comparison study of superconductivity in zirconium and hafnium based electron-doped layered chloronitrides

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ARTICLE INFO

Article history:
Received 29 May 2015
Received in revised form
15 June 2015
Accepted 23 June 2015
Available online 24 June 2015

Keywords:
Superconductors
Layered nitrides
Superconductivity
Thermodynamic properties

ABSTRACT

The transition-metal chloronitrides form a fairly large family of superconductors. Motivated by the potential high-temperature superconductivity in electron-doped layered systems we investigated the thermodynamic properties of β-$Li_{0.5}HfNCl$ and β-$Li_{0.5}ZrNCl$ compounds. A systematic comparative study was carried out using the strong-coupling Eliashberg theory. In dependence on the chemical composition (Zr- or Hf-based system), a marked change in parameters of the superconducting state was observed. Moreover, the obtained results indicate that due to the existence of the strong-coupling and retardation effects the studied systems cannot be quantitatively described within the framework of classical Bardeen–Cooper–Schrieffer (BCS) theory.

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1. Introduction

The layered superconductors have attracted much attention owing to the observation of superconductivity with a high value of the superconducting transition temperature (T_C). There have been many types of layered superconductors e.g. the graphite intercalation compounds, the high-temperature cuprates, the magnesium diboride, the borocarbides, the iron pnictides, and the intercalated metal nitride halides. An interesting point is that the chemical doping or substitution is the way to enhance the T_C in this type of superconductors [1]. Unfortunately, the fundamental mechanism responsible for high temperature superconducting state induced in layered copper oxides and new Fe-based pnictides is still debated, which prevents the progress of searching superconductors with higher values of T_C [2–10]. Nonetheless, other systems are widely accepted to be a conventional electron–phonon interaction mediated superconductor.

Especially interesting subject of study are layered nitrides, which in the normal conditions are band insulators with a band gap of 3–4 eV [11]. However, when electrons are doped by intercalation of alkali, alkaline-earth or rare-earth metals into the interlayer site, the crystals changed from a semiconductor to a metal and a superconducting state can occur [12,13]. The superconductivity in rhombohedral layered nitrides β–HfNCl and β–ZrNCl is observed after electron-doping the crystal by intercalation of lithium between the chloride layers [13,14]. It was also found that the electronic structure of above isostructural compounds is very similar, but their transition temperatures are different. The maximum T_C is equal to ~15 K for β–LiZrNCl system and ~25.5 K for β–LiHfNCl system [14,15].

In present paper we compared the thermodynamic properties of superconducting state induced in electron-doped layered chloronitrides β–$Li_{0.5}HfNCl$ and β–$Li_{0.5}ZrNCl$. Due to the high value of the electron–phonon coupling constants, observed in above compounds [16], our calculations were carried out in the framework of the strong-coupling Eliashberg theory of superconductivity [17]. This approach allows us to provide a quantitative estimations and comparative studies of the most important thermodynamic properties of the superconducting phase such as critical temperature, energy gap at the Fermi level, specific heat, thermodynamic critical field and the electron effective mass.

2. The theoretical model

The Eliashberg equations for the order parameter function $\phi(\omega)$ and for the wave function renormalization factor $Z(\omega)$ defined in the mixed representation (simultaneously on the imaginary and real frequency axis) take the following form [18]:

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http://dx.doi.org/10.1016/j.physb.2015.06.023
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$$\phi(\omega) = \frac{\pi}{\beta}\sum_{m=-M}^{M}\frac{\left[\lambda(\omega-i\omega_m)-\mu^{\star}\theta(\omega_c-|\omega_m|)\right]}{\sqrt{\omega_m^2 Z_m^2+\phi_m^2}}\phi_m + i\pi\int_0^{+\infty} d\omega' \alpha^2F(\omega,')[[N(\omega,')+f(\omega'-\omega)]\times K(\omega,-\omega')\phi(\omega-\omega')] + i\pi\int_0^{+\infty} d\omega' \alpha^2F(\omega,')[[N(\omega,')+f(\omega'+\omega)]\times K(\omega,\omega')\phi(\omega+\omega')] \quad (1)$$

and

$$Z(\omega) = 1+\frac{i\pi}{\omega\beta}\sum_{m=-M}^{M}\frac{\lambda(\omega-i\omega_m)\omega_m}{\sqrt{\omega_m^2 Z_m^2+\phi_m^2}}Z_m + \frac{i\pi}{\omega}\int_0^{+\infty} d\omega' \alpha^2F(\omega,')[[N(\omega,')+f(\omega'-\omega)]\times K(\omega,-\omega')(\omega-\omega')Z(\omega-\omega')] + \frac{i\pi}{\omega}\int_0^{+\infty} d\omega' \alpha^2F(\omega,')[[N(\omega,')+f(\omega'+\omega)]\times K(\omega,\omega')(\omega+\omega')Z(\omega+\omega')], \quad (2)$$

where

$$K(\omega,\omega') \equiv \frac{1}{\sqrt{(\omega+\omega')^2Z^2(\omega+\omega')-\phi^2(\omega+\omega')}}. \quad (3)$$

The order parameter is defined as $\Delta(\omega) \equiv \phi(\omega)/Z(\omega)$. On the imaginary frequency axis the equations for $\phi_n \equiv \phi(i\omega_n)$ and $Z_n \equiv Z(i\omega_n)$ functions take the following form [17]:

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

and

$$Z_n = 1+\frac{1}{\omega_n}\frac{\pi}{\beta}\sum_{m=-M}^{M}\frac{\lambda(i\omega_n-i\omega_m)}{\sqrt{\omega_m^2Z_m^2+\phi_m^2}}\omega_m Z_m, \quad (5)$$

where $\omega_n \equiv (\pi/\beta)(2n-1)$ is the Matsubara frequency, with $n = 0, \pm 1, \pm 2, \ldots, \pm M$, where $M=1100$ and $\beta \equiv (k_BT)^{-1}$. The symbol k_B represents the Boltzmann constant and the pairing kernel is given by

$$\lambda(z) \equiv 2\int_0^{\Omega_{\max}} d\Omega \frac{\Omega}{\Omega^2-z^2}\alpha^2F(\omega). \quad (6)$$

The Eliashberg spectral function $\alpha^2F(\omega)$ models the electron–phonon interaction and $\Omega_{\max}$ is the maximum phonon frequency (for investigated systems $\Omega_{\max} \approx 80$ meV). In the case of the analyzed electron-doped layered chloronitrides β–$Li_{0.5}HfNCl$ and β–$Li_{0.5}ZrNCl$, the Eliashberg functions were calculated in the paper [16] using the QUANTUM ESPRESSO package [19], where the local density approximation with the parametrization by Perdew and Zunger and the Troullier–Martins norm-conserving pseudopotentials were employed [20,21]. The function $\mu^{\star}(\omega_n) \equiv \mu^{\star}\theta(\omega_c-|\omega_n|)$ describes the depairing Coulomb interaction, where $\mu^{\star}$ represents the Coulomb pseudopotential [22]. Symbol θ is the Heaviside unit function and ω_c denotes the cut-off frequency, we have chosen 10 times the maximum phonon frequency: $\omega_c = 10\Omega_{\max}$. Moreover, $N(\omega)$ and $f(\omega)$ denote the Bose–Einstein and the Fermi-Dirac distribution function, respectively. The solutions of $\phi(\omega)$ and $Z(\omega)$ functions are stable for $T \geq T_0$, where $T_0 = 2$ K.

3. The numerical results and discussion

The experimental results of the superconducting critical temperature for β–$Li_{0.5}HfNCl$ (T_C=25.5 K) and β–$Li_{0.5}ZrNCl$ (T_C=11.5 K) allow us to estimate the critical value of the Coulomb pseudopotential $\mu_C^{\star}$. In the Eliashberg theory, the exact value of $\mu_C^{\star}$ is defined as the Coulomb pseudopotential at which the order parameter vanishes at critical temperature. In particular, on the basis of the expression: $[\Delta_{m=1}]^{T=T_C}_{\mu=\mu_C^{\star}} = 0$, we obtained $\mu_C^{\star} = 0.08$ for

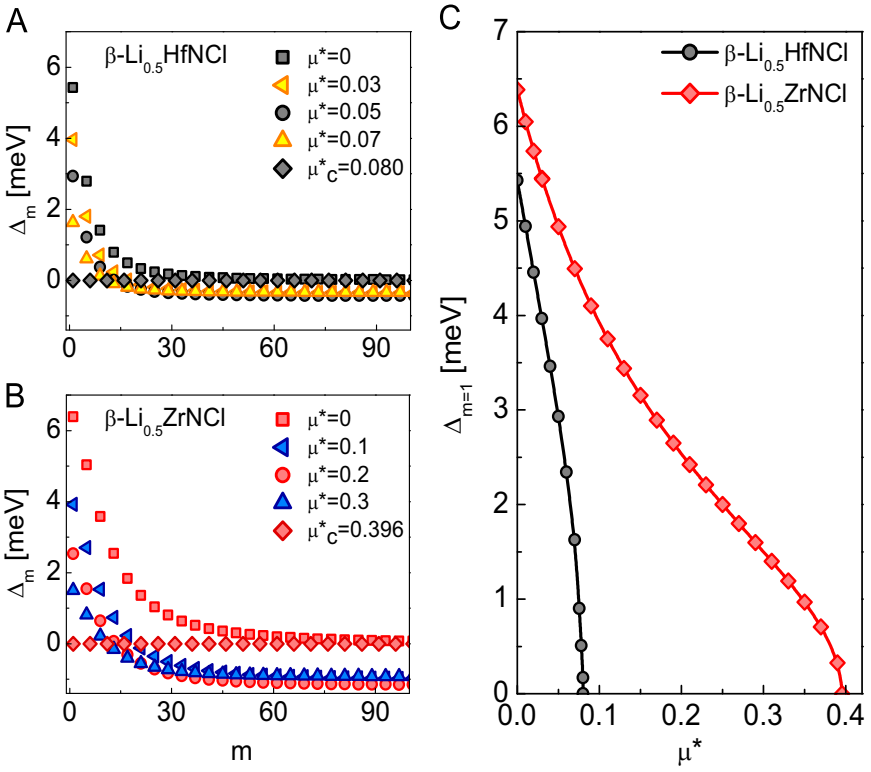

Fig. 1. (A) and (B) The order parameter on the imaginary frequency axis for the selected values of the Coulomb pseudopotential. (C) The full dependence of the maximum value of the order parameter on the Coulomb pseudopotential for investigated systems.

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