Magnetoelastic properties and quadrupolar ordering in the magnetic superconductor $TmNi_2B_2C$

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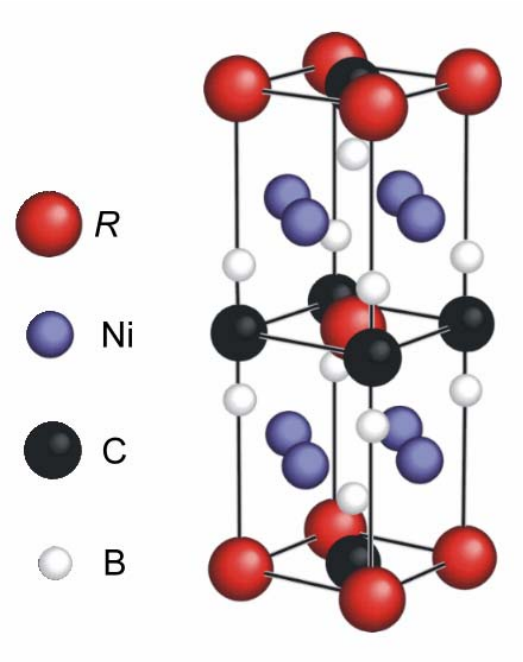
Introduction

The rare-earth borocarbides RNi$_2$B$_2$C show the coexistence of
- antiferromagnetic ordering of the rare-earth moments (below T_N)
- superconducting ordering of the conduction electrons (below T_c)

when R = Dy, Ho, Er, and Tm (discovered in 1994).



Crystal structure of RNi$_2$B$_2$C

The rare-earth moments are mutually coupled via the conduction electrons (the RKKY- interaction)

Magnetic ordering ➡ strong effects on the superconducting properties.

Superconducting ordering ➡ weak effects on the magnetic properties.

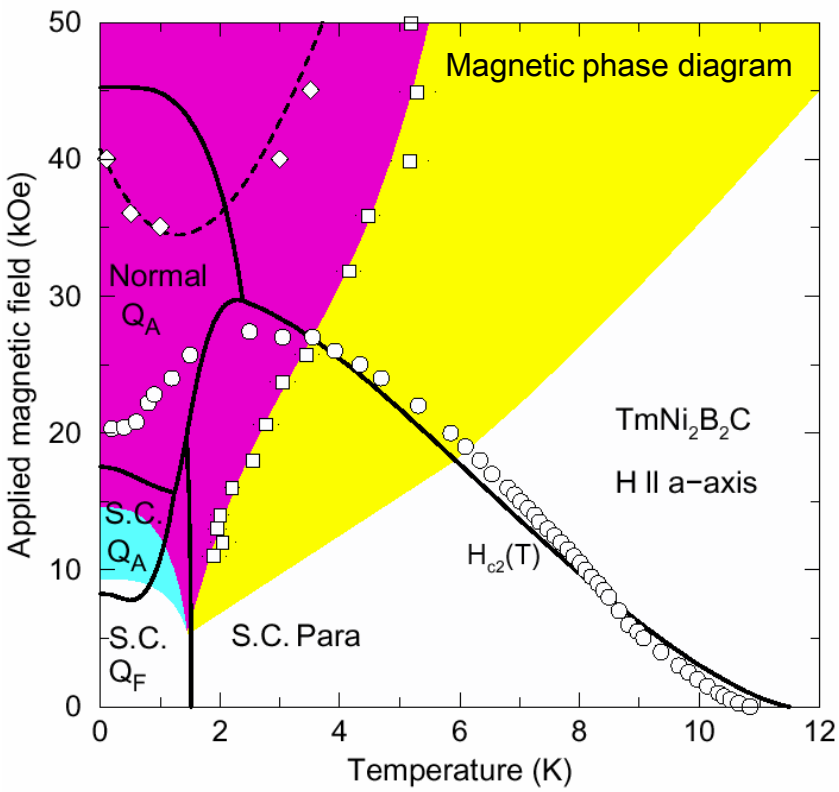
TmNi$_2$B$_2$C: T_c = 11 K and T_N = 1.52 K

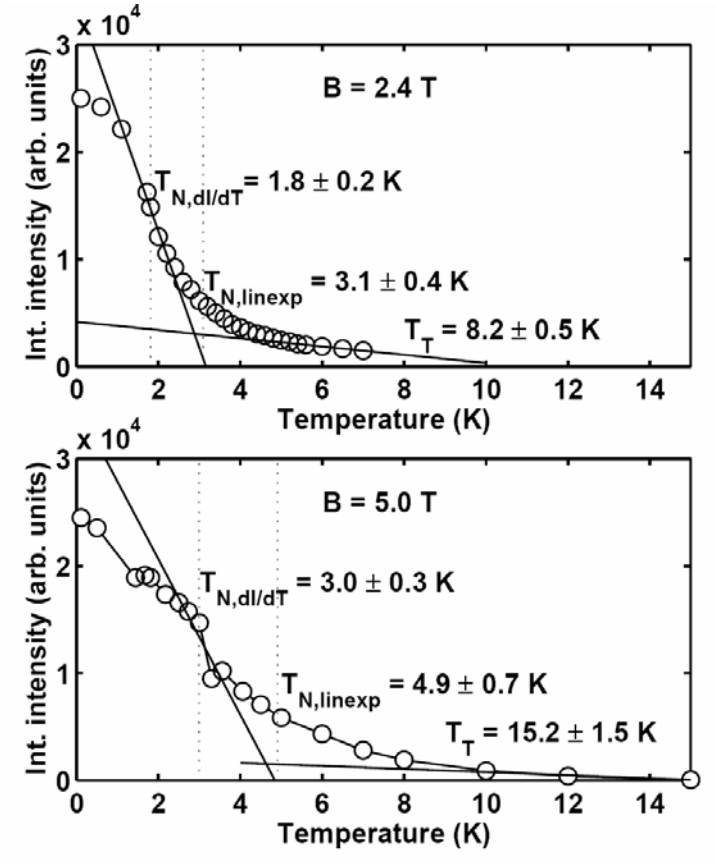
Magnetic ordering:

$$\langle J_z(i)\rangle = M_Q \cos(\mathbf{R}_i \cdot \mathbf{Q}_F + \phi),$$
$$z \parallel c\text{-axis},\ \mathbf{Q}_F = (0.09, 0.09, 0).$$

$TmNi_2B_2C$ in a magnetic field

Field along [100]:





Nesting wave vector: $\mathbf{Q}_A$ = (0.48, 0, 0) ll **H**.

Quadrupolar ordering induced by a lattice distortion at $\mathbf{Q}_A$: $\langle O_2^1(i)\rangle = \langle J_x J_z\rangle \cos(\mathbf{Q}_A \cdot \mathbf{R}_i + \phi)$

Field along the *x* axis, i.e. [100], implies: $\langle J_x(i)\rangle = M_0 \quad \Rightarrow \quad \langle O_2^1(i)\rangle \approx \langle J_x(i)\rangle\langle J_z(i)\rangle = M_0\langle J_z(i)\rangle$

Soft phonons in superconducting $LuNi_2B_2C$

The non-magnetic "rare-earth" borocarbides $LuNi_2B_2C$ and YNi_2B_2C are BCS-like type-II superconductors: $T_c \approx 15$ K, $\xi(0) \approx 100$ Å, $\lambda(0) \approx 1000$ Å, $\kappa \approx 10$, $H_{c2}(0) \approx 100$ kOe.

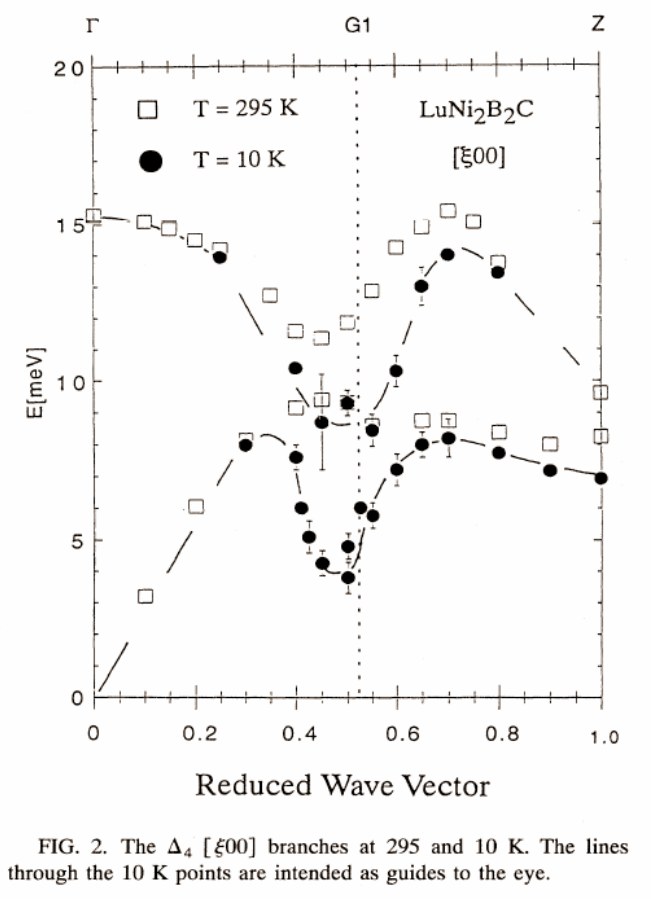


FIG. 2. The Δ_4 [ξ00] branches at 295 and 10 K. The lines through the 10 K points are intended as guides to the eye.

Band-structure calculations indicate nesting features at the Fermi surface around the wave vectors **Q** ≈ (0.5,0,0) and (0,0.5,0).

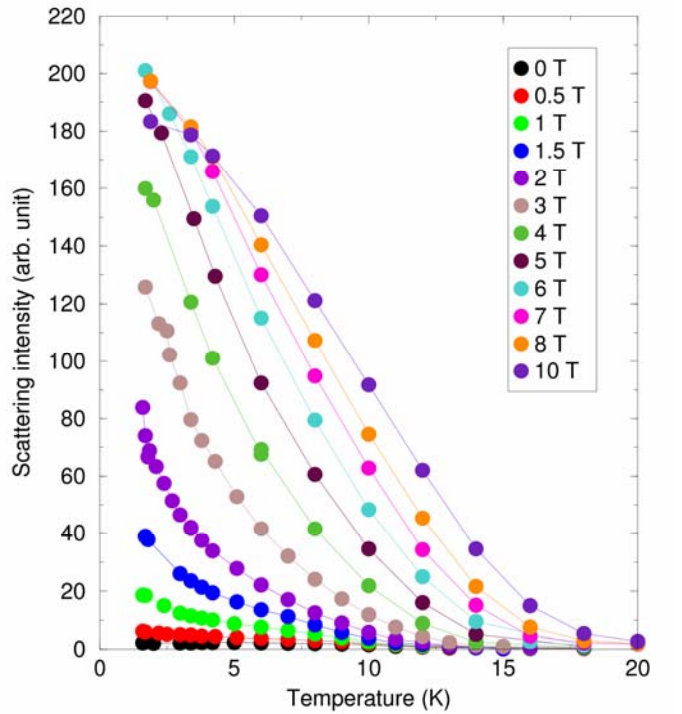
This nesting is important for the phonon mediated coupling of the electrons. A softening of the transverse phonons around these wave vectors has been observed [Dervenagas et al., Phys. Rev. B **52**, R9839 (1995)].

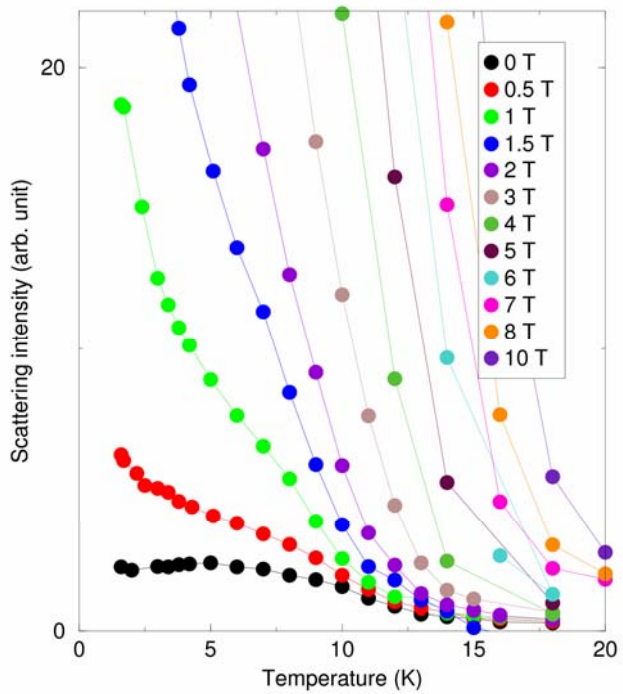
The Δ_4-mode: Transversal displacement u_3 of the Lu (or Tm) ions along axis

$$\Delta\mathcal{H} = -B_{13}O_2^1(i)E_{13}(i)$$

$$E_{13}(i) = \frac{u_3(i)}{a/2} = E_{13}\cos(\mathbf{Q}_A \cdot \mathbf{R}_i + \phi)$$

X-ray scattering experiments on $TmNi_2B_2C$

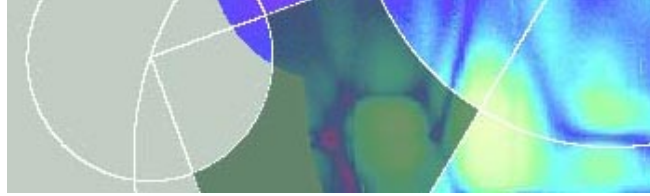




Intensity of elastic x-ray scattering at **Q** = (0.48, 0, 8) obtained at HASYLAB, Hamburg, when applying a magnetic field along [100].

The intensity of 200 (max. value) corresponds to a strain E_{13} of about 6 x 10^{-3}.

Model for the quadrupolar ordering in $TmNi_2B_2C$



Magnetic system: $\mathcal{H}_0 = \mathcal{H}_{CF} - \frac{1}{2}\sum_{ij}\mathcal{J}(ij)\mathbf{J}_i \cdot \mathbf{J}_j - \sum_i g\mu_B \mathbf{H}\cdot\mathbf{J}_i$

The crystal-field Hamiltonian is well determined and $\mathcal{J}(\mathbf{Q}_F) \approx \mathcal{J}(\mathbf{0}) = 0.0087$ meV.

The quadrupolar, magnetoelastic mean-field Hamiltonian is assumed to be described by 4 terms:

$$\mathcal{H}_Q(i) = -B_{13}O_2^1(i)E_{13}(i) + c_E E_{13}^2(i) + \tfrac{2}{3}B_E E_{13}^4(i) - K(Q_A)\langle O_2^1(i)\rangle(O_2^1(i) - \tfrac{1}{2}\langle O_2^1(i)\rangle)$$

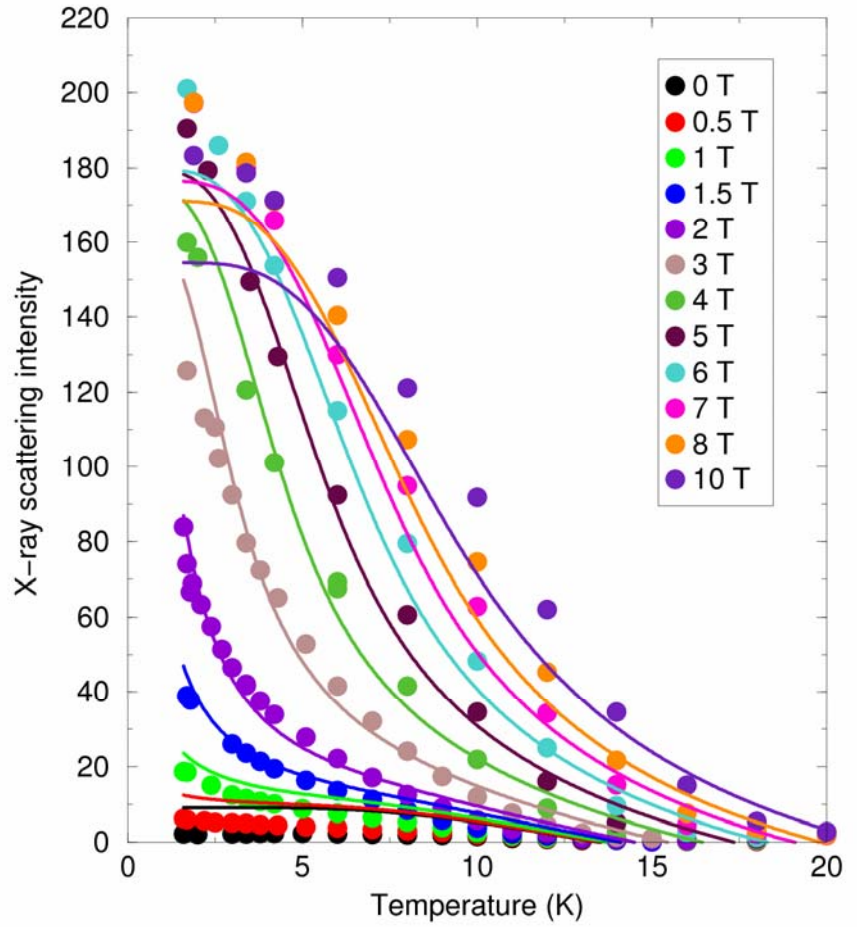
B_E is important because of the small value of c_E (as derived from the strong softening of the corresponding phonon mode produced by the electronic system). This term and the strong increase of the quadrupolar susceptibility with field at the lowest temperatures (a CF effect) are the two main factors for explaining the extreme variation of E_{13} with field.

The transition at the temperature T_Q = 13.5 K at zero field implies that the value of the effective quadupolar coupling has to be equal to the inverse quadrupolar susceptibility at 13.5 K and zero field: $K_{\text{eff}} = K(Q_A) + B_{13}^2/(2c_E) = 0.0187$ meV

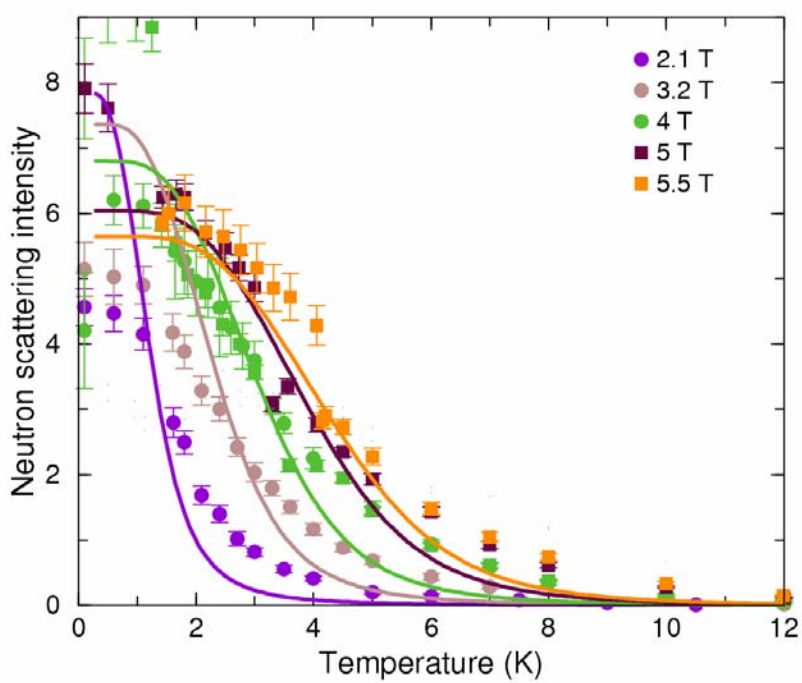
Final model: $K(Q_A)$ = 0.0086 meV, B_{13} = 1.91 meV, c_E = 360 meV (fonon mode at 2.4 meV), and B_E = 4.8 x 10^7 meV, and finally $\mathcal{J}(\mathbf{Q}_A) = -0.0029$ meV.

Comparison between experiments and theory

Quadrupolar ordering



Magnetic ordering



Conclusion

1. A quadrupolar phase at the "nesting wave vector" $\mathbf{Q}_A$ = (0.48, 0, 0) was predicted and has now been observed in $TmNi_2B_2C$. The transition temperature is T_Q = 13.5 K at zero field.

2. The transition temperature increases with field along [100], and the induced displacement of the Tm ions is 7 - 10 times larger at 6 T than at zero field.

3. The presence of the quadrupolar ordering implies that a magnetic field applied along [100] induces an antiferromagnetic magnetic moment at the wave vector $\mathbf{Q}_A$ = (0.48, 0, 0), but not at (0, 0.48, 0).

4. The corresponding quadrupolar charge-ordering is close to occur (is occurring?) in the non-magnetic Lu and Y borocarbides.

5. The present discovery have implications for the understanding of the magnetic properties of the other borocarbides.

The tendency for the quadrupolar ordering might be the basic reason for the magnetic ordering at $\mathbf{Q} \approx (0.5,0,0)$ observed in these compounds, rather than a strong maximum in the RKKY interaction at $\mathbf{Q}$ due to Fermi-surface nesting.

One example is, why is the antiferromagnetic ordering in Tb-borocabide longitudinally polarized, in spite of that the classical dipole-dipole interaction strongly favors the transverse polarization?