Thermodynamic Properties of SmCu₂

J. Vejpravová a,1, P. Svoboda a, M. Rotter b, M. Doerr b, M. Loewenhaupt b

a Charles University, Dept. of Electronic Structures, Ke Karlovu 5, 1221 16-Praha 2, The Czech Republic
b IAPD, TU Dresden, D-01062 Dresden, Germany

Abstract

SmCu₂ intermetallic compound crystallizes in the orthorhombic CeCu₂-type structure (space group Imma) and orders antiferromagnetically (AF) below the Néel temperature \( T_N = 23 \text{ K} \). A high-quality single crystal of SmCu₂ was grown and the temperature dependence of specific heat was measured in the low-temperature region to determine the magnetic phase transitions. The detailed analysis of SmCu₂ specific heat data in the low-temperature region was performed in comparison with that of non-magnetic analogues LuCu₂ and YCu₂.

Key words: rare-earth intermetallic compounds; magnetic phase transitions; specific heat

1. Introduction

The series of orthorhombic intermetallic compounds \( R\text{Cu}_2 \) (\( R = \) rare earth metal) has attracted new attention within last years and are systematically investigated namely due to their unusual magnetoelastic behavior - the so-called conversion of the Ising axis [1]. Almost all of them order AF and exhibit a variety of different AF phases in the ordered state [2]. Here we present the detailed study of the specific heat of SmCu₂ (magnetically ordered) in comparison with that of YCu₂ and LuCu₂ (its non magnetic analogues). The aim of this work was to extract the acoustic and optical phonon parts for all the three investigated compounds as well as the magnetic contribution to the specific heat of SmCu₂. This can show the similarity of the phonon spectra within the isostructural \( R\text{Cu}_2 \) series and to show the convenience of the comparative analysis of the specific heat, namely in the case when large contribution to the specific heat from frequent magnetic phase transitions is present.

2. Experimental Results and Discussion

All the compounds were prepared by arc melting from high purity constituents under the protective Ar-atmosphere. The single crystal of SmCu₂ was then grown by Czochralski pulling method, for details see [4]. Homogeneity and stoichiometry of all prepared compounds were checked by microprobe and powder X-ray diffraction. This analysis did not reveal any foreign phase. The lattice parameters and the atomic positions yielded by the Rietweld analysis are in a good agreement with the published values [5]. The residual resistivity ratios \( RRR = 175, 155 \text{ and } 78.5 \) along \( a, b \) and \( c \) axes, respectively, point to the high quality of the grown crystal.

The specific heat measurements were performed on PPMS using the relaxation method [6] in the temperature range \( T = 1.5 - 300 \text{ K} \) in zero magnetic field. We have not observed any anomalies on the specific heat of nonmagnetic compounds YCu₂ and LuCu₂. Four sharp peaks corresponding to the Néel temperature and to additional order-to-order magnetic phase transitions were detected on SmCu₂ at temperatures \( T = 22.3, 17.7, 16.4 \text{ and } 3.7 \text{ K} \) (see the inset of Fig. 1).

The analysis of the phonon specific heat - including both the Debye and the Einstein models as well as

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1 Corresponding author. E-mail: jana@mag.mff.cuni.cz

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the correction on the anharmonic contribution to the phonon spectrum (for details see [3]) - had substantially improved the fit of the phonon specific heat of nonmagnetic YCu$_2$ and LuCu$_2$. The acoustic part and the optical branches of the phonon spectrum are described by the Debye $\theta_D$ and the Einstein $\theta_E$ temperatures, respectively.

From the electronic part of the specific heat we have obtained the $\gamma$-values as 8.2, 5.7 and 6.0 mJ/molK$^2$ for YCu$_2$, LuCu$_2$ and SmCu$_2$, respectively.

Their respective Debye temperatures and anharmonic corrections are then $\theta_D = 156$, 145 and 148 K and $\alpha_D = 2.9$, 0.8 and $2.2 \times 10^{-4}$ K$^{-1}$). The 6 optical branches of each phonon spectrum were described by a superposition of 2-times degenerated Einstein branches of each phonon spectrum were described by the Debye $\theta_D$ and the Einstein $\theta_E$ temperatures, respectively.

The magnetic contribution (caused by crystal field (CF) and magnetic phase transitions) to the specific heat of SmCu$_2$ (CF) and magnetic phase transitions) had significantly improved our understanding of the thermodynamic properties of the $RCu_2$ series.

As expected, the characteristic parameters of both the phonon and the electronic part do not substantially differ through the investigated series. This result, in agreement with [7] allows us to use the YCu$_2$ and LuCu$_2$ compounds as nonmagnetic analogues for the comparative analysis of the specific heat of other $RCu_2$. In comparison with [4] we have to say, that the full phonon spectrum analysis of the SmCu$_2$ had improved the fit, namely decreasing the $\gamma$ value of the electronic part, while the magnetic part remain roughly unchanged.

The magnetic contribution (caused by crystal field (CF) and magnetic phase transitions) to the specific heat of SmCu$_2$ was obtained using the comparative analysis. The CF level scheme is then described by the energy gap $\Delta_i$ of the excited level from the ground state. The fit of the Schottky contribution gives the positions of the three Kramer’s doublets of Sm$^{3+}$ as: $\Delta_1 = 100$ K and $\Delta_2 = 120$ K.

The deduced saturated magnetic entropy (see Fig. 1) then corresponds well to the theoretical value which is $R \ln(2J + 1)$. ($R$ is the gas constant and $J$ means the total angular momentum of the Sm$^{3+}$ ion). We may conclude that such detailed approach to the specific

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<tr>
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<th>YCu$_2$</th>
<th>LuCu$_2$</th>
<th>SmCu$_2$</th>
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<td>$\theta_E$ (K)</td>
<td>166</td>
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<td>265</td>
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<td>2.9</td>
<td>2.9</td>
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</tbody>
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References