

SOME PECULIARITIES OF NIOBIUM LATTICE DYNAMICS IN SUPERCONDUCTING TRANSITION REGION

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In order to understand the characteristic features of electron-phonon (e-ph) interaction and carrier coupling mechanism in cuprate high- T_c superconductors as well as to obtain useful scaling conditions it seems relevant to make a detailed analysis of lattice dynamics for the conventional metal superconductors in the critical transition region. We have chosen a niobium as the object of investigation since it is also a type II superconductor, it has the highest transition temperature ($T_c = 9.25$ K) among the metals and exhibits the hole conductivity. As is known, niobium possesses the body-centred cubic lattice with the unit cell including two atoms. This results in the appearance of an optical branch in the phonon spectrum along with the acoustic one [1].

A theoretical model of phonon spectrum with dispersion [2] is used for the description of thermodynamic properties of phonon subsystem of niobium without using fitting parameters. Characteristic frequencies of phonon spectrum have been determined from the experimentally measured lattice elastic constants and they have matched the resonant frequencies, obtained by the methods of neutron spectroscopy [3].

Analytical expressions for the generalized and partial phonon densities of states are derived, thus enabling one to calculate the complete set of phonon thermodynamic functions. Numerical calculations of the phonon heat capacity have been accomplished and the contribution of acoustic and optical lattice vibrations has been studied in wide temperature range 0-250 K. Using the phonon heat capacity thus calculated, the unambiguous contribution of the carrier subsystem to the measured heat capacity of niobium has been reconstructed.

Then we have calculated the average values of frequency, wavelength, wave vector, phase and group velocities, effective mass of the acoustic and optical phonons as a function of temperature. The corresponding quantities, determined for the phonon subsystem of niobium in the superconducting transition region ($T \approx T_c$) are presented in the Table:

T=7-9 K	frequency ω , meV	wave- length λ , Å	wave vector k , cm ⁻¹	phase velocity v , cm/s	group velocity $ u $, cm/s	effective mass $ m_{eff} /m_e$
Acoustic branch	1.6-2.1	220-280	$(2.2-2.9) \times 10^6$	6×10^5	6×10^5	2500-3100
Optical branch	17.5	14	4.5×10^7	6×10^5	4×10^5	160

The main results derived for the niobium in critical region are as follows:

- 1) mean wavelength of the heat acoustic phonons is close to the coherence length value $\xi_0 \approx 250$ Å;
- 2) the equality of the acoustic and optical phonon phase velocities is obtained, that corresponds to the condition of phase resonance with energy exchange among the different branches of lattice vibrations. It can lead to the generation of additional harmonics with the frequencies $\omega = \omega_{bp} + \omega_{ac}$, belonging to the optical branch of phonon spectrum, as well as influence the e-ph interaction.

1. N.B.Brandt, S.M.Chudinov, Electrons and phonons in metals, Moscow, MSU, 1990, 335 p.
2. I.N.Kudryavtsev, Report on XII Trilateral German-Russian-Ukrainian Seminar on HTS, 25-29 October 1999, Kiev, Ukraine.
3. Y. Nakagawa, A.D.B.Woods, Phys. Rev. Lett. **11** (1963) 271.