Research Article

Calculated Changes in the Elastic Properties of MgCNi_3 at the Superconducting Transition

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Received 29 November 2012; Accepted 8 January 2013

Academic Editor: Mark Blamire

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We calculated the elastic properties of MgCNi_3 at the superconducting transition (T_c) using various thermodynamic and acoustic data. From the calculations, a step discontinuity of 8 ppm in the bulk modulus, 7 ppm in the Young's modulus, and 3 ppm in the longitudinal sound velocity (v_l) is expected at T_c . The step discontinuities at the transition temperature indicated the importance of lattice changes to the superconducting mechanism of MgCNi_3 . The Debye temperature was calculated to be 460 K. The electron-phonon coupling constants calculated in the weak and strong coupling limits of the BCS theory and the van Hove scenario showed that MgCNi_3 is a moderately strong coupled superconductor.

1. Introduction

Superconductivity in MgCNi_3 with transition temperature (T_c) near 8 K is of interest especially from the pairing mechanism point of view. The electron-phonon coupling constant of MgCNi_3 has been determined using specific heat measurements [1]. Evidence of strong electron-phonon coupling and the van Hove type singularity in the electronic density of states near the Fermi energy has also been suggested [2].

The nature of superconductivity in this material is still controversial. A step discontinuity in the longitudinal sound velocity indicating lattice softening has been observed in the conventional superconductors. Thus, information on the lattice properties at T_c is very useful in understanding the MgCNi_3 superconductor. The acoustic method is a sensitive probe of phonon states and electron-phonon coupling in materials. The elastic properties of MgCNi_3 have also been reported [3, 4].

The objectives of this work were to estimate the electron-phonon coupling constant, changes in the elastic properties, and sound velocity at the transition temperature of MgCNi_3 . The elastic properties of MgCNi_3 including the change in the bulk and Young's moduli and discontinuity in the longitudinal sound velocity at T_c were calculated using various sound velocity and thermodynamic data. The acoustic Debye

temperature was also calculated and compared to reported values determined by other methods. The electron-phonon coupling constant in various scenarios is also reported.

2. Basic Formulation

The standard isotropic elastic medium approximation can be applied to the polycrystalline samples. In this case, two independent elastic moduli, namely, the shear modulus G can be written as $G = \rho v_s^2$, and the bulk modulus B can be written as $B = \rho v_l^2 - (4/3)\rho v_s^2$, where ρ is the mass density, v_s is the shear velocity, and v_l is the longitudinal velocity [5]. The longitudinal modulus can be written as $L = \rho v_l^2$, and the Young's modulus is $Y = G(3L - 4G)/(L - G)$.

For the superconducting transition in zero fields, the thermodynamics of second-order phase transition [6, 7] gives the following anomalies:

$$\frac{\Delta B}{B} = -\frac{\Delta C_p}{T_c} B \left(\frac{\partial T_c}{\partial P} \right)^2, \quad (1a)$$

$$\frac{\Delta Y}{Y} = -\frac{\Delta C_p}{T_c} Y \left(\frac{\partial T_c}{\partial \sigma_i} \right)^2, \quad (1b)$$

where σ_i is the i th component of the stress, ΔC_p is the discontinuity in specific heat at T_c , and P is the pressure. B

TABLE 1

Sample	T_c (K)	v_l (m s ⁻¹)	v_s (m s ⁻¹)	θ_D (K)	$\Delta B/B$ (ppm)	$\Delta v_l/v_l$ (ppm)	$\Delta Y/Y$ (ppm)
MgCNi ₃ (this work)	8	7980	4800	460	8	3	7
LaFeAsO _{0.89} F _{0.11} [16]	26	5090	2900	367	16	5	—
MgB ₂ [19]	39	9650	5070	880	66	21	76
LaOFeP [20]	5.8	7980	4800	491	59	15	101
LiFeAs [20]	18	8250	4820	509	25	7	38

is expected to show a step discontinuity, and G is supposed to show a change in the slope at T_c from the mean-field transition [6]. The change in B can be written as

$$\frac{\Delta B}{B} \approx \frac{v_l^2 (2\Delta v_l/v_l) - (4/3) v_s^2 (2\Delta v_s/v_s)}{v_l^2 - (4/3) v_s^2}. \quad (2)$$

3. Results and Discussion

Several papers have reported the elastic moduli of MgCNi₃ [3, 4, 8] with a considerable spread in values. Because this material is usually prepared in the polycrystalline form, in this paper, we have used values for polycrystalline form as reported by Shein et al. [3]. Using bulk modulus $B = 171.05$ GPa, shear modulus of $G = 61.46$, and Young's modulus $Y = 168.16$ GPa as published previously [3], the longitudinal sound velocity was calculated to be $v_l = 6270$ m/s and shear sound velocity $v_s = 3100$ m/s.

The sound velocities can be used to calculate the acoustic Debye temperature by using the standard formula $\theta_D = (h/k_B)(3N/4\pi V)^{1/3} v_m$, where h is the Planck's constant, k_B is the Boltzmann's constant, N is the number of mass-point, V is the atomic volume, and v_m is the mean velocity given by $3/v_m^3 = 1/v_l^3 + 2/v_s^3$. Using this expression, the acoustic Debye temperature of MgCNi₃ is calculated to be 460 K. This is near to the θ_D values calculated theoretically [4, 8, 9] but much higher than the value determined from specific heat measurement [10, 11].

The BCS theory for weak coupling gives $T_c = 1.13\theta_D e^{-1/\lambda}$, where λ is the electron-phonon coupling. The electron-phonon coupling constant for the weak coupling case calculated using the previous acoustic Debye temperature is $\lambda = 0.25$.

The relevance of van Hove density of states has been suggested for MgCNi₃ [2]. The singularity in the density of states at the Fermi level was taken into account in the van Hove scenario of a two-dimensional system. In this scenario, T_c is given as $T_c = 2.72T_F e^{(-1/\sqrt{\lambda})}$, where $T_F = E_F/k \approx 10\theta_D$ (E_F is the Fermi energy) [12]. The electron-phonon coupling constant calculated using this formula is $\lambda = 0.018$.

The McMillan expression for the strong coupling BCS case is given as [13] $T_c = (\theta_D/1.45) \exp[-1.04(1 + \lambda)/(\lambda - \mu^*(1 + 0.62\lambda))]$, where μ^* (with conventional values of 0.05–0.1) is the screened Coulomb repulsion between electrons in a Cooper pair. The electron-phonon coupling constant derived from this expression ranged from 0.49 to 0.59. This is consistent with most measured values for MgCNi₃

[1, 10]. Thus, this material is a moderately strong coupled superconductor.

The following is a discussion on the elastic properties of MgCNi₃ at T_c . Using (1a), $\Delta C_p/T_c = 66$ mJ/mol K² [10], and $\partial T_c/\partial P = 0.15$ K/GPa [14], the calculated step discontinuity in the bulk modulus is 8 ppm. Using (2), the discontinuity in the longitudinal velocity is 3 ppm. By assuming that $\partial T_c/\partial \sigma_i \approx \partial T_c/\partial P$, the expected discontinuity in the Young's modulus calculated using (1b) is 7 ppm. These discontinuities are similar to Pb [15] and LiFeAsOF [16] superconductors but are much smaller than the calculated [17] and observed [18] values in the cuprate-based high T_c superconductors and MgB₂ [19]. Table 1 shows the sound velocity and changes in bulk and Young's modulus at T_c of MgCNi₃ and other superconductors.

The second-order phase transition does not allow step discontinuity in the shear velocity at T_c in zero fields; hence, the shear velocity was assumed continuous at T_c . In these calculations, the thermodynamic data used are representative of the various reported values, which are of the same order of magnitude. The expected step discontinuity in the longitudinal velocity in MgCNi₃ is similar to the measured value of Pb which is a BCS-type superconductors and are within the resolution range of most ultrasonic apparatus. Our calculations showed that MgCNi₃ is a moderately strong coupled BCS-type superconductor.

Acknowledgments

The author thanks Dr. W. Kong (KLIUC) for the assistance. This work has been supported by the Ministry of Higher Education of Malaysia (Grant no. ERGS/1/2011/STG/UKM/01/25) and Universiti Kebangsaan Malaysia under Grant no. DIP-2012-32.

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