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Structural instabilities in rare earth intermetallic compounds with CsCl structure

B. Lüthi and R. Sommer

Physikalisches Institut der Universität, D-6000 Frankfurt a.M., F.R.G.

and P. Morin

Laboratoire L.-Néel, C.N.R.S., Grenoble Cedex, France

Résumé. — Un grand nombre de composés de terres rares métalliques et de structure de type CsCl présentent des transitions de structure cristallographique. Les mécanismes responsables de ces transitions sont un couplage du réseau avec des bandes 5d (effet Jahn Teller de bande) ou avec les moments quadrupolaires 4f (effet Jahn Teller). Les mesures récentes de la vitesse de propagation du son ont permis d'étudier l'amollissement du mode normal de déformation tétragonale dans l'état paramagnétique de TmZn et TmCd. Les coefficients magnétoélastiques et d'échange quadrupolaire sont déduits. Le comportement sous champ magnétique est aussi discuté.

Abstract. — Many intermetallic rare earth compounds with CsCl structure undergo structural phase transitions. The responsible mechanisms for these transitions are a deformation potential coupling for 5d bands (band Jahn Teller effect) or a strain coupling to 4f quadrupoles (Jahn Teller effect). Recent measurements of the soft elastic modes in the paramagnetic region for TmZn and TmCd enable us to determine magnetoelastic and quadrupolar coupling constants. Magnetic field effects on elastic constants are also discussed.

In intermetallic rare earth compounds one can have two kinds of structural instabilities, one due to an electronic ordering of 4f shell electrons (cooperative Jahn Teller effect) and a martensitic type of transformation due to a strain deformation potential coupling to the 5d electrons (band Jahn Teller effect). The latter effect has been investigated in some detail in the CsCl-structure $\text{LaAg}_x\text{In}_{1-x}$ [1] system and somewhat less in LaCd [1], CeAg [2]. For the cooperative Jahn Teller effect one has to distinguish between cases where the structural transition temperature T_a and the magnetic transition temperature T_C , T_N are equal or different. Up to the present only two cases have been identified in which $T_a > T_C$: TmCd [3] and TmZn [4]. In other cases [5] ErZn, DyZn $T_C = T_a$ as well as also for the pnictides [6] (DySb, HoSb, TbP, etc.). It is no lucky coincidence that TmCd, TmZn show a pure cooperative Jahn Teller effect. The Tm^{3+} ion with $J = 6$ has $L = 5$, $S = 1$ which favors quadrupolar coupling over exchange effects. Indeed all the Tm-pnictides are nonmagnetic and

TmCd, TmZn show structural transitions at temperatures higher than T_C (see table I). We would like to give a brief account of a recent ultrasonic study of these latter two materials.

In figure 1 we present the temperatures dependence of some elastic stiffness constants for TmZn. One notices the strong softening of the $c_{11} - c_{12}$ mode indicating a cubic-tetragonal transition at low T . The c_{44} mode only gives a small anomaly at T_a , but $c_L = \frac{1}{2}(c_{11} + c_{12} + 2c_{44})$ exhibits a somewhat larger softening. The $c_{11} - c_{12}$ and c_L mode we can quantitatively account for with the soft elastic mode formula [6]:

$$(c_{11} - c_{12})_T = (c_{11} - c_{12})_0 - \frac{g_r^2 N \chi_s}{1 - g' \chi_s} \quad (1)$$

where g_r is the magnetoelastic coupling constant in the strain Hamiltonian

$$\mathcal{H}_{\text{str}} = - \sum g_r \varepsilon_r O_r(i)$$

Table I. — Magnetic dipolar and quadrupolar ordering temperatures, background elastic constants, magnetoelastic and magnetic quadrupolar exchange constants in TmCd and TmZn.

	T_a	T_C	c_0	$g^2 N/c_0$	g'
	(K)		(10^{11} erg/cm ³)	Γ_5 g.s. (mK)	Γ_3 g.s. (mK)
TmCd	3.16	—	3.28	0.66	0.34
TmZn	8.55	8.12	5.06	3.6	—

Fig. 1. — Temperature dependence of elastic constants $c_{11} - c_{12}$ and c_L for TmZn. The solid lines are theoretical fits using eq. (1) and the parameters listed in table I.

and g' the quadrupolar interaction constant

$$g' = \sum' G_{ij}$$

in the quadrupole Hamiltonian

$$\mathcal{H}_a = - \sum G_{ij} O_T(i) O_T(j)$$

and χ_s is the one ion strain susceptibility. Formula (1) was particularly successful in interpreting elastic softening for cooperative Jahn Teller phase transitions [6]. Knowing χ_s from the CEF level system one

can determine the important parameters g_R^2 , g' from a temperature fit of c_T .

This gives the values of $g_R^2 N/c_0$, g' quoted in table I. Both $c_{11} - c_{12}$ and c_L give excellent agreement with theoretical fits using the same parameters g_R , g' . For TmZn inelastic neutron scattering results give a Γ_5 ground state for the Tm^{3+} ion followed by a Γ_3 and Γ_4 . In the ordered phase Γ_5 splits into a lower singlet and a higher doublet. For TmCd it was assumed that a nonmagnetic Γ_3 is the ground state in order to account for the cubic-tetragonal structural transition and the specific heat in the mK region [3]. This level scheme gives one set of parameters shown in table I. For a Γ_5 ground state, in analogy to TmZn, one also gets a cubic-tetragonal transition and with the nonmagnetic singlet lower than the magnetic doublet one can equally well account for the hyperfine specific heat. The second set of values for $x = -0.35$, $W = 0.9$ K stems from this level scheme. Since inelastic neutron scattering is not possible in TmCd other experiments have to decide on those two competing schemes. From the values of table I one sees that TmCd had to order structurally in a second order transition at $T'_a = 2.88$ K for a Γ_3 ground state and at $T'_a = 2.90$ K for a Γ_5 ground state. Likewise TmZn would order at $T'_a = 6.6$ K in a second order transition. However the triplet ground state gives always a first order structural transition [7, 4].

With magnetic fields applied in the easy [100]-direction one can shift the structural transition temperature T_a to higher temperatures. This has been observed for TmCd [3] and TmZn. In TmCd T_a changes from 3.16 K to more than 6 K in a field of 3 T and in TmZn similar strong effects are observed. Isochamps of the $c_{11} - c_{12}$ elastic constant show pronounced minima at $T_a(H)$.

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