The Thermal Stability and Nitrogen Distribution in Epitaxial (110) FeTiN Films

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Objectives

- Investigate the distribution of interstitial nitrogen atoms inside epitaxial bcc $\alpha$-FeTi lattices

- Study the origin of the anisotropy of FeTiN thin films

- Study the role of nitrogen in the thermal stability of the anisotropy of polycrystalline FeTiN thin films
Background

- Origin of the anisotropy:
  free energy induced by interstitial nitrogen in bcc α-Fe lattice\[^1\]:

\[
F' = D(\alpha_1^2 C_x + \alpha_2^2 C_y + \alpha_3^2 C_z) + \frac{RT}{2VC_0}(C_x^2 + C_y^2 + C_z^2)
\]

- Mobility of nitrogen atoms cause instability \[^2\]

- Study the thermal stability of nitrogen atoms: WHERE are the nitrogen atoms?

\[^1\] G. De Vries, Physica 25, 1211 (1959)
Experimental

Deposition:
Sputtering deposition on KEY system
H-Si(100)/Cu(100) 2000Å/FeTiN(110) 1000Å
The FeTiN was sputtered at 35W, 0.45mT, 1.2 Å/S[1]

Lattice fit:

Cu<110> 5.112 Å//
Si(100) 5.431 Å
Fe<111> 4.965 Å//
Cu<110> 5.112 Å

Lattice Structure

Four-fold lattice structure

X-Ray $\phi$ angle scan of FeTi(200) with $2\theta=64.5^\circ$ and $\psi=45^\circ$. The angle $\phi$ is relative to Cu[100] direction.
Lattice Distortion

Calculation of lattice constant $a$ (x-axis) by

$$a = \frac{C_x (1.01) - 2(C_y + C_z)0.12}{C_{FT}} + a_0$$

Where $C_x$, $C_y$, $C_z$ are N concentrations and $C_{FT}$ is the amount of Fe and Ti

Fit is good below 4% N

The $d(200)/d(020)$ spacings measured at $\psi = 45^0$ and $d(002)$ values measured at $\psi = 88^0$. 
Lattice Distortion

Calculation of lattice constant \( d(110) \) by assuming

\[
a(b) = \frac{C_x (1.01) - 2(C_y + C_z)0.12}{C_{FT}} + a_0 (b_0)
\]

Then

\[
d(110) = \sqrt{a^2 - (\sqrt{2}c / 2)^2}
\]

\[
\Delta d(110)/d(101) \sim \frac{1}{2} \Delta d(110)
\]

Fit is reasonable below 4% N.

The \( d(110) \) spacings measured at \( \psi=0^\circ \), and \( d(110)/(d101) \) values measured at \( \psi= 60^\circ \).
FMR Measurement

K band FMR $f_0=25.67\text{GHz}$

In-plane measurement geometry

Resonance field vs. direction of DC field relative to Cu[100] direction ($\theta$)
The calculation of crystalline anisotropy constant $K_1$

$$F = K_1(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2)$$

Inside (110) plane:

$$F = K_1\left(\sin^4 \theta + \sin^2 \theta \cos^2 \theta\right)$$

Consider four lattice orientations:

$$K_1 = Ms \cdot \left[\hat{H}(\theta' = 45^\circ) - \hat{H}(\theta' = 0^\circ)\right]/2.34$$

Figure: Anisotropy constant $K_1$ vs. nitrogen concentration
Conclusions

• In epitaxial FeTiN (110) films, at low nitrogen concentration (<~4at%), nitrogen atoms tend to occupy the sites between (110) planes (x,y sites), this trend seems to be growth related.

• At higher nitrogen concentration (>~4at%), the sites inside (110) planes (z sites) are preferred.

• In-plane magnetocrystalline anisotropy tends to decrease when z sites are preferentially occupied.

• Direct coupling between magnetization and an occupied site was observable due to the four-fold lattice structure, so single crystal films will be deposited in further studies. (manuscript in press, J. Appl. Phys. 2002)