Local magnetic structural analysis on frustrated magnets using magnetic pair distribution function

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Magnetic pair distribution function (mPDF) shows a real space magnetic correlation between magnetic moments with a distance r. The mPDF analysis is appropriate for the determination of magnetic structures of the materials with short-range orderings, for example, spin glass, frustrated magnets, magnetic nanoparticles, and so on. We show results of the local magnetic structural analysis on the frustrated magnet, Mn₃RhSi. Figure 1(a) shows the mPDF of Mn₃RhSi at 220 K where the system is paramagnetic and exhibits large diffuse like magnetic scattering. The mPDF has large negative peak at about 2.7 Å corresponding with the nearest neighboring Mn-Mn distance. Based on the observed mPDF, we suggest the magnetic structure model shown in Fig. 1(b). The 120 degree structure is put on four regular triangles in the unit cell, and the moments in two triangles shown by red circles are reversed. The mPDF calculated from this magnetic structure can reproduce the observed negative peak, as shown by red line in Fig. 1(a).

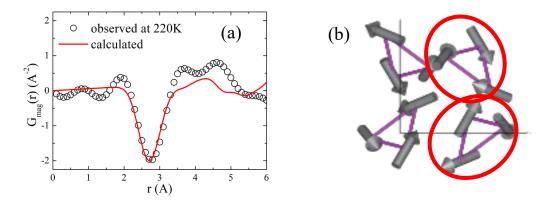


Fig. 1(a) Open circles and red line show observed and calculated mPDFs of Mn₃RhSi, respectively. (b) Magnetic structure determined by mPDF analysis.