Magnetic Structures of *R*NiSi$_3$ (*R* = Gd, Tb and Ho)

R. Tartaglia[1], F. R. Arantes[2], C. W. Galdino[1], D. Rigitano[1], U. F. Kaneko[3], M. A. Avila[1], and E. Granado[1]

[1] "Gleb Wataghin" Institute of Physics, University of Campinas – UNICAMP, Campinas, São Paulo, Brazil,
[2]CCNH, Universidade Federal do ABC (UFABC), Santo André, São Paulo, Brazil,
[3]Brazilian Synchrotron Light Laboratory, Brazilian Center for Research in Energy and Materials (CNPEM),
Campinas, São Paulo, Brazil

rodolfotartaglia.s@gmail.com

The competing or cooperative character between different degrees of freedom lead to different ground states in strongly-correlated systems. Even simple systems, such as pure rare earth compounds, present multiple phase transitions with complex magnetic structures in some of them, resulting from a strong interplay between magnetic dipolar interaction and temperature dependence of crystal field parameters [1]. So, it is expected that some rare-earth-based compounds also have rich magnetic phase diagrams. One example is the series of intermetallic compounds *R*NiSi$_3$ (*R* = rare earth), which shows anisotropic antiferromagnetic ground states evolving with *R* [2-4]. The microscopic magnetic structures must be determined to rationalize such rich behavior. Here, resonant X-ray magnetic diffraction experiments are performed on single crystals of GdNiSi$_3$, TbNiSi$_3$ and HoNiSi$_3$ at zero field. The primitive magnetic unit cell matches the chemical cell below the Néel temperatures $T_N = 22.2, 33.2$ K, for Gd- and Tb-based compounds, respectively. The magnetic structure is determined to be the same for both compounds (magnetic space group *Cmmm'*) and could be fully described by a single one-dimensional irreducible representation of the *Cmmm* space group. It features ferromagnetic *ac* planes that are stacked in an antiferromagnetic + − + − pattern, with the rare-earth magnetic moments pointing along the **a** direction [5]. For HoNiSi$_3$, the situation is more complicated, since this compound show two well-defined λ-shape anomalies at $T_{N1} = 6.3$ K and $T_{N2} = 10.4$ K. Additionally, different components of the total magnetic moment order at different temperatures. The **a** component orders at T_{N2}, and after further cooling above T_{N1}, the **c** component orders. For this compound, our results show that at temperatures between T_{N1} and T_{N2} (phase II), the ordered magnetic moment points along the **a**-axis, while below T_{N1} (phase I), the ordered magnetic moments have components both along with **a** and **c**. Remarkably, while at phase II the possible magnetic structure is the same as found in GdNiSi$_3$ and TbNiSi$_3$, at phase I two irreducible representations are needed to account the total magnetic moment direction. In this phase, the magnetic structure is consistent with *C2'/m* magnetic structure. Lastly, those magnetic structures contrasts with the + − − + stacking and moment direction along the **b** axis previously reported for YbNiSi$_3$ [6]. This indicates a sign reversal of the coupling constant between second-neighbor *R* planes as *R* is varied from Gd, Tb and Ho to Yb. The long b lattice parameter of GdNiSi$_3$ and TbNiSi$_3$ shows a magnetoelastic expansion upon cooling below T_N, pointing to the conclusion that the + − + − stacking is stabilized under lattice expansion. A competition between distinct magnetic stacking patterns with similar exchange energies tuned by the size of *R* sets the stage for the magnetic ground state instability observed along this series.

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