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Crystal structure and physical properties of NpRh_2Sn , a new Np-based ternary compound

T Klimczuk^{1,2}, J-C Griveau¹, P Gaczy ski¹, R Eloirdi¹, E Colineau¹, and R Caciuffo¹

¹European Commission, Joint Research Center, Institute for Transuranium Elements, Postfach 2340, Karlsruhe, D-76125 Germany

²Faculty of Applied Physics and Mathematics, Gdansk University of Technology, Narutowicza 11/12, 80-233 Gdansk, Poland

E-mail: Tomasz.Klimczuk@ec.europa.eu

Abstract. We report on the synthesis and physical characterization of a new compound, NpRh_2Sn , prepared by arc-melting under argon atmosphere. Rietveld analysis of the powder x-ray diffraction pattern reveals an orthorhombic, Fe_3C -type structure, with lattice parameters that are the shortest among the $An\text{T}_2\text{Sn}$ series ($An = \text{U}, \text{Np}, \text{Pu}$, and $T = \text{Pd}, \text{Rh}$). A fit of the high-temperature magnetic susceptibility curve, $\chi(T)$, gives a Curie-Weiss temperature $\Theta_{\text{CW}} = -29\text{K}$, and an effective magnetic moment $\mu_{\text{eff}} = 2.42\mu_{\text{B}}$. The stabilization of the antiferromagnetic order below $T_{\text{N}} = 34\text{K}$ is revealed by a cusp in $\chi(T)$ and by a small anomaly in the specific heat curve, $C_{\text{p}}(T)$. An enhanced value of the Sommerfeld coefficient, $\gamma \approx 107\text{ mJ mol}^{-1}\text{ K}^{-2}$, indicates a moderate heavy-fermion state. NpRh_2Sn is the first member of the $An\text{Rh}_2\text{Sn}$ family, and a rare representative of heavy-fermion systems amidst Np- intermetallics.

1. Introduction

The large family of the ternary actinide compounds $An\text{T}_2\text{M}$, where An is an actinide element, T is a transition element, and M is a metalloid, forms mainly in the orthorhombic Fe_3C - type crystal structure (Pnma, s.g. 62). The uranium based alloys (UT_2M) have attracted considerable attention due to a wide range of physical properties, which originates from the sensitive nature of the uranium $5f$ -electrons. Very few compounds with An other than uranium have been reported, and most of them contain palladium as the transition element.

Here, we present the crystal structure and physical properties of a new intermetallic NpRh_2Sn compound, which is the first member of the $An\text{Rh}_2\text{M}$ family.

2. Experimental

Polycrystalline NpRh_2Sn sample was synthesized by arc-melting stoichiometric amounts of elements under a zirconium gettered ultra pure argon atmosphere. The purity of the product was verified by powder X-ray diffraction (Bruker D8 Focus, $\text{CuK}\alpha$ radiation, graphite monochromator). Data were collected in the 2θ range of $10^\circ - 100^\circ$ with a step size of 0.01° . The FullProf Suite package was used for Rietveld structure refinement [1]. The magnetic susceptibility was measured using a Magnetic Property Measurement System (MPMS, Quantum Design), whereas the specific heat and electrical

resistivity were determined using a Physical Properties Measurement System (PPMS, Quantum Design).

3. Results and discussion

The as-cast sample extracted from the batch was studied by x-ray powder diffraction and the result is presented in Figure 1. The known crystal structure of URh₂Sn was employed as a starting structural model [2]. As shown in Fig. 1, there is good agreement between the model and the data, suggesting that NpRh₂Sn is isostructural to the U analogue. The lattice parameters for NpRh₂Sn were calculated to be $a=9.7208(6)$ Å, $b=4.4221(3)$ Å and $c=6.9043(4)$ Å and are smaller than the reported ones for NpPd₂Sn [3]. It was found that 8% of Np substitutes the Rh(1) site and 8% of Rh are located on the Np site.

Selected physical parameters for NpRh₂Sn and other members of the AnT₂M series are given in Table 1.

Table 1. Lattice parameters, An-An distance ($d_{\text{An-An}}$), Néel temperature (T_N) and Curie-Weiss temperature (Θ_{CW}) for 5 members of AnT₂Sn family

	a (Å)	b (Å)	c (Å)	$d_{\text{An-An}}$ (Å)	T_N (K)	Θ_{CW} (K)
NpRh₂Sn	9.7208(6)	4.4221(3)	6.9043(4)	3.9702	34	-29
NpPd₂Sn [3]	10.004(3)	4.535(2)	6.961(1)	4.0606	15	-80
PuPd₂Sn [4]	10.053(9)	4.502(4)	7.065(6)	---	11	-30
URh₂Sn [2,5]	9.7923(2)	4.37474(7)	6.9639(1)	3.935	---	-200
UPd₂Sn [6]	9.9787(1)	4.58843(5)	6.89166(8)	4.1817	---	-77

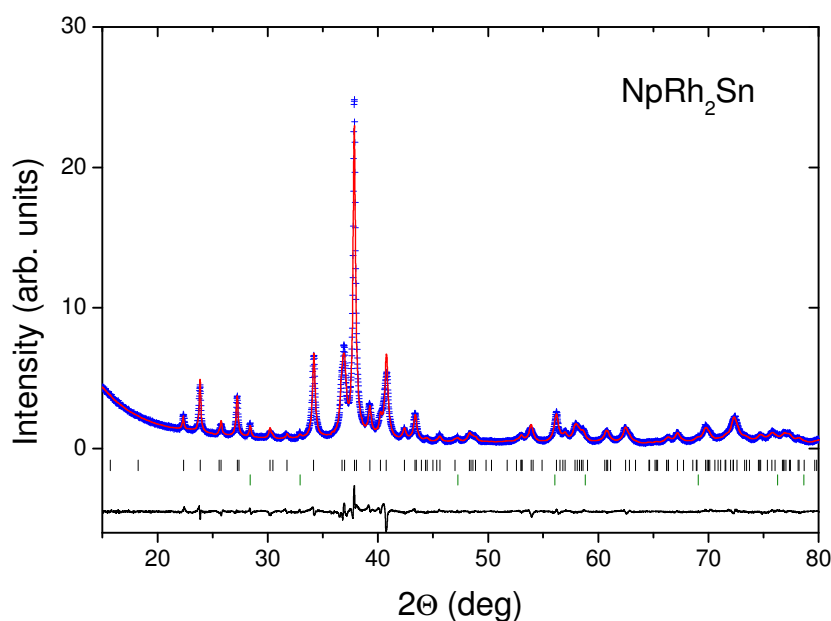


Figure 1. Rietveld refinement of room temperature the x-ray diffraction pattern for NpRh₂Sn. Crosses represent observed data, red solid line is the calculated intensity. The black tick marks correspond to NpRh₂Sn and green set refers to the NpO₂ impurity (~2% wt.). Figure of merits: $R_p = 4.04$, $R_{\text{wp}} = 5.97$, $R_{\text{exp}} = 2.60$ and $\chi^2 = 5.28$.

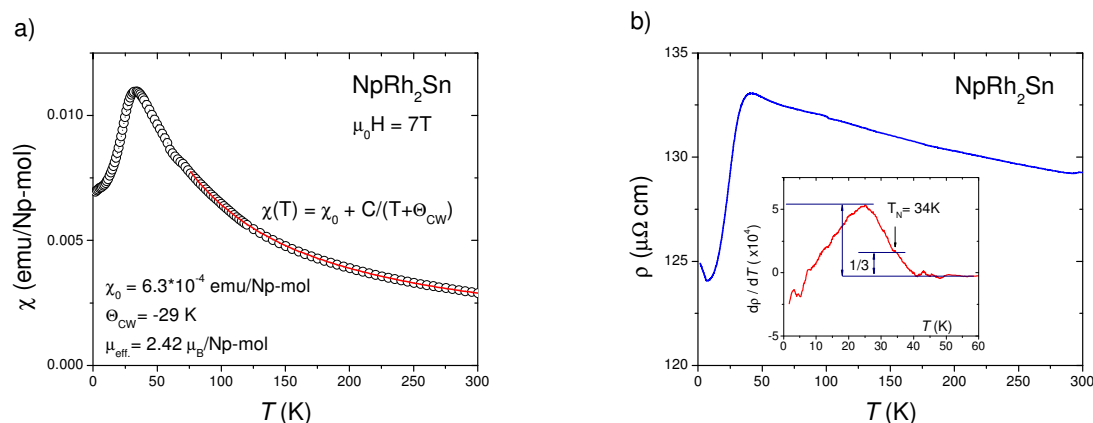


Figure 2. The temperature dependence of the a) magnetic susceptibility ($\chi(T)$) and b) electrical resistivity ($\rho(T)$) of NpRh_2Sn . The solid red line in panel a) is a fit by the modified Curie-Weiss law. The inset in panel b) shows the derivative of the electrical resistivity ($d\rho/dT$) vs. temperature. The Néel temperature, defined as shown in the inset, is 34K.

In Figure 2 we show the temperature dependence of magnetic susceptibility (a) and electrical resistivity (b) of NpRh_2Sn . The Curie-Weiss fit of the $\chi(T)$ data above 75 K (red solid line) gives a Curie-Weiss temperature $\Theta_{\text{CW}} = -29$ K, and an effective magnetic moment $\mu_{\text{eff}} = 2.42 \mu_{\text{B}}$ /Np-mol. This is close to the value expected for Np^{+3} ($2.68 \mu_{\text{B}}$). The measurement indicates an antiferromagnetic anomaly at T_{N} around 35 K.

Electrical resistivity as a function of temperature (main panel) and the temperature derivative of the resistivity (inset) for NpRh_2Sn are plotted in Figure 2b. At room temperature the resistivity is $129 \mu\Omega \text{ cm}$ which is very close to what is observed for PuPd_2Sn [4] and NpPd_2Sn [3]. With decreasing temperature the electrical resistivity slightly increases and at 50 K reaches a value of $133 \mu\Omega \text{ cm}$. Interestingly the non-metallic behavior in the high temperature region was also reported for NpPd_2Sn whereas PuPd_2Sn exhibit metallicity in the whole temperature range. Below 40 K a rapid drop of resistivity, and a pronounced positive peak of $d\rho/dT$, are visible. This behavior is caused by the antiferromagnetic transition. Using the derivative of the electrical resistivity we can determine the ordering temperature (1/3 of the $d\rho/dT$ peak). We found $T_{\text{N}} = 34$ K, which is very close to the magnetic ordering temperature.

The temperature dependence of the specific heat (C_p) and specific heat over temperature (C_p/T) of NpRh_2Sn are shown in Figure 3. At room temperature C_p reaches a value that corresponds to the Dulong-Petit law: $C_p = 3nR = 99.77 \text{ J mol}^{-1} \text{ K}^{-1}$, where $n=4$ and $R=8.314 \text{ J mol}^{-1} \text{ K}^{-1}$. The magnetic phase transition discussed above is not well pronounced in the specific heat measurement. Close to $T=30\text{K}$ only a slight change of slope, as shown in the inset of Fig. 3a, is observed on the specific heat curve $C_p(T)$. Similar result, notably a marginal evidence of a specific heat anomaly was reported also for $\text{UPd}_{2-x}\text{Sn}$ ($x=0.05$ and 0.15), as discussed in ref. [7].

Figure 3b shows C_p/T versus T^2 (only low temperature region) where the Debye temperature (Θ_{D}) and Sommerfeld parameter (γ) can be estimated from the linear fit: $C_p/T = C_{\text{el}}/T + C_{\text{ph}}/T = \gamma + \beta T^2$, where $\beta = \frac{12\pi^4}{5} \frac{nR}{\Theta_{\text{D}}^3}$. Although the experimental data were fitted only up to 10K, which is three

times lower than T_{N} , we are aware of the magnetic contribution (C_{mag}) to the specific heat. Subtracting C_{mag} should not change the value of γ , but might slightly change β , and consequently the Debye temperature. The calculated Sommerfeld parameter for NpRh_2Sn , $\gamma = 107 \text{ mJ mol}^{-1} \text{ K}^{-2}$ indicates

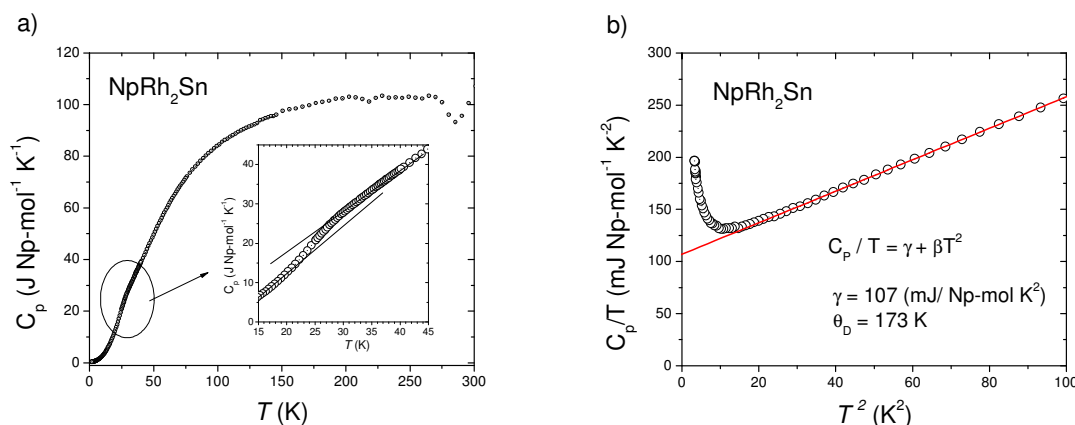


Figure 3. Temperature dependent specific heat (a) and specific heat over temperature (b) of NpRh_2Sn . The inset of the figure a) emphasises the magnetic transition region.

moderately heavy fermion state, and is of the same order of magnitude as reported for PuPd_2Sn and NpPd_2Sn , which are $180 \text{ mJ mol}^{-1} \text{ K}^{-2}$, and $400 \text{ mJ mol}^{-1} \text{ K}^{-2}$ respectively.

To summarize, we have synthesized and studied a new Np-based ternary NpRh_2Sn compound. Its properties are similar to those of NpPd_2Sn , although a shorter Np-Np distance causes an increase of the Néel temperature. NpRh_2Sn is a rare representative of heavy-fermion systems amidst Np-intermetallics.

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