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Layer-by-layer growth of thin epitaxial Fe_3Si films on GaAs (001)

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Abstract

Molecular beam epitaxy of Fe_3Si films on GaAs (001) is studied in situ by grazing incidence X-ray diffraction. Fe_3Si grows layer-by-layer. During deposition the growth front roughens as indicated by the damping of the X-ray oscillations and corresponding atomic force micrographs. The X-ray oscillations are modified during growth at substrate temperatures of 180 °C and below.

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Keywords: MBE; X-ray diffraction; Surface topography; Ferromagnetic materials

1. Introduction

The combination of magnetic and semiconducting materials is investigated for the development of semiconductor devices utilizing the spin of the carriers [1]. Epitaxial ferromagnet/semiconductor heterostructures should possess a rather perfect interface [2] as well as high thermal stability. These properties are regarded as prerequisites for high performance operation. Fe_3Si on GaAs is a promising candidate for spintronics applications [3–5]. It can be grown by molecular beam epitaxy (MBE) at GaAs substrate temperatures near 200 °C [6]. The Curie temperature of Fe_3Si is as high as 567 °C [7]. Spin injection at room temperature has been demonstrated [8]. The lattice misfit between stoichiometric Fe_3Si and GaAs is rather small [6]. The interface between Fe_3Si and GaAs is found to be smooth and of good structural perfection [9]. Fe_3Si has the face centered cubic $D0_3$ structure [10,11,18]. This structure is an fcc lattice with a basis consisting of four atoms A, B, C, and D with the coordinates A(0, 0, 0), B(0.25, 0.25, 0.25), C(0.5, 0.5, 0.5), and D(0.75, 0.75, 0.75). In the ordered Fe_3Si crystal, Fe atoms occupy the three sublattices A, B, and C, while Si atoms fill the sublattice D. The ordered alloy can be regarded as a magnetic Heusler alloy $Fe(B)Fe(A, C)_2Si(D)$ with the two distinct Fe sites (A, C) and (B) [11,12]. The order in Heusler alloys [13] has significant influence on their electric and magnetic properties: the magnetic moments of the Fe atoms at the positions Fe(A, C) linearly depend on the number of nearest Fe neighbors [14,15]. A highly ordered and stoichiometric Fe_3Si matrix is the starting point for most experiments with Fe_3Si.

The layer-by-layer growth mode during MBE allows the controlled fabrication of epitaxial layer sequences with very sharp interfaces between them. The aim of the present work is the in situ characterization of the Fe_3Si epitaxial growth process in the layer-by-layer growth mode by surface diffraction methods. The long-range order in the films is monitored as well. We utilize grazing incidence X-ray diffraction (GID). It is ideally suited for thin film investigation, since it gives access to reflections which cannot be measured by conventional diffraction methods and can be tuned to high surface sensitivity by using bulk forbidden diffraction maxima.

2. Experimental

The Fe_3Si films were grown by solid source MBE in the chamber built into the diffractometer at the wiggler beamline U125/2 KMC (PHARAO) [16] at the storage ring BESSY in Berlin, Germany. The GaAs (001) templates were prepared in a separate III–V growth chamber using standard GaAs growth techniques. The sample was then capped by As and transferred into the system at BESSY for the Fe_3Si deposition by means of an UHV shuttle. The As cap was removed by annealing the sample in the preparation chamber before transferring it into the growth chamber. Then the Fe_3Si layers were grown under X-ray

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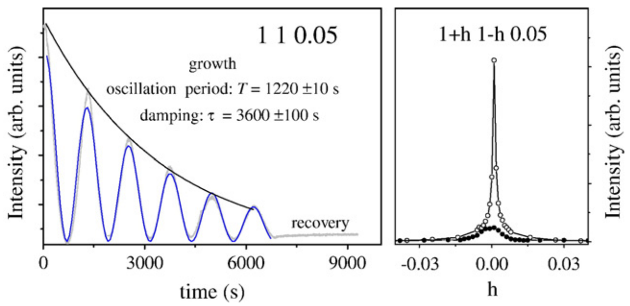

Fig. 1. (a) (Color online) X-ray oscillations (gray line) with a period T observed by GID during the MBE growth of an Fe_3Si epitaxial layer on GaAs (001) at a substrate temperature of 220 °C. For the determination of the period T and the decay time τ the measured curve is approximated by a function $\sim \sin^2(\pi t/T) \exp(-t/\tau)$ (blue line). (b) Scans across the diffraction peak near a maximum (hollow circles) and a minimum (full circles) of the oscillations. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

control on the As-rich GaAs surface at different substrate temperatures near 200 °C with a growth rate of 3 ML h^{-1}, similar as described in Ref. [6]. The Si and the Fe cell temperatures were tuned in order to obtain perfect stoichiometry of the films. During this process the Si content of the film was obtained from the position of the Fe_3Si layer peak on the X-ray diffraction curve. We obtained optimum temperatures of 1239 °C and 1370 °C for the Fe and the Si cells, respectively, and achieved an almost perfect stoichiometry of the samples during and after the growth. An anneal of the surface at 310 °C for about 1 h together with the growth of 1 ML of Fe_3Si improved the quality of the Fe_3Si surface considerably, i.e. the intensity of the X-ray surface reflection increased. All the X-ray oscillations shown in this work were obtained after such an annealing procedure. For the X-ray measurements a double crystal Si (111) monochromator and a six-circle X-ray diffractometer [16] were used. The energy of the radiation was 10 keV. The incidence angle was 0.3°. The acceptance angle of the detector was 0.1° both perpendicular and parallel to the surface. Some of the samples were characterized ex situ by AFM almost immediately after the growth. A Dimension 3100

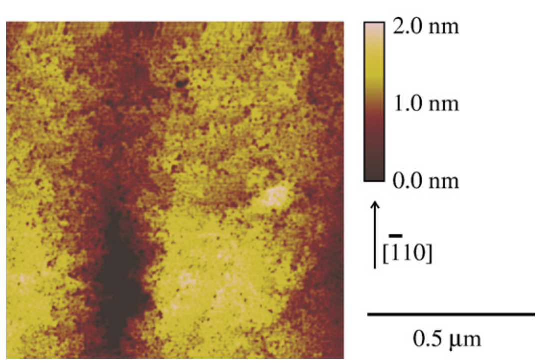

Fig. 2. (Color online) AFM micrograph of the Fe_3Si epitaxial layer surface after quenching. Details are described in the text. Terrace widths of about 50 nm can be recognized. The terrace edges are not straight but show a dendritic shape with many kinks. Small islands are visible as well. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

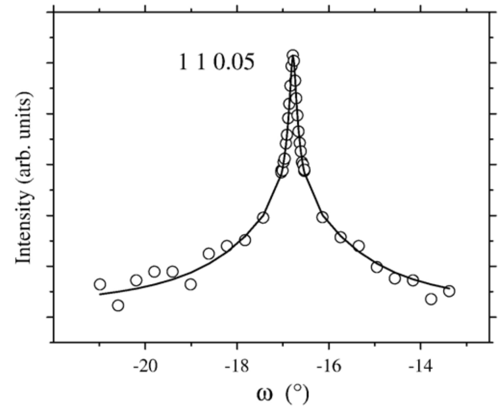

Fig. 3. Diffraction curve (circles) obtained near the maximum 1 1 0.05 by an in-plane rocking scan around the surface normal of the sample immediately before quenching the sample and transferring it to the AFM measurement. The curve can be fitted by two Lorentzian functions (full line) of the different widths 0.12° and 2.0° corresponding to length scales of 55 nm and 3 nm in real space.

scanning probe microscope supplied by Veeco was used for this purpose.

3. Results

During deposition of Fe_3Si by MBE, layer-by-layer growth oscillations are observed (see Fig. 1). For the filling Θ of each terrace level a parabolic dependence of the Bragg diffracted intensity $I_B = (1-2\Theta)^2$ is expected in the ideal two level case [17]. However the measured curve exhibits a damping, indicating that several terrace levels contribute to the diffracted intensity as confirmed by AFM measurements shown in Fig. 2. For practical determination of the oscillation period T and the time constant of the intensity decay τ we approximated the intensity oscillations by a function $\sin^2(\pi t/T) \exp(-t/\tau)$. We see from the oscillations

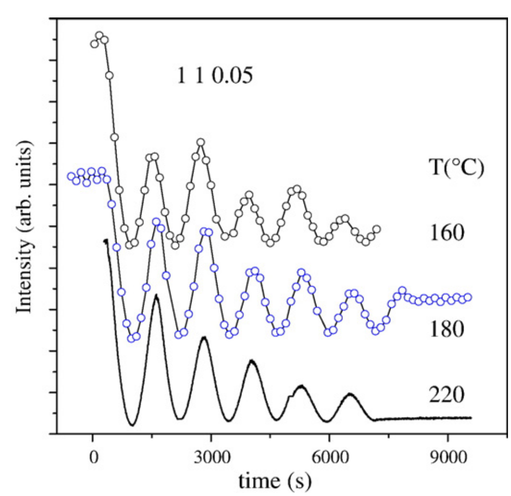

Fig. 4. (Color online) Comparison of the X-ray oscillations measured at the maximum 1 1 0.05 during Fe_3Si growth at the different substrate temperatures 160 °C (black circles), 180 °C (blue circles), and 220 °C (full line). Each open circle corresponds to a rocking curve measurement like in the previous figure. The curve for 220 °C is a measured time dependence of the diffracted intensity. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)