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Magnetic ordering of $CeNi_{0.78}Sn_2$ and $Ce_3Ni_2Sn_7$ compounds by neutron diffraction

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Abstract

The magnetic ordering of the orthorhombic $CeNi_{0.78}Sn_2$ and $Ce_3Ni_2Sn_7$ compounds has been studied by neutron diffraction. $Ce_3Ni_2Sn_7$ has two Ce sites of distinct symmetry. Only the Ce2 moments with a trigonal prism arrangement were found to order below $T_N=3.8$ K with a collinear antiferromagnetic moment arrangement along the *a*-axis associated with the wave vector $q=(0,1,0)$. At 1.5 K the ordered moment value is $1.9(1)\mu_B$/Ce atom. The compound $CeNi_{0.78}Sn_2$ with a single Ce site but with a similar trigonal prism arrangement as $Ce_3Ni_2Sn_7$ was found to order at 1.5 K with two coexisting magnetic phases in equal amounts. One of these is ferromagnetic $T_C=2.3$ K while the other phase is a transversal sine wave modulated phase with $q_2=(0q_y0)$ ordering at $T_N=4.0$ K. The ordered magnetic moment value/amplitude at 1.5 K in both phases is $2.0\mu_B$/Ce atom and points to the same direction along *c*. The observation of two magnetic phases so far observed in several off stoichiometric phases of the $CeNi_xSn_2$system is attributed to the concentration fluctuations associated with the Ni deficiency.

Keywords: Rare earth alloys; Phase diagram; Thermodynamic modelling

1. Introduction

The Ce–Ni–Sn systems were reported [1,2] to comprise a wealth of binary and ternary crystal structures with interesting magnetic properties, which are connected to the valence instability displayed by Ce. In recent investigations our interest was focused on the $CeNi_xSn_2$ type of compounds which form a range of solid solutions characterized by a different degree of Ni deficiency with the upper limit of x as 0.74 [3]. The prototype structure $CeNiSn_2$ [1,4] (*Cmcm* space group $a=4.485$ Å, $b=17.74$ Å, $c=4.513$ Å, $Z=4$) comprises a single Ce site with a trigonal prismatic arrangement. The magnetic properties on the basis of specific heat and magnetic susceptibility measurements for the apparently stoichiometric $CeNiSn_2$ compound reveal two magnetic transitions [5]. The first transition to an antiferromagnetic phase (labelled II in [5]) occurs at $T_N^{II}=3.9$ K, and the second one to another antiferromagnetic phase (labelled I) at $T_N^{I}=3.2$ K, similarly to the isomorphic $CeNiGe_2$ compound. From plots of unit cell volumes vs. atomic number of the lanthanides for the $RNiGe_2$ and $RNiSn_2$ series both Ce compounds show no anomaly indicating a valence fluctuation.

Previously we have studied the magnetic properties of a sample of nominal composition $CeNiSn_{2.1}$ by magnetization measurements and neutron diffraction [6]. The refinements of the neutron data have shown that this compound is Ni-deficient $CeNi_{0.840(4)}Sn_2$ and that the sample contains a small amount of Ni_3Sn_2. Surprisingly, at 1.5 K two coexisting magnetic phases were observed in equal amounts. One of these is ferromagnetic with $T_C=3$ K. The other phase is an antiferromagnetic modulated phase described by a wave vector $(0q_y0)$ with a temperature variable length which at 1.5 K locks-in at the commensurate value $1/3b^*$ and the modulated structure squares up. The 1.5 K magnetic phase was described by us as an antiphase domain structure with two amplitudes as the third harmonic (010) could be observed. Subsequent studies [7] on the interdependence of magnetic properties and Ni content in the system $CeNi_xSn_2$, led to a generali-

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zation of this mictomagnetic behavior. The compound $CeNi_{0.75}Sn_2$ investigated by means of measurements of the specific heat, the magnetization, the a.c. and d.c. susceptibility [7] was found to undergo two magnetic phase transitions at 4.0 K and 2.3 K. It was of interest to study the nature of these transitions in the light of the low-temperature neutron diffraction results obtained for the more Ni-rich samples. The structure of the second orthorhombic (*Cmmm*) compound of this investigation $Ce_3Ni_2Sn_7$ displays a resemblance with the $CeNi_xSn_2$ compounds as it comprises two Ce sites one of which has the same Ce trigonal prism arrangement centered by Sn atoms while the other Ce site is located at the center of a [Sn12] cubooctahedron also found in the $CeSn_3$ and Ce_3Sn_7 compounds [8–10]. The Ce atoms residing in this latter position in both compounds were found to have an intermediate valence state and do not show magnetic order. $Ce_3Ni_2Sn_7$ orders antiferromagnetically below $T_N = 3.8$ K [10].

2. Experimental procedures and results

The investigated powder sample of nominal composition $CeNi_{0.75}Sn_2$ is the same as used in [8], prepared by arc melting followed by vacuum annealing at 800°C for 3 weeks. In order to suppress Ni–Sn impurity phases as far as possible the nominal composition was $CeNi_{0.75}Sn_{1.9}$

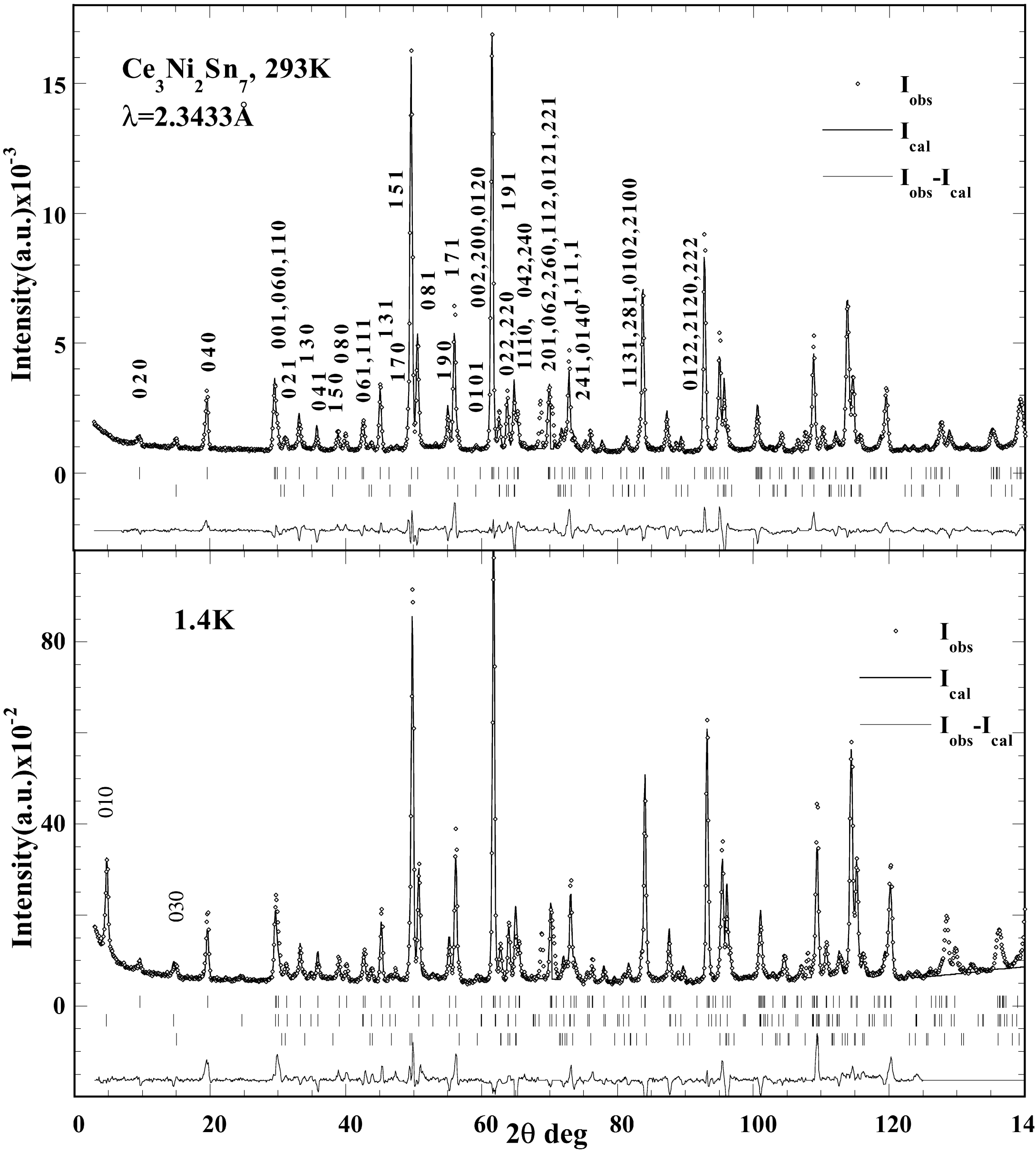

Fig. 1. Observed and calculated HR (G42 instrument) neutron patterns of $Ce_3Ni_2Sn_7$, in the paramagnetic state at 293 K (top part) and the magnetically ordered state at 1.4 K (bottom part). The sample contains 6% of $CeNi_{0.7}Sn_2$ impurity phase, which does not order down to 1.4 K.

Table 1
Crystal and magnetic structure refinement results of $Ce_3Ni_2Sn_7$ from high-resolution (G42: 293 K and 1.4 K) neutron data and high-flux (G4.1: 10 K and (1.5–10 K)) data

Atom site	293 K G42				1.5 K G42		10 K G4.1	1.5–10 K
	x	*y*	*z*	*occ*	*y*	$\mu_x[\mu_B]$	*y*	$\mu_x[\mu_B]$
Ce1 *2c*	0.5	0.0	0.5	1.0	0.0	0.0	0.0	0.0
Ce2 *4i*	0.0	0.1872(2)	0.0	1.0	0.1856(3)	1.8(1)	0.1827(5)	1.89(1)
Ni *4j*	0.0	0.3717(1)	0.5	0.864(4)	0.3715(2)		0.3713(3)	
Sn1 *2a*	0.0	0.0	0.0	1.0	0.0		0.0	
Sn2 *4i*	0.0	0.4106(2)	0.0	1.0	0.4118(3)		0.4129(4)	
Sn3 *4j*	0.0	0.0896(2)	0.5	0.908(8)	0.0904(3)		0.0910(4)	
Sn4 *4j*	0.0	0.2821(2)	0.5	1.0	0.2833(3)		0.2839(5)	
a [Å]	4.5683(3)				4.5504(4)		4.5562(4)	
b [Å]	27.323(1)				27.216(1)		27.219(2)	
c [Å]	4.5718(3)				4.5538(4)		4.5522(4)	
B $[Å]^2$	3.08(6)				0.68(8)		0.0	
R_n, R_m%	6.9, −				9, 15		6.6, −	−, 17
R_{wp}, R_{exp}	16.6, 4.5				20, 5		17.2, 1.7	17.1, 5

Space group *Cmmm* with R_n, R_m, R_{wp}, R_{exp} are the residuals for the integrated nuclear and magnetic, the weighted profile and the experimental intensities. $\mu_x[\mu_B]$ is the refined moment value.

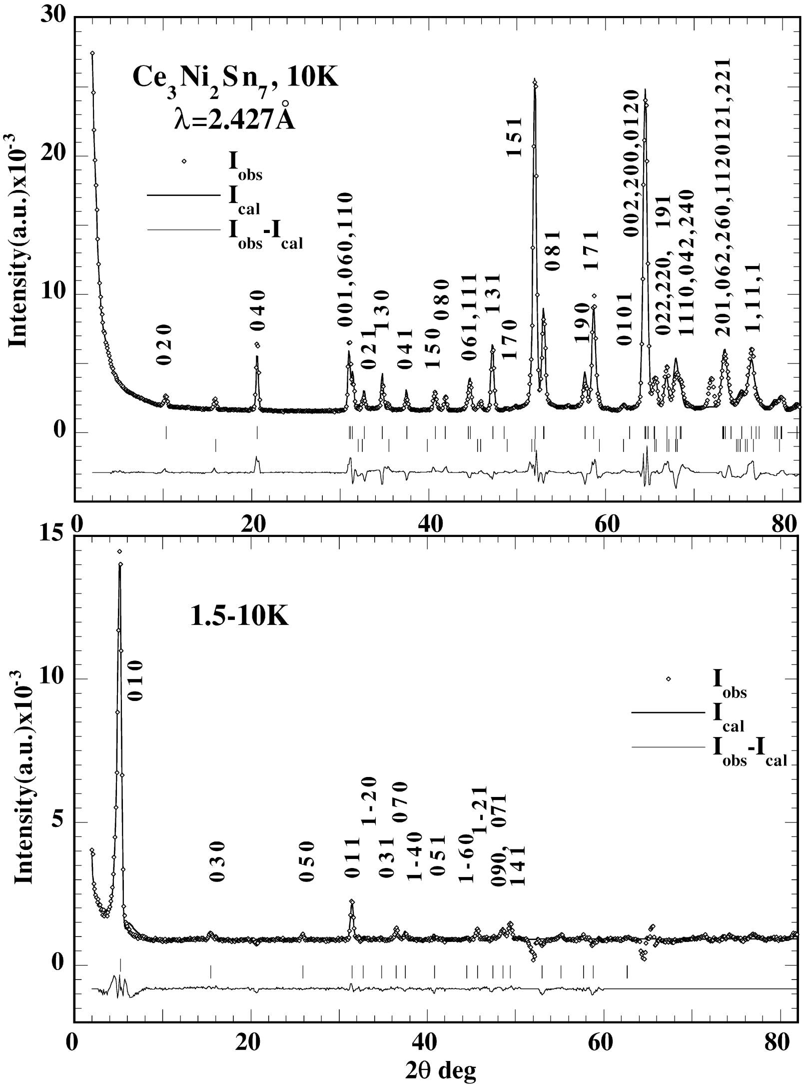

Fig. 2. Observed and calculated (G4.1 instrument) neutron patterns of $Ce_3Ni_2Sn_7$, in the paramagnetic state at 10 K (top part). In the difference diagram pertaining to the magnetically ordered state, 1.5 K–10 K, only magnetic reflections are visible (bottom part).

while the actual composition derived from EPMA analysis was $x=0.77$ and from neutron diffraction (at 293 K), $x=0.780(4)$, as will be further discussed below. In the following the refined composition $CeNi_{0.78}Sn_2$ on the basis of neutron data will be used. The $Ce_3Ni_2Sn_7$ compound was prepared in the same way but it was annealed at 800°C only for 2 weeks.

2.1. Neutron diffraction

Neutron diffraction experiments of $Ce_3Ni_2Sn_7$ were carried out in the temperature range 1.5–293 K at the facilities of the Orphée reactor (LLB-Saclay). The data were collected on the G42 (high resolution: HR 70 detectors with Sollar collimators) and the G4.1 (800-cell Position Sensitive Detector: PSD) diffractometers using the wavelengths of 2.3433 Å and 2.426 Å, respectively. The step increment in 2θ was 0.1°. The G4.1 data were collected in the 2θ region 2–81° for a full set of temperatures in the range 1.5–10 K in steps of 0.3 K in order to study more precisely the magnetic transitions. The G42 data were collected in the 2θ region 2–170° for structural refinements. The $CeNi_{0.78}Sn_2$ neutron data were collected at the temperatures 1.5, 3 and 10 K at the facilities of the ILL in Grenoble with the D1B (double axis multicounter diffractometer, $\lambda=2.52$ Å in the 2θ range 1–81° with the step 0.2°). The data were analysed with the program FullProf [11].

2.1.1. Crystal structure of $Ce_3Ni_2Sn_7$

The refinement of the diffraction pattern of $Ce_3Ni_2Sn_7$ collected in the paramagnetic state at 293 K has shown that

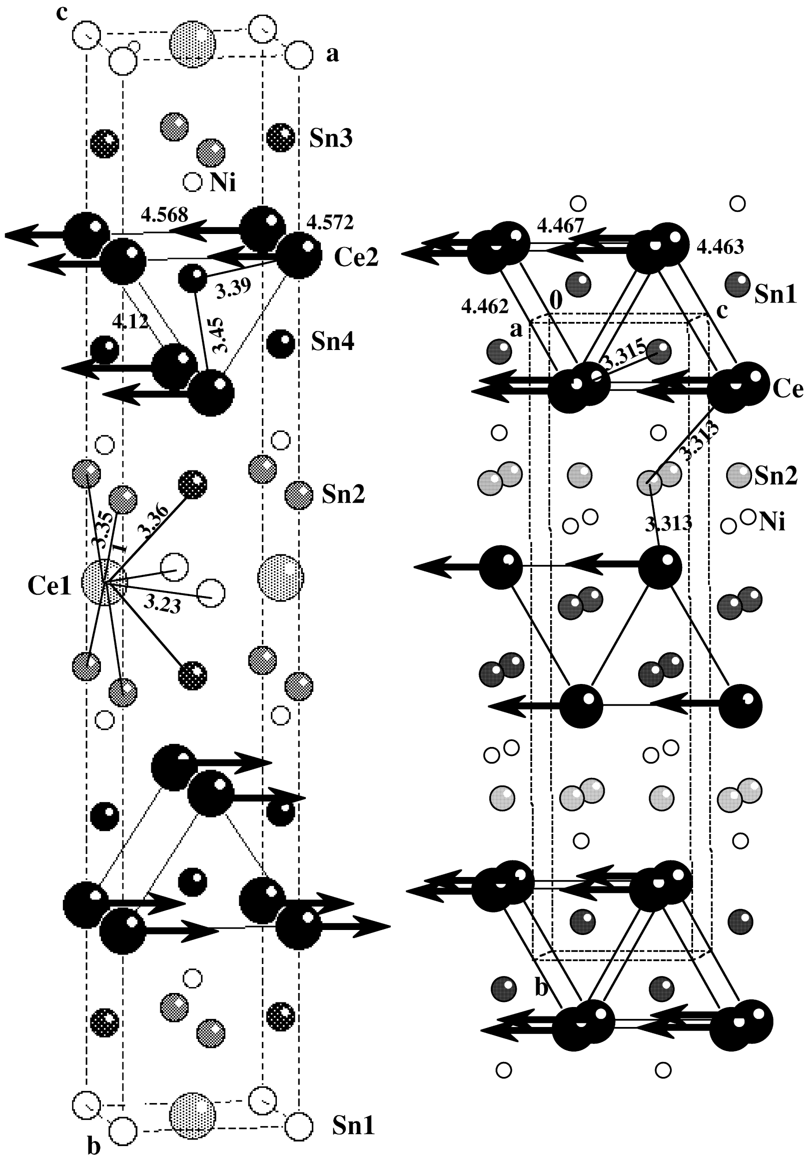

Fig. 3. Schematic representation of the $Ce_3Ni_2Sn_7$ magnetic structure with exclusively ordering of the Ce2 moments with the trigonal prism arrangement (left part). Also shown is the ferromagnetic Ce moment arrangement in $CeNi_{0.78}Sn_2$ with the same orientation relatively to the trigonal prisms (right part).

the sample contains a small amount of two impurity phases. One of the impurity phases (about 6%) was identified as $CeNi_{0.7}Sn_2$ and was included in the refinements (*Cmcm* space group, $CeNiSi_2$ structure-type $a=4.487$ Å, $b=17.67334$ Å, $c=4.480$ Å). This phase orders magnetically below 1.5 K. The second phase was not identified and the two non-overlapping reflections at 2θ 68.5° and 71° were excluded from the refinements. Results are summarized in Fig. 1 and in Table 1 and confirm the $Ce_3Ni_2Sn_7$ structure [2,8]. However the refinement has indicated that there is some Ni and Sn deficiency corresponding to the composition $Ce_3Ni_{1.72}Sn_{6.81}$ as the profile factor improved by 5% when the occupation parameters for those sites were refined.

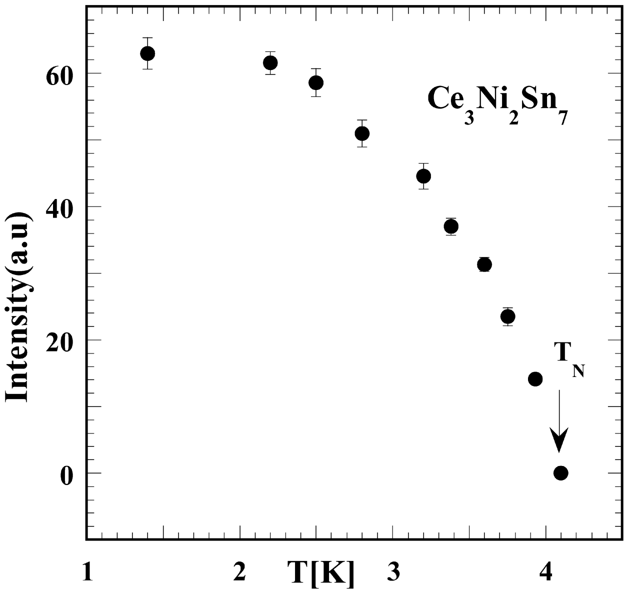

Fig. 4. Thermal variation of the magnetic intensity of the (010) reflection of $Ce_3Ni_2Sn_7$.

2.1.2. Magnetic ordering of $Ce_3Ni_2Sn_7$

The main feature of the $Ce_3Ni_2Sn_7$ neutron patterns below $T_N=3.8$ K is the presence of a strong (010) magnetic line at low angles 5° and of several weak lines, which do not obey the *C*-lattice reflection conditions. This is clearly shown in the difference diagram (1.5–10 K) of the G41 data (Fig. 2). The magnetic peak topology remains the same over the entire ordered regime. The wave vector $q=(010)$ describing the magnetic ordering corresponds to the anticentered lattice C_P. Symmetry analysis shows that the space group *Cmmm* has eight one-dimensional real representations for the wave vector $q=(010)$. In the decomposition of the magnetic representation for the Ce1 *2a* site only the representations τ_3, τ_5, τ_7 appear and each of these only once. For the Ce2 *4i* site the six representations τ_2, τ_3, τ_4, τ_5, τ_7, τ_8 appear and each of these only once. The basic vectors are given for the two Ce sites in Table 2. Both atoms are located at special positions, Ce1 at *2c* site:(*mmm*) is located at a center of symmetry in the intersection of three mirror planes and its magnetic ordering is compatible with the magnetic space groups with odd labels, which comprise a center of symmetry. From Table 2 it can be disclosed that only collinear structures can be realized for both Ce sites. The representations τ_3, τ_5, τ_7 lead for both Ce sites to moment arrangements constrained along the *x*, *y*, *z* axes, respectively. The representations with even labels would be compatible with collinear structures for only the Ce2 positions as atoms related by the center of symmetry have opposite moments.

From the strong (010) intensity the τ_2 and τ_5 representations can be ruled out, as they would constrain the moments along *y*. The best agreement between experimental and calculated intensities was achieved for a collinear structure of only the Ce2 magnetic moments along the *x* direction invariant under the representation τ_8 corresponding to the magnetic space group $C_pmm'm'$, P_Cmmn (Sh_{59}^{415}) [12]. The resulting ordered moment value of $1.89(1)\mu_B$/Ce atom is close to the free ion value of Ce^{3+}, $gJ\mu_B=2.14\mu_B$. Fig. 3 shows the collinear moment arrange-

Table 2
Basic vectors of the irreducible representations for the *Cmmm* space group and the wave vector $q=(010)$ for the sites: Ce1: at *2c* and Ce2: at *4i*

	x y z	*x y z*	Magnetic group
Ce1	*(1/2, 0, 1/2)*		
τ_3	(1 0 0)		$C_pmm'm'$, P_Bmna (Sh_{53}^{334})
τ_5	(0 1 0)		$C_pm'mm'$, P_Bmna (Sh_{53}^{334})
τ_7	(0 0 1)		$C_pm'm'm$, P_Cbam (Sh_{55}^{363})
Ce2	*(0,0.18,0)*	*(0,0.82,0)*	
τ_2	(0 1 0)	(0 −1 0)	$C_pm'm'm'$, P_Cban (Sh_{50}^{287})
τ_3	(1 0 0)	(1 0 0)	$C_pmm'm'$, P_Bmna (Sh_{53}^{334})
τ_4	(0 0 1)	(0 0 −1)	$C_pm'mm$, P_Bmma (Sh_{51}^{302})
τ_5	(0 1 0)	(0 1 0)	$C_pm'mm'$, P_Bmna (Sh_{53}^{334})
τ_7	(0 0 1)	(0 0 1)	$C_pm'm'm$, P_Cbam (Sh_{55}^{363})
τ_8	(1 0 0)	(−1 0 0)	$C_pmm'm'$, P_Cmmn(Sh_{59}^{415})

The atoms related by the *C*-centering operation have their moments inverted.

ment of the Ce2 site with the trigonal prism arrangement. Within each trigonal prism block the Ce2 moments point into the same direction and change sign collectively along the *b* axis due to the anticentering translation. Successive Ce2 trigonal prism blocks are separated by the non-magnetic Ce1 layers with the cubooctahedral surrounding. The thermal variation of the strongest magnetic intensity (Fig. 4) confirms the ordering temperature of 3.8 K reported in [10].

2.2. Magnetic structure of $CeNi_{0.78}Sn_2$

A comparison of the 10 K neutron data of the compound with refined composition $CeNi_{0.78}Sn_2$ in the paramagnetic state with those of the 1.5 K data (Fig. 5) shows that the latter comprises only a few weakly resolved magnetic reflections in the low 2θ range, similar to the previously studied sample of refined composition $CeNi_{0.84}Sn_2$ [6]. These reflections are better visible in the difference diagram (1.5 K–10 K) displayed in Fig. 6. In Fig. 6 one observes two sets of reflections. One set pertains to ferromagnetic ($q_1=0$) overlapping reflections. The second set, which is not well resolved, consists of very weak antiferromagnetic $q_2=(0,q_y,0)$ reflections. The refinement of the 1.5 K magnetic intensities was made under the assumption of coexisting domains as found in the sample with $x=0.840(4)$ [6]. Results are given in Table 3. The refined ferromagnetic ($\mu_z=1.44(7)\mu_B$/Ce) component and

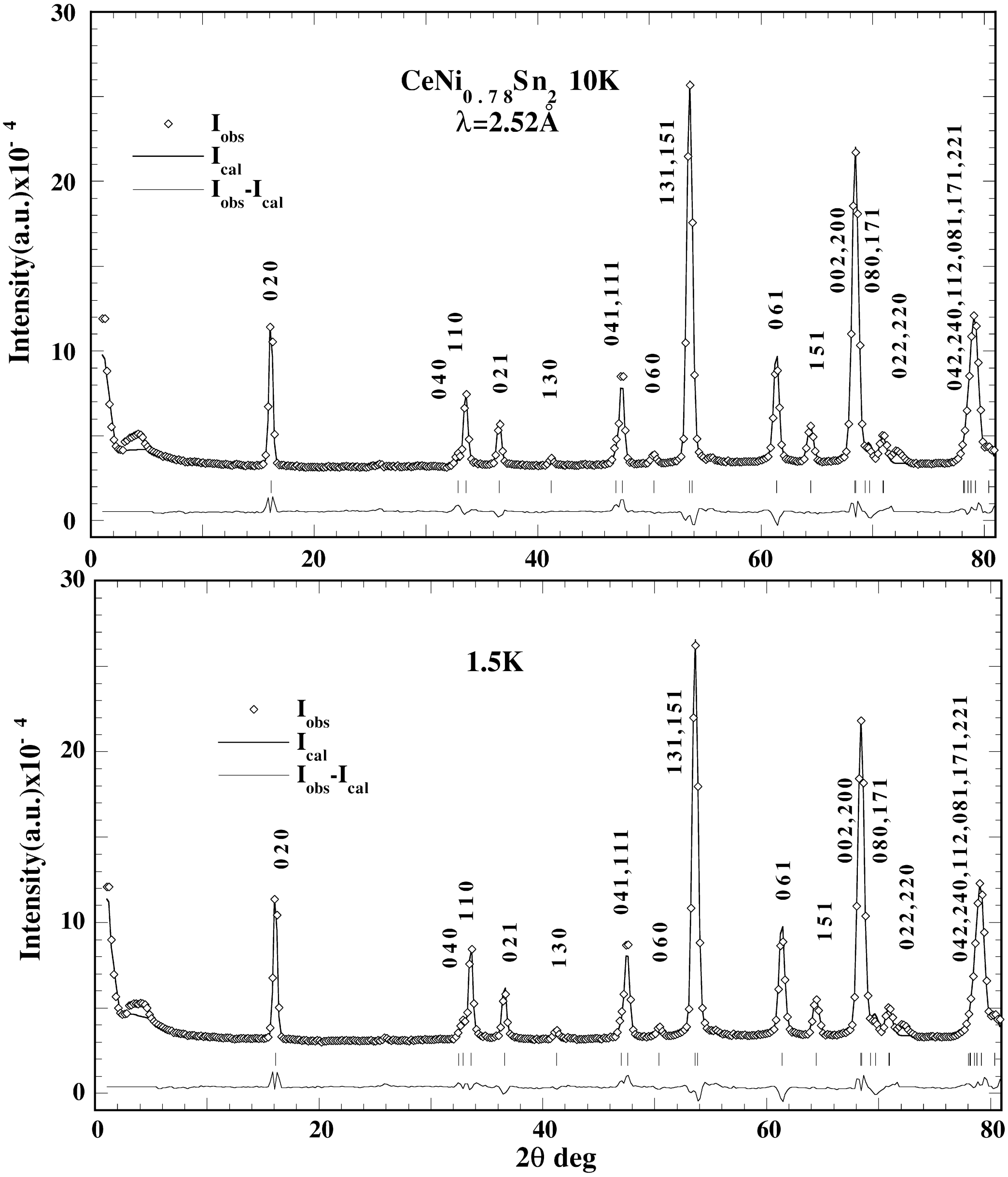

Fig. 5. Observed and calculated neutron intensities of $CeNi_{0.78}Sn_2$ in the paramagnetic state at 10 K (top part) and in the magnetically ordered state at 1.5 K (bottom part) with only ferromagnetic reflections.

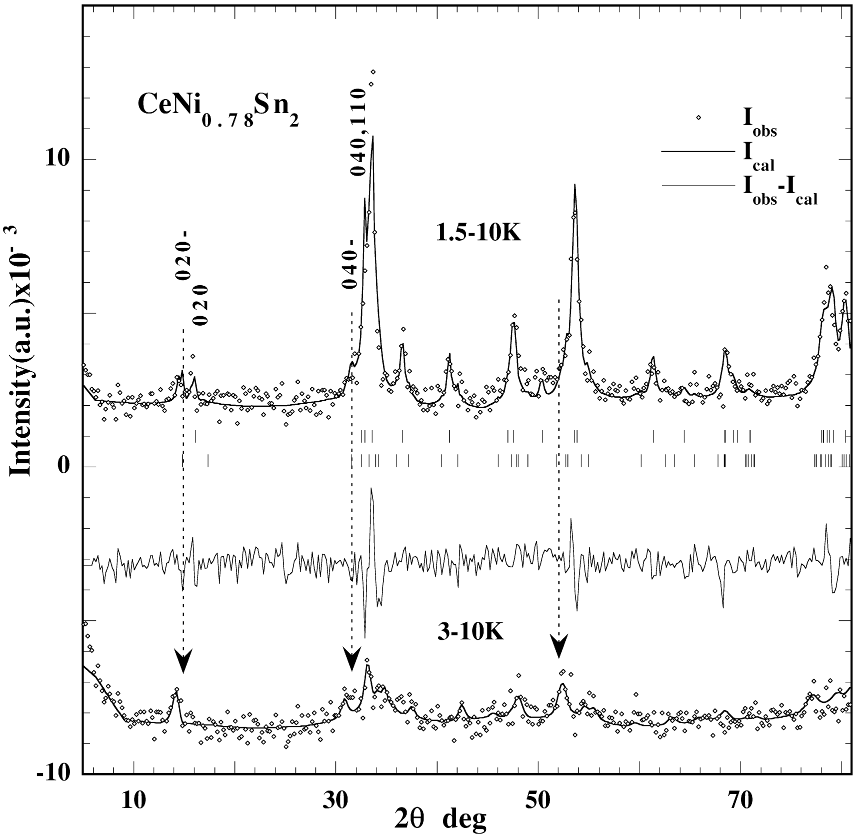

Fig. 6. Observed and calculated difference diagram of $CeNi_{0.78}Sn_2$ (1.5 K–10 K) comprising two sets of magnetic reflections associated with the wave vectors $q_1=0$, $q_2=(0q_y0)$. Also included are the observed and calculated difference diagram 3–10 K comprising only a few weak satellites (indicated by arrows) pertaining to the wave vector $q_2=(0q_y0)$.

the amplitude of the modulated structure (1.6(2)μ_B/Ce) have very comparable values which suggests that the two phases are present in equal portions. Fig. 3 displays the Ce magnetic moment arrangement of the ferromagnetic phase.

Table 3
Refined parameters of the $CeNi_{0.78}Sn_2$ compound in the paramagnetic state at 10 K and in the magnetically ordered state at 1.5 K and 3 K

Parameter	10 K	1.5 K	3–10 K
y_{Ce}	0.1093(5)	0.1093	0.1093
y_{Ni}	0.3186(3)	0.3168	
y_{Sn1}	0.4479(5)	0.4479	
y_{Sn2}	0.7479(4)	0.7479	
$\mu_z[\mu_B]$	−	1.44(7)	−
$\mu_{(2)}[\mu_B]$		1.6(1)	1.24(4)
q_y [r.l.u.]		0.153(5)	0.232(3)
a (Å)	4.4625(8)	4.4628(8)	4.4628
b (Å)	17.669(2)	17.671(2)	17.671
c (Å)	4.4669(7)	4.4664(7)	4.4664
B_{of} (Å)^2	0.53(5)	0.53	0.53
R_n, $R_{m1,}R_{m2}$%	3.87, −, −	3.6, 9	−, 12, 17
$R_{wp,}$ R_{exp}%	8.7, 1.2,	8.9, 1.2	32, 21

μ_z is the ferromagnetic moment value ($q_1=0$). $\mu_{(2)}$ is the Fourier component giving rise to the transversal amplitude modulated structure along c ($q_2=(0,q_{y,}0)$) refined from the difference diagrams.

In contrast to $Ce_3Ni_2Sn_7$ the ferromagnetic trigonal prism blocks are stacked ferromagnetically along the b axis. A rough estimate of the relative amounts of the two magnetic phases can be achieved by assuming that Ce has the same moment value 2.0 μ_B as in $CeNi_{0.84}Sn_2$ [6]. Then the volume of the present ferromagnetic phase would correspond to $(1.44/2.0)^2=51\%$ and that of the antiferromagnetic phase to 49%. The refined wave vector value of $q_y=0.153$ r.l.u. at 1.5 K is much smaller than that found in $CeNi_{0.84}Sn_2$ ($1/3b^*$) with the same ordering temperature which explains that the peaks were less well resolved. The reflections of the sine wave modulated structure at 3 K are very weak and therefore the wave vector length can not be precisely defined.

3. Discussion

In previous investigations of off-stoichiometric compounds of the type $CeNi_xSn_2$ we have obtained indications that an antiferromagnetic phase coexists with a ferromagnetic phase at 1.5 K and that the relative amount of these phases depends on the Ni concentration. In the compound with refined composition $CeNi_{0.84}Sn_2$ the relative proportions of the ferromagnetic and antiferromagnetic phase were found to be roughly equal [6], whereas the relative amount of the ferromagnetic phase had dropped to only 16% in the compound with refined composition $CeNi_{0.86}Sn_2$ [7]. This led us to propose that the relative amount of the ferromagnetic phase decreases strongly with increasing Ni content. Unfortunately, these two compounds were prepared in different ways. Whereas a slight excess of Sn was used in the former compound, we found that the Ni_3Sn_2 impurity phase could be much more suppressed by using a slight Sn deficiency rather than an excess in the preparation (the amount of the Ni_3Sn_2 impurity phase dropped from 4.3 wt% to 1.3 wt%). In order to avoid this uncertainty, we have used the same preparatory conditions now as in [7]. For this reason the result obtained for the present compound with $x=0.78$ is directly comparable to that obtained previously on the compound with $x=0.86$. The strong drop of the relative amount of the ferromagnetic phase when going from the former compound to the latter implies that our statement regarding the dependence of the amount of ferromagnetic phase on Ni content is still valid.

We mentioned already in the introduction that the crystal structure of the second compound studied in this investigation ($Ce_3Ni_2Sn_7$) displays a resemblance with the $CeNi_xSn_2$ compounds as it comprises two Ce sites one of which (Ce2) has the same Ce trigonal prism arrangement centered by Sn atoms. The other Ce site (Ce1) is located at the center of a [Sn12] cubooctahedron also found in the $CeSn_3$ and Ce_3Sn_7 compounds [8–10]. The Ce atoms residing in this latter position in both compounds were found to have an intermediate valence state and do not show magnetic order. This opens the possibility to explain the absence of magnetic ordering observed by us for the Ce1 position by a similar mechanism. However, this possibility can be excluded by the observation that the temperature dependence of the reciprocal susceptibility of $Ce_3Ni_2Sn_7$ follows Curie–Weiss behavior with an effective moment close to the free Ce^{3+} ion value [10]. Concentrating on the number of nearest Ce neighbors one may derive from the left part of Fig. 3 that Ce2 has four near Ce neighbors at distances of about 4.57 Å and two nearest neighbors at distances of about 4.14 Å. By contrast, Ce1 has only the four near Ce neighbors at distances of about 4.57 Å and lacks the nearest neighbors at the much shorter distance. Consequently, the molecular field experienced by the Ce1 moments is much smaller than that felt by the Ce2 moments. This is possibly the reason why we did not observe any magnetic ordering of the Ce1 moments in the temperature range considered. The magnetic ordering is dominated by the Ce2–Ce2 interactions and the crystal field anisotropy in the $Ce_3Ni_2Sn_7$ compound. Within each Ce2 trigonal prism block the exchange is ferromagnetic similarly to the ferromagnetic $CeNi_{0.78}Sn_2$ compound. The difference between the two structures is that in $Ce_3Ni_2Sn_7$ successive Ce2 trigonal prism blocks are related by the anticentering translation. The Ce1 site sandwiched between two antiparallel Ce2 blocks experiences geometrical frustration. The Ce2 site was found to order according to the τ_8 representation ($C_p mm'm'$, $P_C mmn$ (Sh_{59}^{415})) in a collinear arrangement along the a axis. The fact that Ce1 was not found to order down to 1.5 K is in agreement with the restrictions imposed by symmetry analysis. As a consequence an eventual ordering of the Ce1 atomic moments below 1.5 K could only be effected by symmetry breaking.

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