Neutron powder diffraction study of the TiNiSi-type GdNiSi and GdNiGe compounds

P. Lemoine[1], N.R. Lee-Hone[2], D.H. Ryan[2], A. Vernière[3], B. Malaman[3]

[1] Department of Physics and Astronomy, University of Manitoba, Winnipeg, MB, Canada
[2] Physics Department and Centre for the Physics of Materials, McGill University, Montreal, QC, Canada
[3] Institut Jean Lamour, dept P2M, équipe 103, CNRS (UMR 7198), Université Lorraine, Faculté des Sciences et Technologies, B.P. 70239, 54506 Vandoeuvre-lès-Nancy Cedex, France

The magnetic structures of the TiNiSi-type GdNiSi and GdNiGe compounds were determined by combining powder neutron diffraction data using a flat plate geometry sample holder [1] and ^{155}Gd Mössbauer spectroscopy measurements. The neutron diffraction patterns recorded in the paramagnetic state (*i.e.* 20 K and 30 K for the GdNiSi and GdNiGe, respectively) confirm the TiNiSi-type structure (top panel of the figure 1 and figure 2) observed with powder X-ray diffraction. Appearance of additional pure magnetic peaks in the 3.6 K neutron diffraction patterns (bottom panel of the figure 1 and figure 2) indicates an antiferromagnetic behavior for these compounds. Fitting the intensity of the strongest magnetic peak from the paramagnetic state down to 3.6 K reveals a magnetic ordering temperature T_N = 13.3(3) K and T_N = 11.5(2) K for GdNiSi (left panel of figure 3) and GdNiGe (right panel of figure 3), respectively. The magnetic behavior and the magnetic temperature ordering of GdNiGe are in fair agreement with the previous reports [2-4], while it is the first time that these of GdNiSi are reported.

At 3.6 K, the magnetic structure of GdNiSi is characterized by the propagation vector k = [0.384, 0.327, 0], with the magnetic moments oriented in a plane close to the (-110) one (bottom panel of the figure 1). Similar propagation vector was already reported for TbNiSi and DyNiSi [5]. For GdNiGe, the magnetic structure at 3.6 K is characterized by the propagation vector k = [0.266, 0.5, 0.5] with the magnetic moments in a plane close to the (011) one (bottom panel of the figure 2). For both compounds, the 3.6 K neutron diffraction pattern can be refined using either a planar helimagnetic structure or a sine-wave modulated magnetic structure. The absence of higher-order harmonic peaks suggests that a square-wave magnetic structure can be rule out. However, this kind of magnetic structure is not excluded taking into account the weak intensity of the first odd integer harmonic magnetic peaks (*i.e.* A(3k) = A(k)/3) and the noise level of the patterns. Similar to the TiNiSi-type GdNiSn magnetic structure study [6], ^{155}Gd Mössbauer spectroscopy measurements are in progress in order to determine the right magnetic structure of these TiNiSi-type compounds.

References

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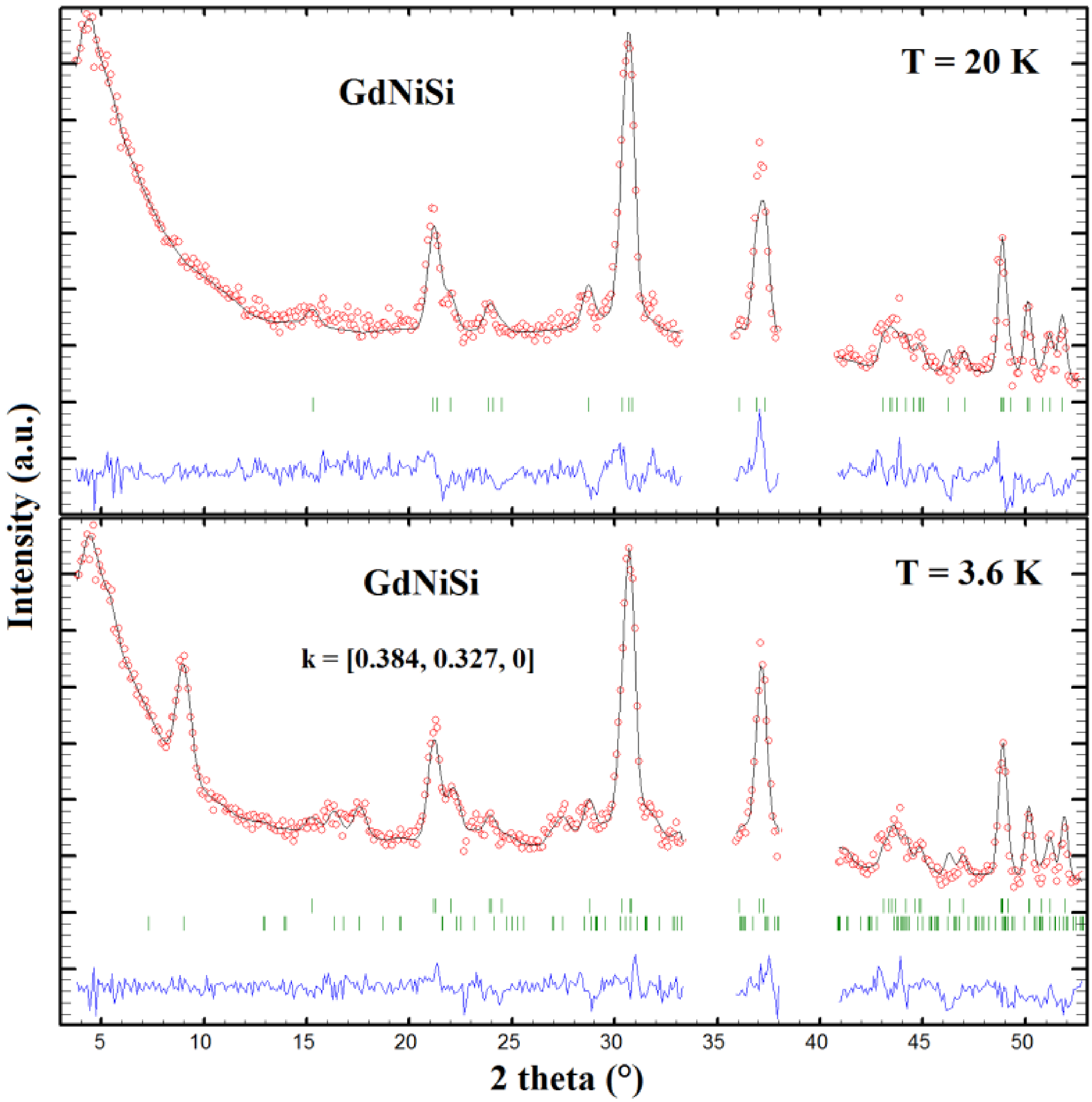

Figure 1 Refinement of the neutron powder diffraction patterns of GdNiSi at 20 K (top panel) and 3.6 K (bottom panel) with λ = 1.3286(1) Å.

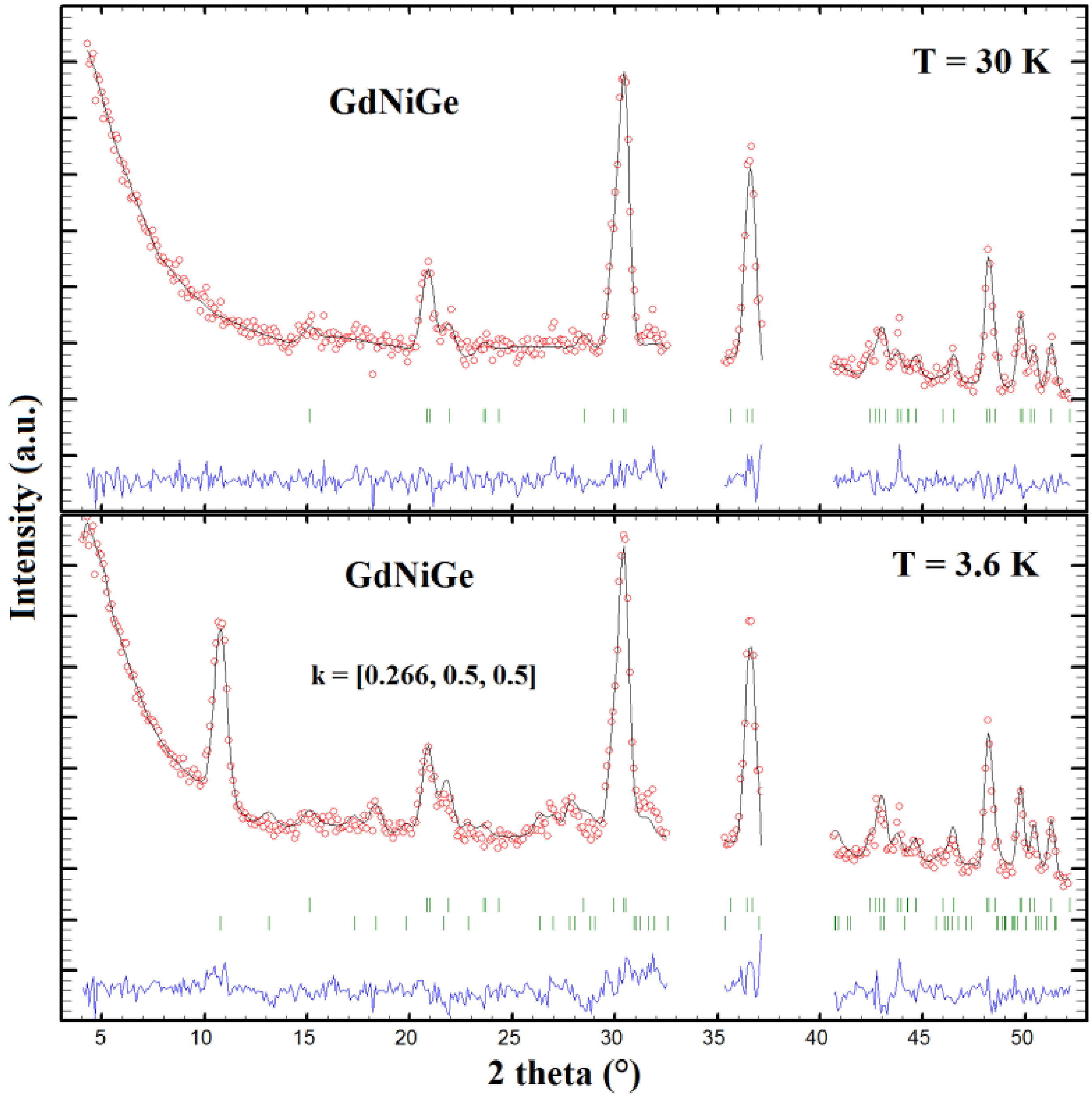

Figure 2 Refinement of the neutron powder diffraction patterns of GdNiGe at 30 K (top panel) and 3.6 K (bottom panel) with λ = 1.3286(1) Å.

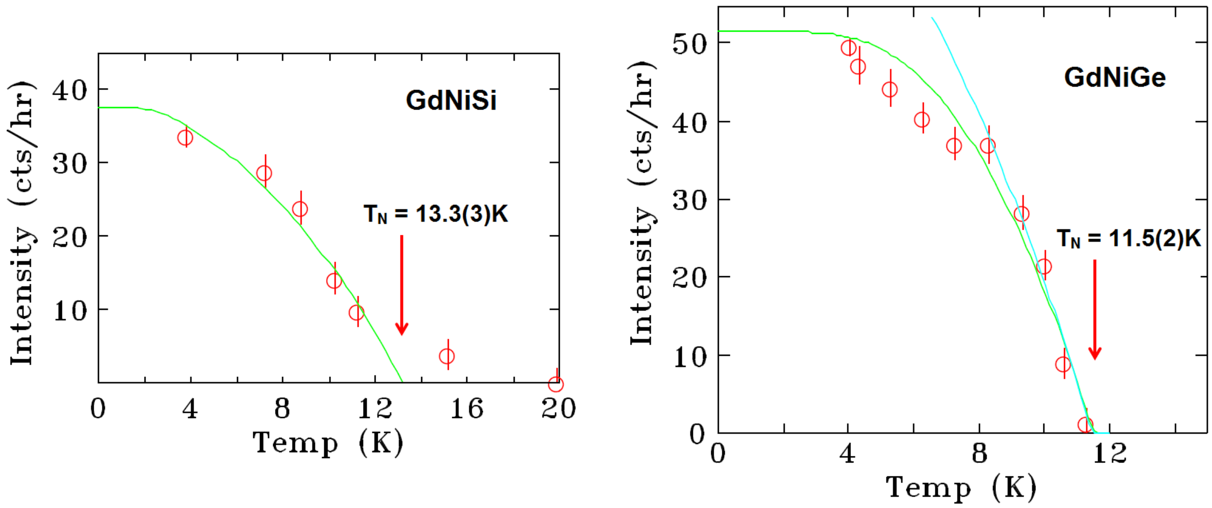

Figure 3 Intensity of the strongest magnetic peak of GdNiSi (left panel) and GdNiGe (right panel) as a function of temperature, showing a Néel temperature of 13.3(3) K and 11.5(2) K, respectively.