Peak Identification of Conventional X-ray Diffraction Patterns for MBE FePt Thin Films on MgO Single-crystal Substrates

H.-C. Lin
Materials Research Laboratory, Industrial Technology Research Institute, Hsinchu, Taiwan
and
H.-C. Chien, Y.-S. Huang, S.-L. Chang, and T.-C. Huang*
Department of Physics, National Tsin-Hua University, Hsinchu, Taiwan

* Visiting Professor from IBM Research Division, Almaden Research Center, San Jose, CA, USA

ABSTRACT

Conventional x-ray diffraction patterns were recorded and used for peak identification and phase determination of MBE multilayer Pt/FePt/Pt thin films on MgO single-crystal substrates. Results showed that both the FePt and the Pt layers were either epitaxially grown or strongly textured with the (110) planes parallel to the surfaces of the MgO (110) substrates. The FePt layer was ordered to the L1₀ (AuCu I) phase. An extra strong peak at 30° was identified to be the λ/2 peak of CuKα for the MgO (220) reflection. The λ/2 peak was greatly reduced using a scintillation counter with a narrow PHA window. To eliminate the λ/2 peak completely, a Xe proportional counter with a high energy resolution of 28% was used.

INTRODUCTION

Intermetallic alloy thin films of FePt have recently been found to show promising characteristics for high density recording application.¹ Magnetic and magneto-optical properties of the films were found to correlate with film structure.²³⁴ The ordered FePt phase with its c-axis in plane showed large magnetic anisotropy. The higher the order, the larger the anisotropy.

In our laboratory, we used X-ray diffraction techniques to determine the structure of FePt films. Crystalline phases presented in the films was first identified using the conventional
This document was presented at the Denver X-ray Conference (DXC) on Applications of X-ray Analysis.

Sponsored by the International Centre for Diffraction Data (ICDD).

This document is provided by ICDD in cooperation with the authors and presenters of the DXC for the express purpose of educating the scientific community.

All copyrights for the document are retained by ICDD.

Usage is restricted for the purposes of education and scientific research.

 DXC Website  
 – www.dxcicdd.com

 ICDD Website  
 - www.icdd.com
symmetric Bragg diffraction technique. In-plane crystalline structure of the films was
determined using grazing-incidence diffraction technique, while thin-film structure
perpendicular to the film surface was obtained using symmetric Bragg diffraction technique. In
this paper, we report the results of peak/phase identification of FePt films deposited on MgO
single-crystal substrates. Results on analyzing epitaxial structure of the films using grazing-
incidence technique is reported in a separated paper at this Denver X-ray Conference.\textsuperscript{5}

**EXPERIMENTAL**

Experimentally, FePt films were grown at 200° to 500° on MgO (110) single-crystals in a
VG Semicon V800M molecular beam epitaxial (MBE) system using e-gun sources for both Fe
and Pt at the IBM Almaden Research Center. The Pt and the FePt layers were grown at the rates
of 0.1 and 0.2 Å per second, respectively. The MgO (110) single-crystal substrates were
supplied by Harrick Inc. The complete structure for the films was Pt (16-32 Å)/FePt (200 Å)/Pt
(10-17 Å)/MgO. The principle layer of the film was the 200-Å FePt magnetic layer. The bottom
10-17 Å Pt layer deposited between the FePt layer and the MgO substrate served as a seed layer
for epitaxial growth of FePt on MgO (110). The surface 16-32 Å Pt layer was deposited on top
of the FePt layer to protect it from possible oxidation.

X-ray diffraction patterns of the MBE FePt films were recorded using a conventional
powder diffractometer equipped with a diffracted-beam graphite monochromator and a
scintillation counter. For high x-ray energy resolution experiments, a Xe proportional counter
was used.

**RESULTS AND DISCUSSION**

Conventional X-ray diffraction patterns for the 1133 and the 1124 films are plotted in Fig. 1.
Each pattern shows strong Cu K\(\alpha\) peaks at 33.2°, 62.4°, 68.5° and 70.5°, and they were
identified to be FePt (110), MgO (220), Pt (220), and FePt (220) reflections, respectively. The
results suggest that the (110) crystal plane of the MBE FePt and Pt layers were grown parallel to
the surfaces of the MgO (110) substrates. This indicates that both the FePt and the Pt layers
were either epitaxially grown or strongly [110] texture. Grazing-incidence X-ray diffraction analysis found the layers were epitaxially grown. The detection of a strong superlattice FePt (110) peak reveals that FePt was ordered to the L1₀ (CuAu I) phase.

![Graph](image)

Fig. 1. Conventional XRD patterns for the 1133 film (top) and the 1124 film (bottom) recorded with the pulse height analyzer (PHA) set at base = 1.0 and window = 4.5 volts.

A weak Cu Kα peak at 40.8° was also detected and identified to be the FePt (111) reflection. This indicates that a minor amount of polycrystalline FePt was also presented in the epitaxial FePt layer. In other words, the FePt layer was not 100% epitaxial. The small but sharp peak at 55.7° was identified to be the MgO (220) Cu Kβ peak from the substrate.
In each of the patterns, there is an asymmetric peak with the third strongest intensity presented at 30°. This peak is neither the Cu Kα nor the Cu Kβ peak for FePt or Pt. The d-spacing of this 30° peak agrees with that of the MgO (110). However, (110) is a forbidden reflection for MgO with Fm3m space group.

It should also be noted that the 30° peak for the 1133 film is slightly stronger than the adjacent 33° FePt (110) peak. While, the 30° peak for the 1124 film is about 25 times stronger than its FePt (110) peak.

To positively identify this extra peak, the pulse height distribution for the 30° peak and the 33° peak for the Cu Kα of FePt (110) peak were measured (Fig. 2). Fig. 2 shows the 30° peak appeared at twice the volts (or energy) of the 33° peak. In other words, the wavelength for the 30° peak was half of that of the Cu Kα radiation for the 33° peak. Thus, the 30° peak can be identified as the λ/2 peak for MgO (220), not the MgO (110) CuKα peak.

![Fig. 2. Pulse height distribution curves for the 30° (right) and the 33° peaks (left).]
Since the energy resolution for the scintillation counter was not high (i.e., 58%, see Fig. 2), it is difficult to eliminate the λ/2 peak completely. The diffraction pattern for the 1133 film recorded using a much narrower PHA window (W) of 2.2 volts is plotted in Fig. 3. The λ/2 peak at 30° has now been greatly reduced (by an order of magnitude) to a very small peak on the low-angle tail of the much stronger 33° peak.

![Diffraction pattern for the 1133 film recorded with W=2.2 volts.](image)

Fig. 3. Diffraction pattern for the 1133 film recorded with W=2.2 volts.
The 28.5°-35.0° section of the diffraction patterns for the 1133 and the 1124 films was plotted at Fig. 4. It shows that the effect in using a small PHA window of \( W = 2.2 \) volts on the 1124 film was less dramatic because the \( \lambda/2 \) peak at 30° was originally much stronger than the FePt (110) peak at 33° (also see Fig. 1).

Fig. 4. A small section of the diffraction patterns for the 1133 and the 1124 films: 
\( W = 4.5 \) volts (light line) and \( W = 2.2 \) volts (heavy line).
To completely eliminate the \( \lambda/2 \) peak, a detector with a high energy resolution such as a solid-state or a proportional counter\(^7\) can be used. For example, the energy resolution of a proportional counter is significantly better than that of a scintillation counter. The pulse height distribution curve for a Xe proportional counter is plotted in Fig. 5. The energy resolution of the counter is 28\%, about a factor of 2 improvement over the scintillation counter. Using the Xe proportional counter, the \( \lambda/2 \) peak at 30\(^\circ\) can be eliminated.

\[ W / H = 28\% \]

![Pulse height distribution curves for the FePt (110) peak at 33\(^\circ\).](image)

Fig. 5. Pulse height distribution curves for the FePt (110) peak at 33\(^\circ\).
A small section (29°-35°) of the diffraction patterns for the MgO (220) $\lambda/2$ peak and the FePt (110) CuKα peak for the 1124 film is plotted in Fig. 6. The $\lambda/2$ peak at 30° was successfully eliminated using the Xe proportional counter, but not when a scintillation counter was used.

Fig. 6. A section of the diffraction patterns for the 1124 film.

REFERENCES