Structure of $GdAl_2$ Nanomagnets by High-energy X-ray Diffraction

V. Petkov,[1] S. J. L. Billinge,[1] S. D. Shastri,[2] D. Leslie-Pelecky[3]
[1]Department of Physics and Astronomy and Center for Fundamental Materials Research,
Michigan State University, East Lansing, MI, U.S.A.
[2]Advanced Photon Source, Argonne National Laboratory, Argonne, IL, U.S.A.
[3]Department of Physics and Astronomy and Center for Fundamental Materials Research,
University of Nebraska-Lincoln, Lincoln, NE, U.S.A.

Introduction

One of the fundamental themes of nanotechnology is that every physical property has a critical length scale and, if the basic structural building block is made smaller than the critical length scale, the property begins to change. A vivid demonstration is nanophase $GdAl_2$. Pristine $GdAl_2$ is a ferromagnet with Curie temperature of 170K. Upon mechanical milling, $GdAl_2$ becomes nanophase material and gradually losses its ferromagnetic properties. Understanding this drastic change in the magnetic properties requires detailed knowledge of the atomic ordering at the nanoscale. Usually the structure of materials is obtained from the Bragg peaks in their diffraction patterns. However, materials constructed at the nanoscale, such as nanophase $GdAl_2$, do not posses the long-range order of conventional crystals. The diffraction patterns of such materials show a pronounced diffuse component and few Bragg peaks. This poses a real challenge to the traditional techniques for structure determination. The challenge can be met by employing nontraditional approaches such as the combination of high energy x-ray diffraction and the atomic pair distribution function (PDF) technique [1, 2].

Methods, Materials, and Results

The experiments were carried out at the SRI-CAT beamline 1-ID by using x-rays with an energy of 80.6 keV. Three samples were measured: pristine $GdAl_2$ (first sample) and nanophase $GdAl_2$ obtained by ball milling for 100 h (second sample) and 400 h (third sample). The so-called experimental structure factors *S(Q)* are shown in Fig. 1, and the corresponding atomic pair distribution functions *G(r)* are shown in Fig. 2. Sharp Bragg peaks are present in the *S(Q)* of pristine $GdAl_2$ up to wave vectors as high as 25-30 $Å^{-1}$. The corresponding PDF also features sharp peaks reflecting the presence of long-range order in this perfectly crystalline material. The lack of long-range atomic order in nanophase $GdAl_2$ is evidenced by the considerable broadening and even disappearance of Bragg peaks (Fig. 1). An analysis of the corresponding PDFs in Fig. 2 shows that the local atomic ordering as well as the cubic (*S.G. Fd3m*) structure type of pristine $GdAl_2$ survives in the nanocrystalline phase. However, the spatial extent of structural coherence, measured by the real space distance at which the PDF decays to zero, changes drastically. This extent is reduced to only 50-60 Å in the nanocrystalline samples (inset in Fig. 2), and they become spin glasses. More detailed analysis of the experimental data is under way. The outcomes will be presented elsewhere.

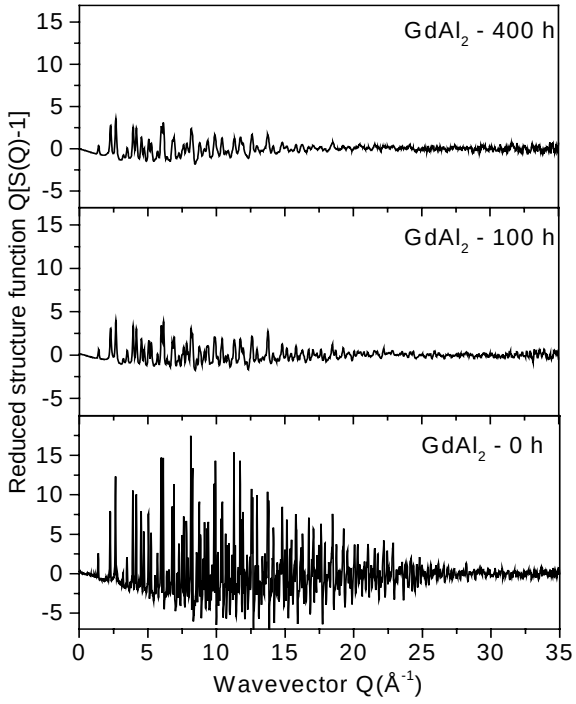

FIG. 1. Experimental structure factors Q[S(Q) - 1] of pristine and ball milled (100 and 400 h) $GdAl_2$.

Acknowledgments

Use of the APS was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. W-31-109-ENG-38.

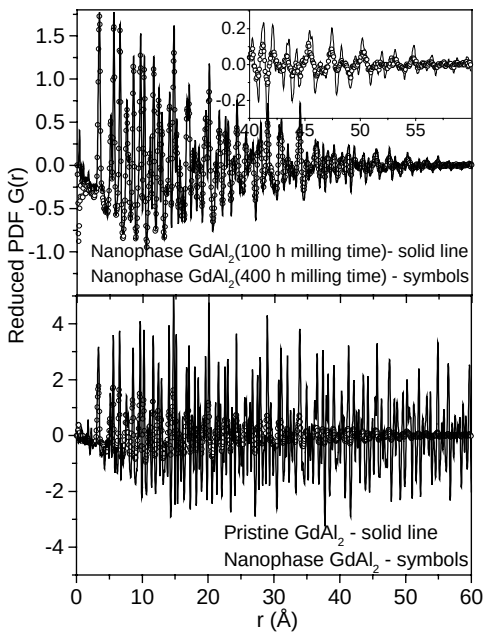

FIG. 2. Experimental PDFs for pristine and nanophase $GdAl_2$.

References

[1] V. Petkov, S. J. L. Billinge, S. D. Shastri, and B. Himmel, Phys. Rev. Lett. **85**, 3436-3439 (2000); V. Petkov, I.-K. Jeong, J. S. Jung, M. F. Thorpe, S. Kycia, and S. J. L. Billinge, Phys. Rev. Lett. **83,** 4089 (1999).

[2] V. Petkov, S. J. L. Billinge, P. Larson, S. D. Mahanti, T. Vogt, K. K. Rangan, and M. G. Kanatzidis, Phys. Rev. B **65**, 092105 (2002).