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Electron–Phonon Interaction and Superconductivity in $NaSn_3$ Intermetallic Compound

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In this study, the superconducting properties of $NaSn_3$ — an intermetallic compound with an $AuCu_3$-type crystal structure and space group $Pm\bar{3}m$ (221), where Na atoms occupy the corners and Sn atoms are in face-centered positions — were investigated. The critical temperature of superconductivity (T_C) in $NaSn_3$ is found to be 7.038 K. The electron–phonon coupling constant has been calculated to assess its role in superconductivity, with the aim of understanding the mechanisms that enable $NaSn_3$ to reach a relatively high T_C. The analysis includes the calculation of the superconducting order parameter, the wave function renormalization factor for the first Matsubara frequency as a function of temperature, and the specific heat in both the superconducting and normal states. The results provide insight into the electron–phonon interaction and its contribution to the superconducting state in $NaSn_3$, offering a detailed perspective on its potential for higher-temperature superconductivity.

topics: electron–phonon coupling, Eliashberg function, high-temperature superconductivity (HTc)

1. Introduction

The intermetallic compound made of sodium and tin, $NaSn_3$, has recently attracted considerable attention due to its intriguing physical properties and potential applications in the field of superconductivity [1–4]. $NaSn_3$ crystallizes in a cubic $AuCu_3$-type structure, providing a platform for studying electron–phonon interactions that play a crucial role in determining its superconducting properties [1, 4–7]. This class of materials is particularly attractive because of its potential for unconventional superconductivity, resulting from complex interactions between lattice vibrations and conduction electrons.

High-temperature superconductors are a significant focus of condensed matter physics, offering promising applications in energy transmission, magnetic levitation, and quantum computing. The critical temperature, T_C, is a fundamental parameter that characterizes the transition to the superconducting state. Understanding and enhancing T_C remain key challenges in the development of new superconducting materials. Although superconductivity in sulfur hydrides has been experimentally observed at temperatures exceeding 200 K [8], the requirement to maintain extremely high pressures currently precludes their practical application. Similarly, the utilization of cuprate superconductors is complicated by their mechanical limitations, particularly their brittleness, which poses significant challenges for technological implementation. Thus, intermetallic superconductors, such as $NaSn_3$, are commonly used for technological applications. Moreover, they provide a fertile ground for exploring these phenomena, as they often exhibit rich electronic and structural behaviors.

In this study, the authors focused on several critical aspects of superconductivity in $NaSn_3$. The spectral function $\alpha^2F(\omega)$ [4, 6, 9, 10], which describes the electron–phonon interaction as a function of frequency, is analyzed to elucidate the underlying mechanisms of superconductivity. The specific heat in the superconducting state is examined, providing insights into the thermodynamic properties of the compound. Additionally, the thermodynamic critical field as a function of temperature is investigated [11, 12], offering a deeper understanding of the energy scales associated with the superconducting phase.

The superconducting order parameter on the imaginary axis is studied for selected temperatures, with particular attention given to its behavior at the first Matsubara frequency as a function of temperature. This provides a comprehensive picture of the pairing mechanism and its thermal evolution. Furthermore, the wave function renormalization factor, which quantifies the strength of electron–phonon coupling, was calculated, as well as the dependence

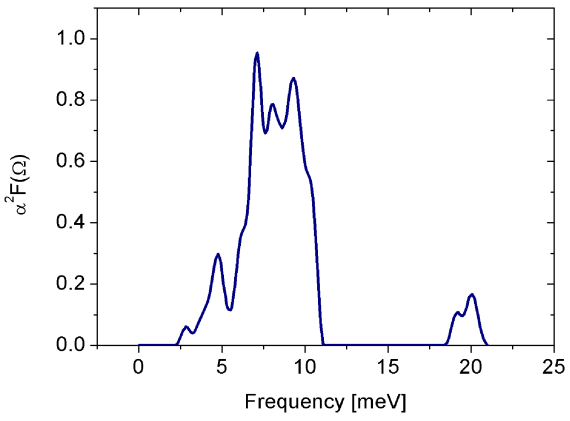

Fig. 1. The Eliashberg function for $NaSn_3$. Source: own research based on [5].

of the renormalization factor at the first Matsubara frequency on temperature, highlighting its relevance to the superconducting state.

By exploring these key properties, this work aims to provide a detailed characterization of $NaSn_3$, contributing to the broader understanding of intermetallic superconductors and their potential for technological applications.

2. Computational details

Firstly, the used model implementing the Eliashberg equations should be presented, which on the imaginary axis take the following form

$$\phi = \frac{\pi}{\beta}\sum_{m=-M}^{M}\frac{\lambda(\mathrm{i}\omega_n-\mathrm{i}\omega_m)-\mu^*\theta(\omega_c-|\omega_m|)}{\sqrt{\omega_m^2 Z_m^2+\phi_m^2}}\phi_m, \tag{1}$$

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

In the above equations, symbols $Z_n \equiv Z(\mathrm{i}\omega_n)$ and $\phi_n \equiv \phi(\mathrm{i}\omega_n)$ denote the wave function renormalization factor and the order parameter function, respectively. Here, ω_n equal to $(\frac{\pi}{\beta})(2n-1)$ is used to represent the n-th Matsubara frequency and the factor $\beta = 1/(k_\mathrm{B}T)$, in which k_B is the Boltzmann constant. Next, the order parameter Δ_n is defined as $\Delta_n = \phi_n/Z_n$. The electron–phonon pairing kernel, which in the Eliashberg theory describes the effective interaction between two electrons via phonon exchange, is given by the following equation

$$\lambda(Z) = 2\int_0^{\Omega_\mathrm{max}}\mathrm{d}\Omega\ \frac{\Omega}{\Omega^2-Z^2}\,\alpha^2F(\Omega). \tag{3}$$

Here, α^2F is the Eliashberg electron–phonon spectral function defined as

$$\alpha^2F(\Omega) = \frac{1}{N(E_\mathrm{F})}\sum_{\boldsymbol{k},\boldsymbol{k}'}|g_{\boldsymbol{k},\boldsymbol{k}'}|^2\,\delta(\Omega-\Omega_{\boldsymbol{k}-\boldsymbol{k}'}), \tag{4}$$

where $N(E_\mathrm{F})$ is the density of electron states at the Fermi level, $g_{\boldsymbol{k},\boldsymbol{k}'}$ — electron–phonon coupling matrix element for the transition from the wave vector $\boldsymbol{k}$ to $\boldsymbol{k}'$, and $\Omega_{\boldsymbol{k}-\boldsymbol{k}'}$ — phonon frequency associated with the momentum transfer vector $\boldsymbol{q} = \boldsymbol{k}-\boldsymbol{k}'$.

The depairing electron correlations are characterized by the Coulomb pseudopotential μ^*. In the calculations, the value of $\mu^* = 0.1$ was assumed, as typical for strongly coupled classical superconductors. The symbol θ in (1) represents the Heaviside unit function, while the ω_c is the cut-off energy set to $\omega_c = 5\Omega_\mathrm{max}$. The Eliashberg functions were solved for the $M = 1100$, and — unless otherwise indicated — solutions for these mentioned equations are stable for $T \geq 0.5$ K. The numerical methods outlined in [13, 14] were employed in that instance.

3. Results and discussion

In the works concerning the study of the superconductivity phenomenon, a common approach is to use the Eliashberg formalism to determine the electron–phonon coupling and to determine the critical temperature [15–17]. In work [5], for $AuCu_3$-type intermetallic compounds, and between them $NaSn_3$, the Eliashberg spectral function was calculated, and the curve of this function is shown in Fig. 1.

The order parameter on the imaginary axis for specific temperature values is illustrated in Fig. 2. This parameter describes the amplitude of the energy gap in the electron spectrum at the Fermi level. Physically, Δ_m is related to the amount of energy needed to break up Cooper pairs (electrons paired together in the superconducting state). As can be seen, the order parameter diminishes with rising temperature (as presented for $T_0 = 0.5$ K to $T = 4.0$ K), and this diminishing is faster the higher the temperature.

The relationship between the order parameter and temperature is evident upon graphing the function $\Delta_{m=1}$ in the insertion placed in Fig. 2. In the Eliashberg theory of superconductivity, the order parameter $\Delta(\mathrm{i}\omega_n)$ is defined on the imaginary axis in terms of the Matsubara frequencies $\mathrm{i}\omega_n$. The first Matsubara frequency corresponds to $n = 0$, which means $\omega_0 = \pi/\beta$. The first Matsubara frequency $\mathrm{i}\omega_0$ is the dominant contribution to the dynamics of superconductivity because its value is associated with the lowest fermion energies in the system.

In Fig. 3, the dependency of specific heat on temperature for the normal and superconducting states is presented. In the normal state, this dependence increases linearly from temperature 0.5 to 10 K, reaching values from 0.5 meV for $T = 0.5$ K to about 12 meV for 7 K ($C/(k_\mathrm{B}\rho(0))$ [meV]). For the superconducting state, it increases nonlinearly, starting at temperature from 0.5 to 7 K, reaching values of 0.5 meV (for 0.5 K) up to 26 meV for 7 K. The

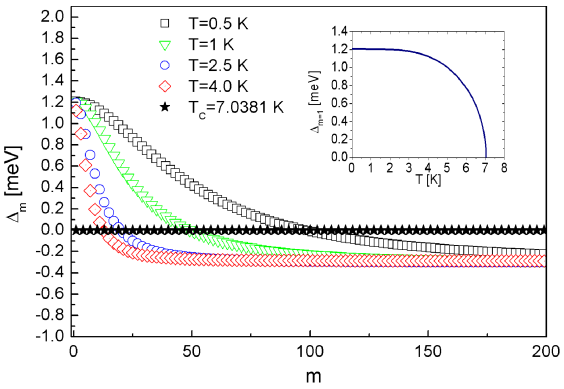

Fig. 2. The order parameter on the imaginary axis for selected temperature values. The insert shows the dependence of the order parameter for the first Matsubara frequency on temperature.

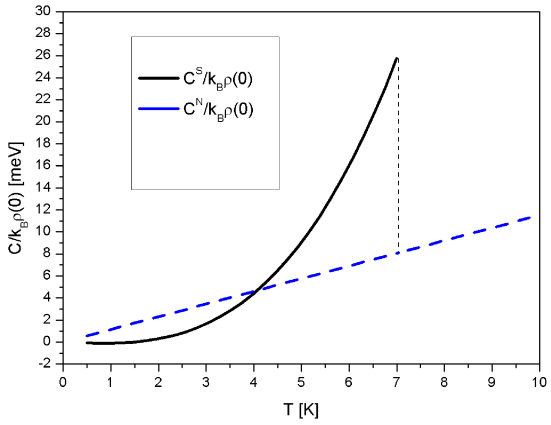

Fig. 3. Dependence of the specific heat of the superconducting and normal state on temperature.

linear increase in the specific heat in the standard state ($C/T \propto T$ in the range from 0.5 to 10 K) is typical for the electronic contribution to the specific heat observed in metals. This value increases linearly because the electron contribution is proportional to the temperature (related to the thermal excitement of electrons). For very low temperatures (e.g., 0.5 K), the specific heat is much smaller than in the normal state, which results from the existence of an energy gap in the superconductor. Electrons in Cooper pairs cannot be easily thermally excited, because this requires energy of at least $2\Delta(0)$, where $\Delta(0)$ is the value of the energy gap at absolute zero. At low temperatures (< 4 K), the specific heat in the superconducting state is smaller than in the normal state because Cooper pairs dominate and there are fewer thermally excited states. At temperatures approaching T_C (> 4 K), as the temperature increases, the energy gap decreases, and the contribution from electrons and phonons in the superconducting state increases dramatically. This leads to a situation where the specific heat in the superconducting state exceeds the normal state.

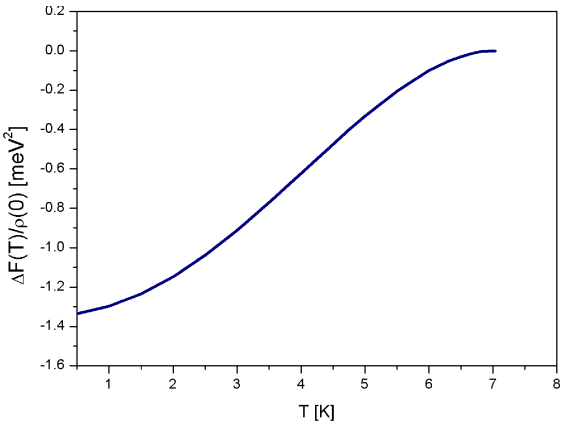

Fig. 4. Free energy difference between the superconducting and normal states as a function of temperature.

In Fig. 4, the difference in free energy of the superconducting and normal states as a function of temperature is shown. As can be seen, in the whole range, the value of free energy difference is negative. This negative value of $\Delta F(T)$ indicates that the superconducting state is thermodynamically more stable than the normal state up to that temperature. The maximum difference ($|\Delta F(T)|$ seen at low temperatures) reflects the energetic advantage of the superconducting state, which is proportional to the number of Cooper pairs formed and the binding energy. The point at which $\Delta F(T)$ reaches zero ($T = T_C$) defines the critical temperature of the second-order phase transition. At this point, the superconducting state becomes unstable and the material transitions to the normal state.

The calculated thermodynamic critical field $H_c(T)$ as a function of temperature is presented in Fig. 5. This relation describes the maximum value of the external magnetic field at which the superconducting state can exist in $NaSn_3$. At the critical temperature T_C, where $H_c(T) = 0$, the superconducting state becomes unstable. The free energy difference between the states disappears and the material transitions to the normal state.

In Fig. 6, the calculated wave function normalizing factor on the imaginary axis for studied temperature values is presented. The wave function renormalization factor describes the influence of electron–phonon interactions on the dynamics and properties of quasiparticles in a superconductor. In the context of the framework of the Eliashberg theory, this factor is a key indicator of the renormalization of the effective electron mass and the strength of electron–phonon interactions. Just as it was in the case of the order parameter, the function Z_m takes the highest value for $m = 1$. Throughout the analyzed temperature range, the wave function renormalization factor reaches relatively high values. These values of Z_m indicate the intensity of electron–phonon interactions at different ω_n

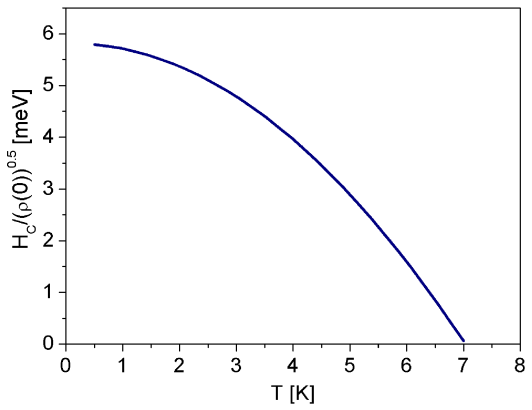

Fig. 5. Thermodynamic critical field as a function of temperature.

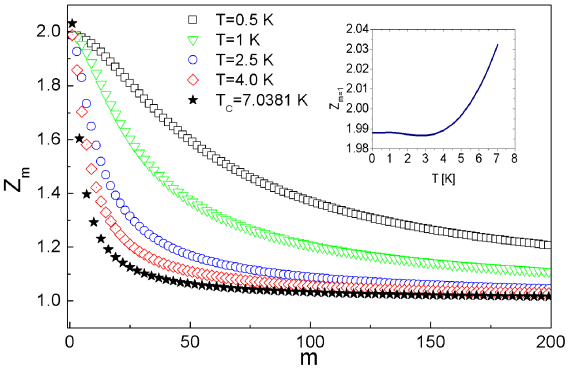

Fig. 6. The factor renormalizing the wave function for selected temperature values. The insert shows the dependence of the factor renormalizing the wave function for the first Matsubara frequency on the temperature.

frequencies. Higher values suggest that it is more difficult for electrons to move in the crystal lattice due to stronger coupling to phonons. The insertion in Fig. 6 presents the dependence of the renormalization factor of the wave function for the first Matsubara frequency on the temperature. This relationship provides information on the influence of electron–phonon interactions on electron dynamics. As can be seen in the graph, this dependence initially decreases slightly (up to 3.5 K) and then increases quite quickly and nonlinearly up to the critical temperature T_C.

At very low temperatures, the energy gap $\Delta(T)$ is close to its maximum value. Most electrons form stable Cooper pairs, and the number of thermally excited quasiparticles is very small. Fewer quasiparticle states are available for electron–phonon interactions, which temporarily reduces the value of $Z_{m=1}$. The number of thermal phonons (responsible for electron–phonon coupling) is very small, which may cause a temporary weakening of the renormalization effect visible in the insert. It is also possible that additional mechanisms (e.g., spin or electron–electron fluctuations) are emerging in the system, which at low temperatures partially compensate for the electron–phonon effect, causing a small decrease in $Z_{m=1}$.

4. Conclusions

In this study, the superconducting properties of $NaSn_3$ have been investigated using the Eliashberg formalism, focusing on the role of electron–phonon interactions in determining its superconducting state. The results indicate that $NaSn_3$ exhibits a relatively high critical temperature of 7.038 K, with a strong electron–phonon coupling, as evidenced by the calculated wave function renormalization factor and superconducting order parameter. The specific heat analysis confirms the thermodynamic stability of the superconducting state, while the computed thermodynamic critical field is consistent with the expected temperature dependence. Additionally, the free energy difference between the superconducting and normal states highlights the energetic advantage of the superconducting phase. These findings provide valuable insight into the mechanisms governing superconductivity in $NaSn_3$, contributing to the broader understanding of intermetallic superconductors and their technological potential.

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