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STRUCTURAL PROPERTIES OF REM_2Sn_2 (RE = La, Ce and M = Ni, Cu)

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The lattice parameters a and c of CeM_2Sn_2 show an anomalous temperature dependence compared to the analogous variations for LaM_2Sn_2. The anomaly Δa of thermal expansion for $CeCu_2Sn_2$ has a maximum around 90 K, whereas Δc has a maximum near 140 K, near to the maximum of the magnetic resistivity $\Delta\rho$.

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1. Introduction

Numerous rare earth (RE)–transition metal (M) intermetallics with the composition REM_2X_2 crystallize with the $CaBe_2Ge_2$ tetragonal structure (space group $P4/nmm$). A large number of compounds with Si and Ge has been studied. More recently, stannides with the same structure have been prepared. One main goal of investigations in these series is to study the influence of the transition metal on the magnetic interactions between rare earth or on the hybridization state of Ce compounds. In the following, we present structural properties of La and Ce stannides with Cu and Ni.

Two crystallographic phases have been identified for $CeNi_2Sn_2$, the parent tetragonal structure and a monoclinic variant [1]. $CeNi_2Sn_2$ is found to be a heavy fermion system with a γ value of 0.6 J/mole K^2. It orders antiferromagnetically at 2.2 K, exhibits a maximum of resistivity at 9 K and a minimum at 30 K.

$CeCu_2Sn_2$ belongs to the tetragonal structure; Ce has a smaller hybridization than in the former compound. It orders at 2.1 K and does not exhibit any resistivity minimum; however, its magnetic resistivity passes through a maximum at about 100 K.

2. Crystallographic properties

All measurements at different T were performed with the X-ray powder diffractometer using Fe K_α radiation. To obtain the profile of a line at room temperature and below, every reflection was measured by a scan method in which the counter moved in steps of 0.01° and the counting time for every point was 10 s. Next, the measured intensity lines were approximated by the Pearson function of the type [2]:

$$I_i(\text{calc}) = \sum_k I_{0k} \left[1 + (2^{1/m_k} - 1) \left(\frac{2\Theta_{0k} - 2\Theta_i}{\Delta_k/2} \right)^2 \right]^{-m_k}$$

where I_{0k} is the maximum intensity at $2\Theta_{0k}$ for each of the k lines in the region of overlap, $2\Theta_{0k}$ is the calculated position of the Bragg peak corrected for the zero-point shift of the counter, Δ_k is the half width at half height, m_k is the shape factor.

The best results were obtained within the interval $1 < m < 2$. For the $K_{\alpha 1}$ profile the intensity was a half of the value for the $K_{\alpha 1}$, whereas all other parameters were the same as used in $K_{\alpha 1}$ profile.

Pearson-type distributions were fitted to the experimental profiles by a least squares method. The best fit to the shape of every (hkl) line with deviation less than 10% was obtained. The lattice parameters a and c of $CeCu_2Sn_2$ show an anomalous temperature dependence comparing with the analogous temperature

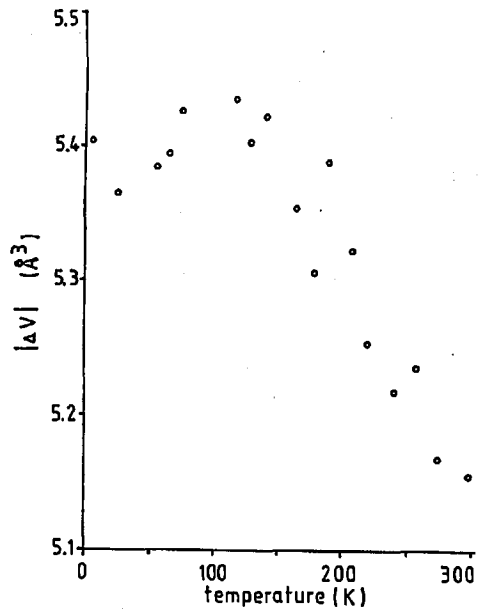

Fig. 1. Volume anomaly of $CeCu_2Sn_2$ as a function of temperature.

dependence of $LaCu_2Sn_2$. These anomalies are clearly seen in the plots of $|\Delta a| = |a(CeCu_2Sn_2) - a(LaCu_2Sn_2)|$ and $|\Delta c| = |c(CeCu_2Sn_2) - c(LaCu_2Sn_2)|$ vs. T.

We observe an anisotropy of lattice thermal expansion of $CeCu_2Sn_2$. $|\Delta a|$ shows a maximum around $T = 90$ K but $|\Delta c|$ shows a maximum at $T = 140$ K. We note also that volume increment $|\Delta V| = |V(CeCu_2Sn_2) - V(LaCu_2Sn_2)|$ plotted vs. T (Fig. 1) is proportional to resistive increment $\Delta\rho = \rho(CeCu_2Sn_2) - \rho(LaCu_2Sn_2)$ [1].

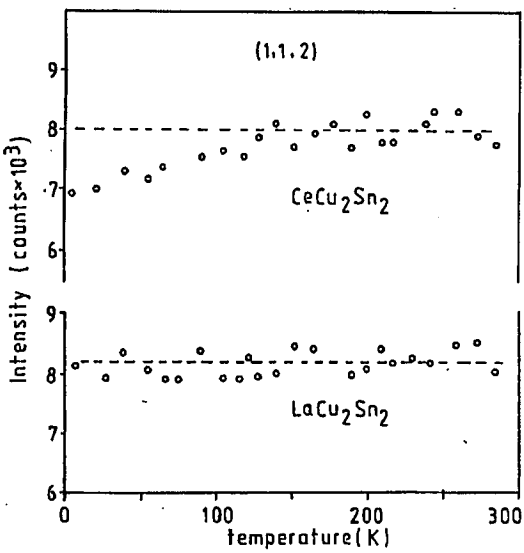

Fig. 2. Intensity of the Bragg line (1,1,2) for Ce and La compounds as function of temperature.

In Fig. 2 we show the temperature dependence of the Bragg (1,1,2) line intensities I of $CeCu_2Sn_2$ and $LaCu_2Sn_2$. Here a weak temperature change of the intensity of X-ray diffraction line for a small diffraction angle is expected. The intensity of (1,1,2) Bragg's line of $LaCu_2Sn_2$ (Fig. 2) nearly does not depend on temperature, however, comparing this I–T plot with the $I(T)$ dependence of $CeCu_2Sn_2$ of the same (h,k,l) Bragg reflection one clearly sees an anomalous decrease in the intensity of the line for Ce-compound below ≈ 130 K. This result correlates with the abnormal lattice parameters temperature dependencies and with the abnormal $\Delta\rho(T)$ of $CeCu_2Sn_2$.

3. Discussion

Anomalous behaviour of thermal expansion has been observed in several heavy fermion systems. For instance, a negative thermal expansion may occur at very low temperatures (i.e. in $CeCu_6$ [3]), which is explained within the Fermi liquid model. The present anomalies occur at higher temperatures, but are believed to be related to cerium hybridization.

First, the Kondo behaviour or mixed-valent character of Ce may result in a difference in cohesion energy and Debye temperature between La and Ce compounds. We also remark that the maxima of Δa and Δc occur in a temperature range close to the maximum of magnetic resistivity, which is a temperature representative of crystal field splitting and where also lattice correlations between Ce sites begin to set up.

The temperature dependence of some Bragg intensities was found anomalous for $CeCu_2Sn_2$, which implies a strong change in the structure factor. Such change may arise from variations in the Ce scattering factor, in the Debye–Waller factors, or may be due to the shifts of atomic positions in the cell as well as to an incipient distortion of the cell, as observed in $CeNi_2Sn_2$ and $CePt_2Sn_2$ [4]. These phenomena are linked to Ce atomic volume which is a function of valency, and possibly to some redistribution of the electronic density due to the anisotropy of the ground state wave function. All these modifications in the $4f$ configuration are strongly correlated to the lattice cohesion, and may explain the different behaviours of $LaCu_2Sn_2$ and $CeCu_2Sn_2$.

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