CRYSTAL FIELD INTERACTIONS IN THE CHIRAL COMPOUNDS RNi_3Ga_9 (R = Tb, Dy, Ho and Er) STUDIED BY INELASTIC NEUTRON SCATTERING

Authors: L. A. Gil[1]; R. Lora-Serrano[1] and co-authors: J. G. dos Santos Duque[2], D. Garcia[3], S. Cadogan[4], K. Rule[5]

[1]Federal University of Uberlandia, Uberlândia, Brazil. [2]Federal University of Sergipe, São Cristóvão, Brazil.

[3]Bariloche Atomic Centre, Bariloche, Argentina. [4]University of New South Wales, Canberra, Australia. [5]ANSTO

Theory

- Crystal Field Hamiltonian (extended Stevens notation):

$$\hat{H}_{CEF} = B_0^2O_0^2 + B_0^4O_0^4 + B_3^4O_3^4 + B_{-3}^4O_{-3}^4 + B_0^6O_0^6 + B_3^6O_3^6 + B_{-3}^6O_{-3}^6 + B_6^6O_6^6 + B_{-6}^6O_{-6}^6$$

- Magnetic susceptibility (Van Vleck equation):

$$\chi_0^\alpha = g^2\mu_B^2 \sum_i \rho_i \left[-2 \sum_{j \neq i} \frac{|\langle i|J_\alpha|j\rangle|^2}{E_i - E_j} + \frac{1}{k_B T} |\langle i|J_\alpha|i\rangle|^2 \right]$$

where: $\hat{H}_{CEF}|i\rangle = E_i|i\rangle$; $\rho_i = e^{-\frac{E_i}{k_B T}} / \sum_i e^{-\frac{E_i}{k_B T}}$; $\alpha = x, y, z$.

- Double differential cross section for unpolarised neutrons (dipole approximation):

$$\frac{d\sigma}{d\Omega d(\hbar\omega)} = \frac{k_f}{k_i} N \left[\frac{1}{2} g^2 F(\vec{Q})\right]^2 e^{-2W} \left(\frac{\hbar\gamma e^2}{mc^2}\right)^2 \times \sum_{i,j} \rho_i \, |\langle i|J_\perp|j\rangle|^2 \delta(\hbar\omega - E_i + E_j)$$

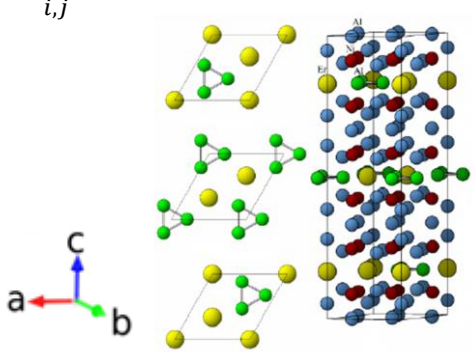

Fig. 1. RNi_3Ga_9 unit cell and RNi_3-layers along the c axis.

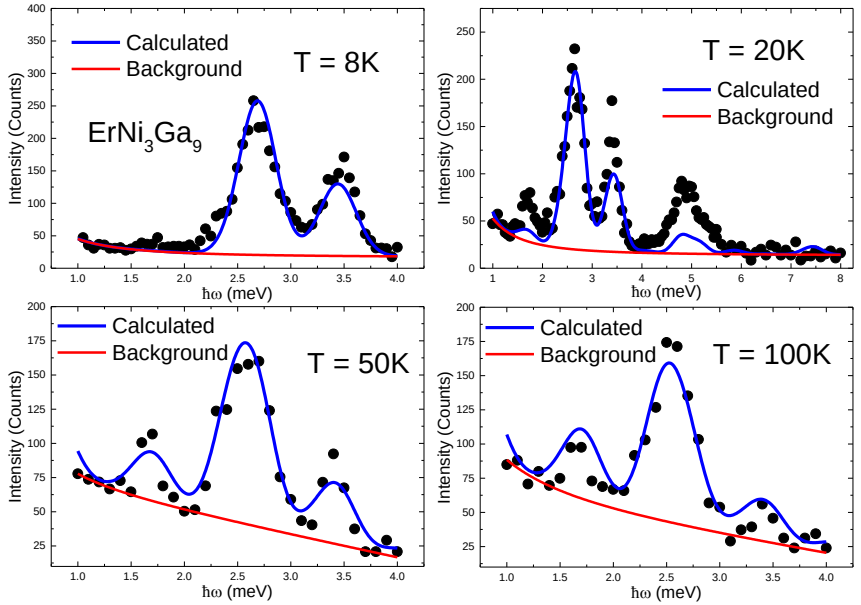

Fig. 2. Inelastic Neutron Scattering (INS) spectra of $ErNi_3Ga_9$ for temperatures T= 8, 20, 50 and 100 K obtained at SIKA. The symbols represent the observed data; solid lines are fits to the INS data using the model above.

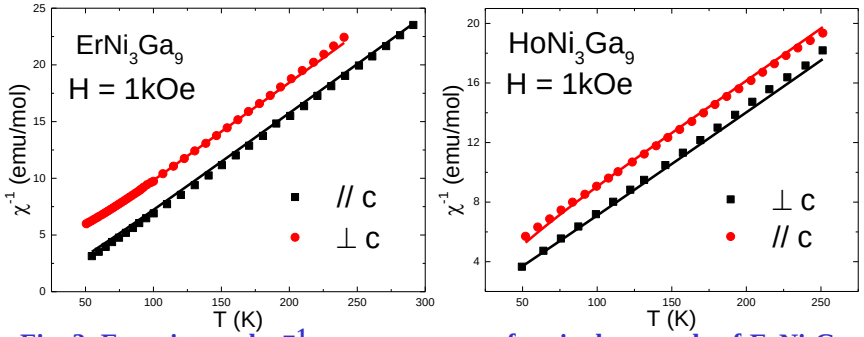

Fig. 3. Experimental χ^{-1} vs. temperature for single crystals of $ErNi_3Ga_9$ and $HoNi_3Ga_9$ in a magnetic field of 1 kOe. χ is the powder (average) susceptibility given by $\chi = \chi_0^x + \chi_0^y + \chi_0^z$.

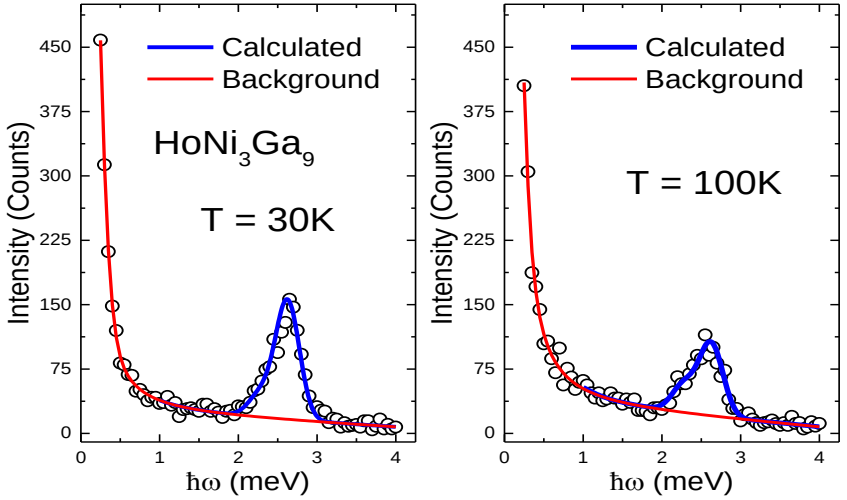

Fig. 4. INS spectra of $HoNi_3Ga_9$ (T = 30 and 100 K). The symbols represent the observed data; solid lines are fits to the INS data using the model above.

Preliminary Conclusions

Our results describe the CEF energy levels' configuration and the relative intensity of the observed peaks in the INS spectrum. The transverse and longitudinal magnetic susceptibilities in the paramagnetic region are reproduced as well.

The results for $TbNi_3Ga_9$ and $DyNi_3Ga_9$ compounds (not shown here) are not yet entirely conclusive; their analysis is ongoing and will be presented elsewhere.

Acknowledgments

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