# BL-9C, 12C/ 2012G033 Structural phase transformation of intermetallic compound GdMn<sub>2</sub> by milling

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We report XAFS study on the structural phase transformation of C15 Laves phase intermetallic compound  $GdMn_2$  by mechanical milling. Milling transforms  $GdMn_2$  into the  $GdMn_{12}$  phase for 40 h; subsequent milling grows the  $Gd_6Mn_{23}$  compound at 150 h.

## 1 Introduction

Gd-Mn alloying system has a variety of intermetallic compounds such as GdMn<sub>2</sub>, Gd<sub>6</sub>Mn<sub>23</sub> and GdMn<sub>12</sub>. The C15 Laves phase GdMn<sub>2</sub> (space group *Fd-3m*) has a Néel temperature of 110 K and becomes ferromagnetic below 40 K with the Mn moment of  $1.6\mu_B$  [1]. Mechanical milling is a technique to introduce a lattice defect and to induce a structural phase transformation. We report here an example of the structural phase transformation of GdMn<sub>2</sub> by milling.

#### 2 Experiment

The ingot of GdMn<sub>2</sub> was prepared from Mn (99.99%) and Gd (99.9%) metals by arc melting. It was ground in a mortar. Milling was made upto 1000 h with a vibratory ball mill in an argon atmosphere. The weight ratio of the powdered GdMn<sub>2</sub> to balls was 1:7. Although x-ray diffraction with rotating Cu anticathode was measured as shown in Fig. 1, reflection peaks disappeared after 15 h milling because of reduced crystallite size.

#### 3 Results and Discussion

Figure 2 shows the radial structure functions for the Mn K edge of milled GdMn<sub>2</sub> at a typical milling time. As indicated by the arrow, the first peak around 2.3 Å corresponds to Mn-Mn pairs and the shoulder around 3.0 Å comes from Mn-Gd ones. These peaks at 5 h milling are exactly the same as those of no milling. The interatomic distance between Mn atoms is 2.74 Å at 5 h milling. This is the same as that of GdMn<sub>2</sub>. Therefore milling for 5 h does not affect GdMn<sub>2</sub> with the Fd-3m structure. After 10 h the first peak does not change, while the shoulder shrinks abruptly. This means that GdMn<sub>2</sub> with the Fd-3m structure is transformed gradually into GdMn<sub>12</sub> (space group *I4/mmm*) because Mn atoms has a much smaller number of Gd neighbor in GdMn<sub>12</sub> than that of GdMn<sub>2</sub>. At 40 h milling the phase transformation has been almost completed and the atomic distance of Mn-Mn pairs is 2.39 Å. Milling after 40 h till 100 h activates no phase transformation. After 100 h another phase transformation occurs and a new phase of Gd<sub>6</sub>Mn<sub>23</sub> (space group Fm-3m) appears. At 120 h the distance between Mn-Mn neighbors becomes 2.58 Å which is longer than that of GdMn<sub>12</sub>. As the Mn coordination number of Gd<sub>6</sub>Mn<sub>23</sub> is about twice larger than that of GdMn<sub>12</sub>, the first peak grows. X-ray diffraction is a powerful technique to complement these prediction about

the structural phase transformation. We will plan a synchrotron x-ray diffraction measurement.



Fig. 1: X-ray diffraction patterns of GdMn<sub>2</sub> at typical milling time.



Fig. 2: The radial structure function of GdMn<sub>2</sub> at typical milling time for the Mn K edge at 300 K.

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### <u>References</u>

[1] Y. Makihara et al., J. Phys. Soc. Jpn. 52, 629 (1983).

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