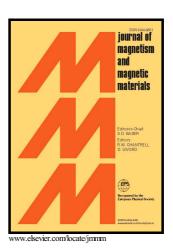
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### ACCEPTED MANUSCRIPT

# Thin film phase diagram of iron nitrides grown by molecular beam epitaxy

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#### Abstract

A low-temperature thin film phase diagram of the iron nitride system is established for the case of thin films grown by molecular beam epitaxy and nitrided by a nitrogen radical source. A fine-tuning of the nitridation conditions allows for growth of  $\alpha'$ -Fe<sub>8</sub>N<sub>x</sub> with increasing c/a-ratio and magnetic anistropy with increasing x until almost phase pure  $\alpha'$ -Fe<sub>8</sub>N<sub>1</sub> thin films are obtained. A further increase of nitrogen content below the phase decomposition temperature of  $\alpha'$ -Fe<sub>8</sub>N (180 °C) leads to a mixture of several phases that is also affected by the choice of substrate material and symmetry. At higher temperatures (350 °C), phase pure  $\gamma'$ -Fe<sub>4</sub>N is the most stable phase.

 $\it Keywords: \,\,$ iron nitride, molecular beam epitaxy, thin films, phase diagram, nitrides, FeN

#### 1. Introduction

The iron nitride system has attracted the interest of researchers for several decades due to the large variety of mechanical, electrical, and magnetic properties of the different occurring phases [1, 2, 3]. Magnetically,  $\alpha$ -Fe is a soft magnetic material with large magnetization of 1714 emu/cm³ (2.15 T) and low magnetocrystalline anisotropy of  $4.8 \times 10^5 \, \mathrm{erg/cm}^3$  ( $4.8 \times 10^4 \, \mathrm{J/m}^3$ ) [4]. For small nitrogen concentrations, the nitrogen interstitial atoms lead to an enhanced volume of the unit cell and induce tetragonality (c/a > 1) into the lattice. The first effect leads to an enhanced absolute magnetization [5], the second effect leads to an increased magnetic anisotropy [6].  $\alpha$ -Fe with nitrogen interstitials,  $\alpha$ -FeN<sub>x</sub>, is not a thermodynamical phase in itself, but the additional nitrogen can be used to tune magnetic properties by distorting the lattice in c-axis direction. Only at a particular nitrogen content, an ordered phase occurs,  $\alpha''$ -Fe<sub>16</sub>N<sub>2</sub> while the unordered equivalent with the same nitrogen content is termed  $\alpha'$ -Fe<sub>8</sub>N.  $\alpha''$ -Fe<sub>16</sub>N<sub>2</sub> exhibits a high ferromagnetic moment with

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