

The Lattice Specific Heat of RENi₅ Compounds at Low Temperatures

Rafea A.Monef

College of science-University of Kirkuk

Abstract

The lattice specific heat, C_L , and Debye temperatures, $\theta_D(0)$, of the rare earth metals with nickel compounds (RENi₅) have been estimated at low temperatures ($T < 30K$) by scaling results of the specific heat of the non-magnetic compound LaNi₅. The magnetic specific heats, C_m , and the magnetic entropy, S_m , in some magnetic RENi₅ compounds have also been recalculated and compared with the other published results.

Introduction

The rare earth Nickel (RENi₅) intermetallic compounds have the $C_a C_{u5}$ structure at room temperature. The magnetic RENi₅ compounds (except PrNi₅ which exhibits a ferro- to paramagnetic transition with Curie temperature of 15 K), the magnetic properties of these compounds have been investigated by many authors. (Wells et al, 1979; Mohammed, 2003; Gorem, 1984; Craig, 1972; Abrahams et al, 1964; Escudler et al, 1977) but the thermal properties, and especially specific heat, have received less attention. (Andres et al, 1975; Wernich, 1959) have the specific heats of TbNi₅, GdNi₅, and ErNi₅ compounds have also been measured.

(Mohammed, 2003; Gorem, 1984) but were studied were the properties in the temperature range from 2 to 50K. In general, the total specific heat of solid materials can be written as ;

$$C_p = C_e + C_L + C_m \quad \dots(1)$$

Where C_e , C_L and C_m represent the electronic, lattice and magnetic specific heats respectively. Studies of the specific heats of RENi₅ compounds have faced a great problem in the separation of the magnetic specific heat C_m from the total specific heat C_p . The accuracy of the resultant values of C_m are in great doubt due to the error in the estimation of lattice specific heat.

These estimation methods can be summarized as follows:

The first method is to measure the specific heat of a similar but non-magnetic compound and then use it as representative of a non-magnetic specific heat (Ushizaka et al, 1984). In this regard, LaNi₅ is the best non-magnetic compound used in this respect. The second method (Seipler et al, 1977)

is a the computer to get the best fit equation for the matezials C_p .

The Lattice Specific Heat Predictions

In order to study the magnetic specific heat more carefully it has to be extracted from the total specific heat, i.e., the lattice specific heat has to be estimated accurately by a reliable method. In this study we have estimated the lattice specific heat and Debye temperatures for all $RENi_5$ compounds by scaling the results of the lattice specific heat of stable, non-magnetic and quite similar compound , $LaNi_5$. The principles of this method(Naji et al, 1989, Lanchester et al, 1987) are based on Debye theyy, which assumes that lattice specific heats of all compound fit a universal functon of $T/ \theta_D(0)$,where the values of the Debye temperature $\theta_D(0)$ should be proportional (according to Lindemanns function) the inverse of square root of the mean atomic mass, i.e.

$$\theta_D(o) \propto M^{-0.5} .$$

Moreover, by using the scling approach , many universal functions have been introduced to characterise the experimental results, such as the specific heat, magnetisation, susceptibility and electrical resistivity(Souletic et al, 1969) This seems to be quite true for similar highly correlated compounds such as $RENi_5$ compounds in which values of the force constants are expected to change gradually from one compound to another . Accordingly, the Debye temperture of any $RENi_5$ compound can be obtained by the following equation.

$$\dots(2) \theta_D(0)(RENi_5) = \theta_D(0)(LaNi_5) \frac{\langle MLaNi_5 \rangle^{0.5}}{\langle MRENi_5 \rangle^{0.5}}$$

where the value of $LaNi_5 \theta_D(0)$ has been found from the C/T versus T^2 plot to be equal to 147K.(Mohammed 2003) Resultant of $\theta_D(0)$ for $RENi_5$ compounds are shown in Table 1 . It is clear from this table that there is a significant difference between values of $\theta_D(0)$ in this stady and that in other investigations. The lattice specific heat of any of these compounds can be estimated by scaling values of C_L for $LaNi_5$ at a temperature T , to a new temperature T' , where

$$T' = T \frac{\theta_D(0)[RENi_5]}{\theta_D(0)[LaNi_5]} \dots(3)$$

where value s of $\theta_D(0)$ for any $RENi_5$ compound can be found from table(1). The lattice specific heats obtained by this method for rare earth-nickle compound are shown in figs.1 and 2 respectively. The variation of the

Debye temperatures $\theta_D(0)$ with temperature for these compounds can now be estimated using the well known relation

$$\theta_D(0) = \left| \frac{1944}{C_L} \right|^{1/3} T..(K) \quad \dots(4)$$

The variation of $\theta_D(0)$ with temperature for some of rare earth-nickel compounds is shown in figs 3,4 and 5 respectively.

Table 1: Values of Debye temperature $\theta_D(0)$ for $RENi_5$ compounds.

	$\theta_D(0) \pm 0.5K^0$	$\theta_D(0) \pm 0.5K^0$
RENi ₅ compounds	work $\theta_D(0)K^0$	$\theta_D(0)K^0$ (other studies)
LaNi ₅	147	142k (Aoyacim et al ,1971)
CeNi ₅	146.79	
PrNi ₅	146.66	
NdNi ₅	146.64	
PmNi ₅	145.64	
SmNi ₅	145.09	
EuNi ₅	144.83	
GdNi ₅	143.97	
TbNi ₅	143.71	
DyNi ₅	143.14	
HoNi ₅	142.76	
ErNi ₅	142.40	
TmNi ₅	142.14	
YbNi ₅	141.52	
LuNi ₅	141.22	

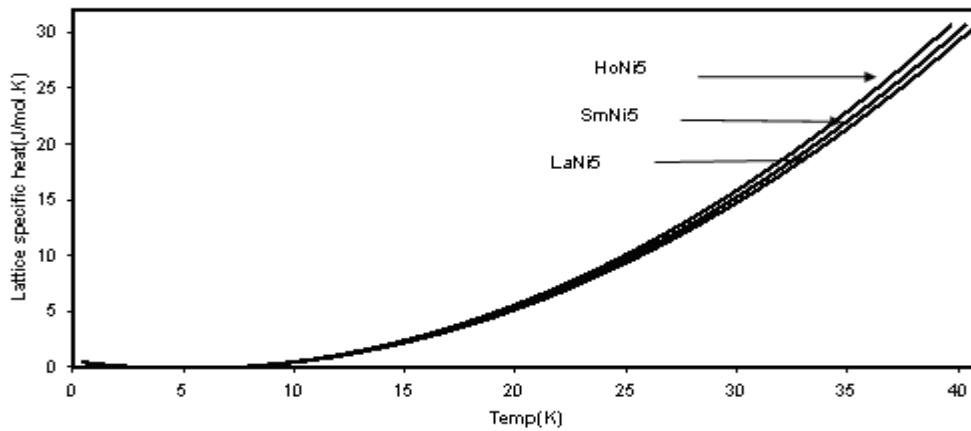


Fig 1: The predicted lattice specific heats, C_L versus temperature T for some rare earth nical ($RENi_5$) compound.

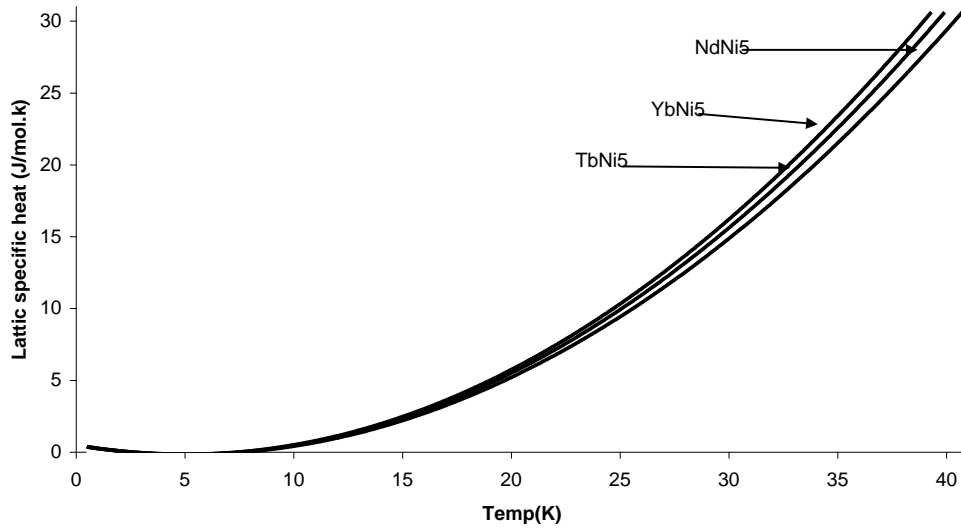


Fig. 2 : The predicted lattice specific heats, C_L versus temperature T for some rare earth nical ($RENi_5$) compound.

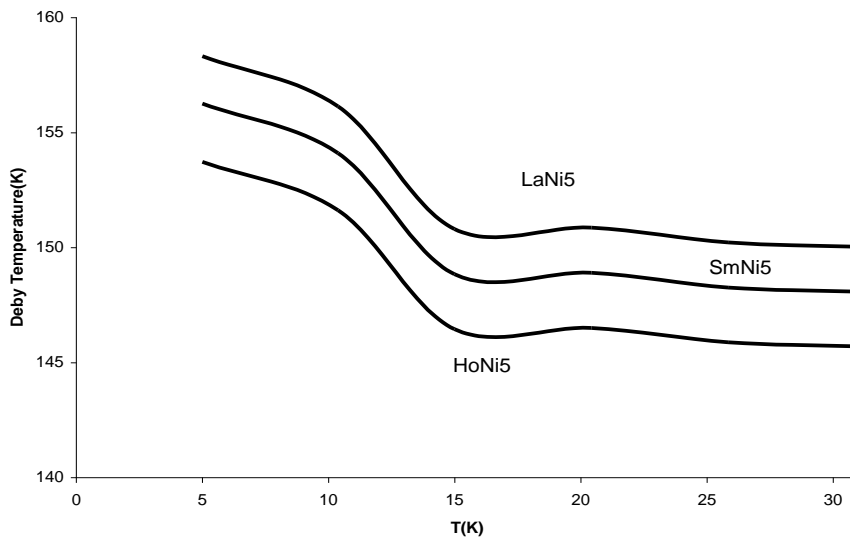


Fig 3: Debye temperature, θ_D (T) temperature T for some rare earth- nical ($RENi_5$) compound.

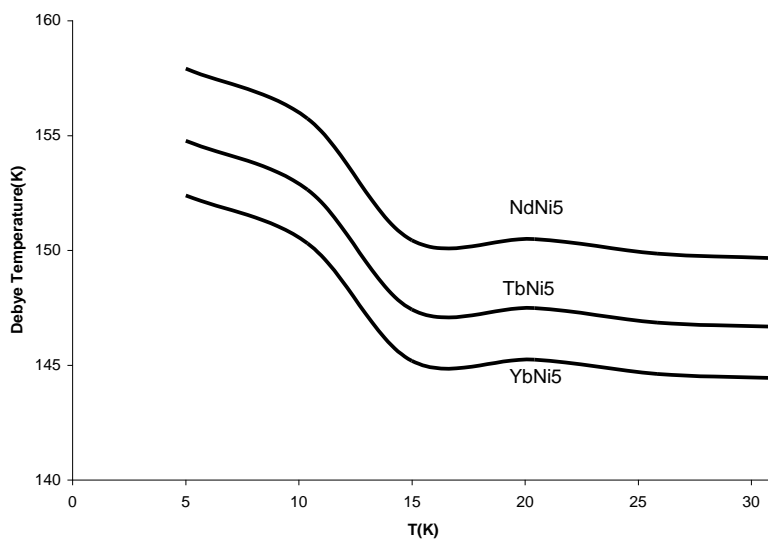


Fig 4: Debye temperature, θ_D (T) temperature T for some rare earth- nical ($RENi_5$) compound.

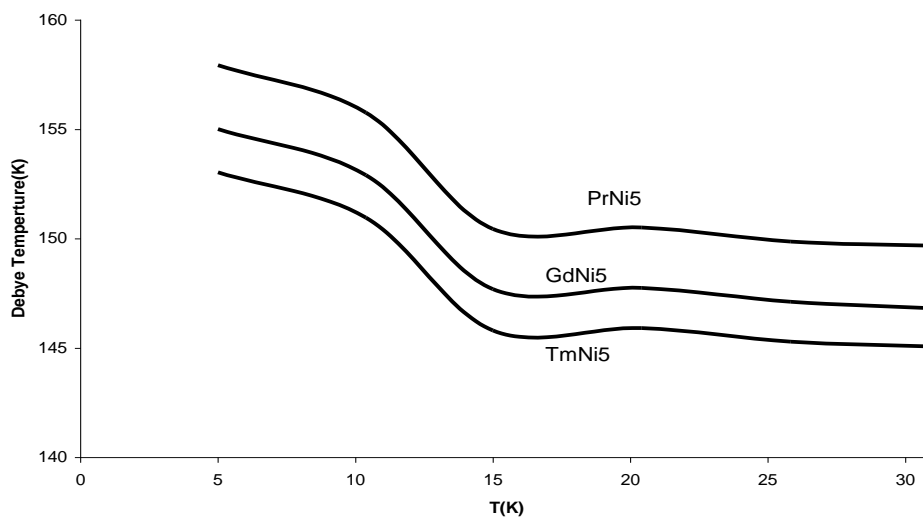


Fig 5: Debye temperature, θ_D (T) temperature T for some rare earth- nical ($RENi_5$) compound.

It has been mentioned earlier that the error estimating the lattice specific heat for $RENi_5$ compounds causes a significant error in the estimation of the magnetic specific entropy changes, especially for compounds with an ordering temperature higher than 10K. In spite of that and in order to show quantitatively the error in C_m caused by using the usual methods we have recalculated the magnetic specific heats C_m of some of these compounds using new values of the lattice specific heats calculated using equation 2. As an example of the magnetic specific heats of some $RENi_5$ compounds are shown in Figs. 6 and 7 for $GdNi_5$, $ErNi_5$ respectively. Moreover, the magnetic entropy S_m changes in these compounds from $T=0$ to $T=T_m$, where T_m is the temperature of the maximum magnetic specific heat, are also recalculated using new values of C_m . Table 2 shows these results.

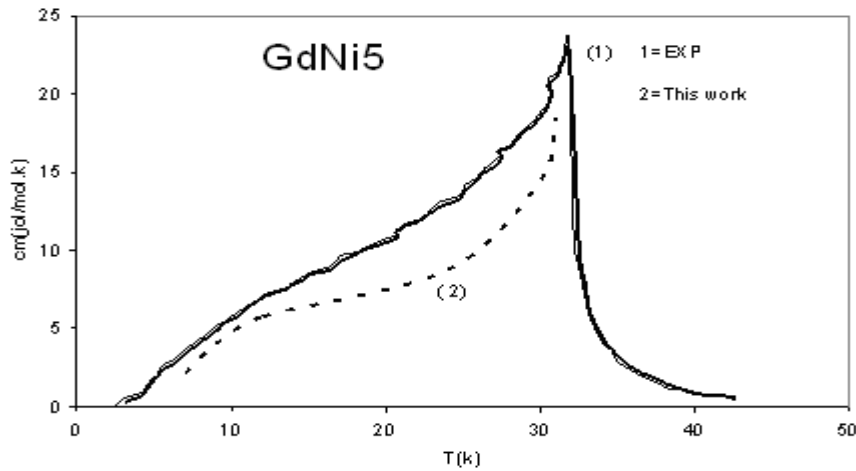


Fig.6: C_m versus T for $GdNi_5$.

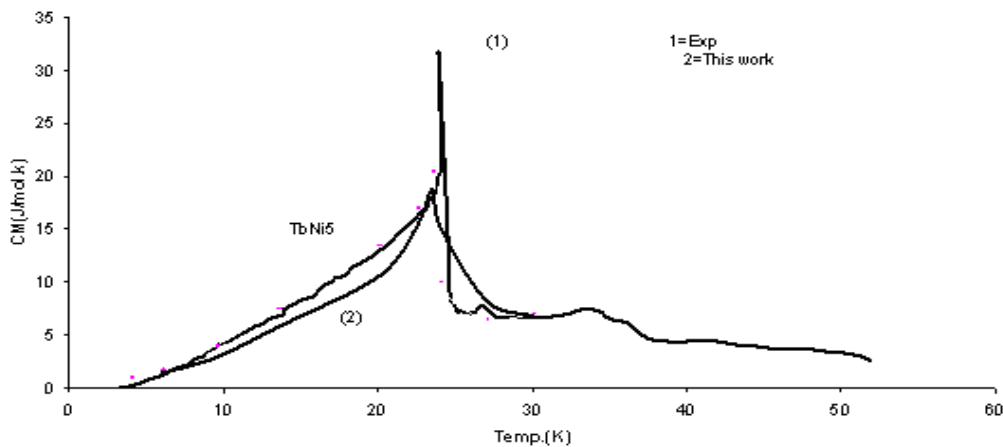


Fig 7: C_m versus T for $TbNi_5$

Table 2: values of magnetic entropy changes S_m for $RENi_5$ compounds.

Some $RENi_5$ Compound	$T_m(K)$	T_c or T_N (K) From other refs	$S_m/R.Ln$ (2J+1) (%)	S_m 0- T_m J/mol.k	This work
$LaNi_5$	Non-magnetic	-----	-----	-----	-----
$GdNi_5$	32	32 (Abrahms,1964)	95	16.4	16
$TbNi_5$	23.7	27(Gignonx etal,1979)	49	10.6	10.2
Gd_2O_3	3.8	3.6(Nasa et al 1971)	-----	-----	-----
Tb_2O_3	2.4	2.4 (Hill,1986)	-----	-----	-----

Conclusions

The principles of Debye theory and Lindemanns equation can be used to estimate the lattice specific heats of $RENi_5$ compounds. The magnetic lspecific heats and magnetic entropy of some of these compounds have also been recalculated using lattice specific heats as obtained by this method .In spite of the rather large mass difference between RE and La metals the use of this method is quite satisfactory and can be used in analysing magnetic heats in other $RENi_5$ cmpounds at low temperature ($< 30K$). It results in an accurate estimation of C_m , which allows studying the validity of the $T^{3/2}$ and T^3 laws for ferro- and antiferromagnetic $RENi_5$ compounds at low temperature .morover, this method might also be shown to be valid for high temperature ranges.

References

- Abrahams .S.C,Bernstin.J.L, Sherwood.R.C and Williams.H.J.,(1969): the crystal structure and magntic properties of the RARE-EARTH Nickel (RNi) compounds.phys.chem.solids pergarmon press,Vol.25, pp.1069-1080.
- Abrahams .S.C, Bernstin.J.L, Sherwood.R.C and Williams.H.J.and Williams H.J., (1964): J.phy. chem.solds .Vol.25, 1069p.
- Andres.K, Ott.H.R, Bucher .E and malta .J.P., (1976): solid state commun.Vol.18,1303p.
- Craig R.S,Sankar S.G,Marzouk N, Rao.Y.U,Wallace W.E and Secal .E., (1972): J .phy.chem.solids,Vol.33, pp.2267-2274.

- Escudier.P,Gignoux .D,Givord .D,Lemaire.R and murani .A.P.,(1977): CRYSTAL FIELD EFFECTS in ErNi₅ .phy.pp.86-88.North-Holland.
- Gignoux.D ,Hennion.B and Nait .A.,(1982): crystalline electric field effects in f-electron magnetism ,new york,485p.
- Gorem E.A., (1984): Crystal Electric field splitting in TbNi₅ and ErNi₅, phy.state .Vol.b.pp.121- 623.
- Hill R.W, Cosier .J and Hukin D.A., (1986):Specific heat of Tb₂O₃ and Tb₄O₇ between 0.5 and 22K.J.phy.C:solid stats physics.Vol.19, 673p.
- Mohameed K.A and Lanchester P.C,(1987): The low temperature Specific heat of Lu-Cu-Y metallic Glasses.J.Magn.Mater. Vol.65, 275p.
- Mohameed K.A and Naji J.S., (1989):J.Sci of Educ. (Mosul un., mosul, Iraq) Vol.8,108p.
- Mohameed K.A., (2003): Specific heat of LaNi₅,GdNi₅ and TbNi₅ compounds between 2 and 50 K, J.Sciences of technologie–N19, pp.27-31.
- Mohameed K.A., (2003): The low temperature Specific heat of Magnetic TbNi₅, Tikrit Journal for pure science, Vol.9.
- Nasa .S, Neumann .N, Marzouk. N, Cralg.R and Wallace .E., (1971): Specific heat of LaNi₅,CeNi₅,PrNi₅, NdNi₅and GdNi₅.bett-ween 1.6 and 4K.J.phys.chem.solids,Vol.32,pp.2779-2883.
- Seipler .D, Bremicker .B,Goebel .U,mappel .H, Hoenig .H.E and perrin.,(1977): J.phys.Vol.7, 599p.
- Souletie.J and Tournier .R.,(1969): J.Low tmp.phys, Vol.1,95p.
- Ushizaka .H,Murayama .S, Miyako.Y and Tazuke .Y., (1984): J.phys .soc.Japan,Vol.53,1136p.
- Wells .P,Lanchester P.C ,Jones D.W and Jordan R.G.,(1976): The low temperature heat capacity of Tb and Y .phy.F:metal phys.Vol.6, 11p.
- Wernickj .H and Geellers.,(1959): Act.Crystallogr.Vol.12,662p.

الحرارة النوعية للشبيكة لمركبات النادرة مع النيكل في درجات الحرارة الواطئة

رافع عبدالله منيف

كلية العلوم – جامعة كركوك

الخلاصة

تم حساب الحرارة النوعية للشبيكة C_L لمركبات العناصر النادرة مع النيكل حيث أن [RE] عنصر نادر، وكذلك تم حساب درجة حرارة ديبياي $\theta_D(0)$ من خلال تدرج الحرارة النوعية للمركب غير المغناطيسي $LaNi_5$. كما تم حساب الحرارة النوعية المغناطيسية C_m والأنتروبي المغناطيسي S_m للمركبات $RENi_5$ المغناطيسية ومن ثم مقارنة النتائج المستحصلة مع نتائج الدراسات السابقة.