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Structural and hyperfine magnetic properties of Fe_3Si thin films grown at low temperature

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Abstract

Fe_3Si thin films were prepared in ultrahigh vacuum by codeposition of ^{57}Fe and Si onto various substrates (Si(100), NaCl(100) and KCl(100)) held at 130 K. The structural properties were determined by X-ray diffraction, transmission electron microscopy and Mössbauer spectroscopy. Our results demonstrate that Fe_3Si films prepared on substrates with a lattice parameter similar to that of Fe_3Si (Si(100) and NaCl(100)) grow in the crystalline disordered B2 structure (with Fe_3Si/Si(100)being epitaxial), while Fe_3Si films on KCl(100) substrates (with a lattice parameter deviating strongly from that of Fe_3Si) grow predominantly in the amorphous structure. The low-T growth of epitaxial Fe_3Si/Si(100) films could be an approach for suppression of interfacial interdiffusion in Fe_3Si/Si(100) heterostructures for potential magnetoelectronics applications.

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1. Introduction

Fe-rich Fe–Si alloys are of great scientific and technological interest [1–7]. The ferromagnetic ordered $D0_3$ structure (space group: $Pm\bar{3}m$) of Fe_3Si has two Fe–Sites;one site (Fe(A)) whose environment is different from that of elemental bcc-Fe, and the other one (Fe(B)) whose nearest-neighbor coordination number is 8, identical to that of elemental bcc-Fe. The Fe(A) atom also has 8 nearest-neighbor (nn) atoms, however, only 4 of them are the iron atoms, which are the Fe(B) atoms, and the other 4 atoms are the Si(C) atoms. Fe_3Si can be regarded as a Heusler alloy: $Fe(B)Fe(A)_2Si(C)$. Heusler alloys in thin film form are currently attracting much interest due to their potential for applications in future magnetoelectronics/spintronics devices, e.g., as possible spin injector electrodes in tunnel magnetoresistance structures [1,2], in spin valves to increase the giant magnetoresistance effect [3], or for spin polarized current injection into semiconductors [4–7].

It is also possible to produce amorphous Fe–Si alloys. Atomic deposition techniques producing high cooling rates led to Fe_xSi_{1-x} amorphous material in a large composition range ($0 \le x \le 0.8$) [8–11]. In the past, amorphous Fe_3Si alloys were obtained by vapour deposition onto liquid nitrogen cooled amorphous substrates being either glass plates, polyimid (kapton) foils, fused silica or carbon covered grids [8,9].

Hitherto no literature reports exist dealing with the question whether *crystalline* Fe_3Si thin films grown by vacuum deposition at low temperature can be stabilized on appropiate substrates. Especially in the case of Si substrates the answer is of great interest, as for high-efficiency electrical spin injection from a ferromagnet to a semiconductor a sharp interface between them is required. Therefore, low-temperature growth at or even below room temperature (RT) might be essential in order to suppress interdiffusion between the Fe_3Si film and the Si substrate.

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In this paper we report on the structural and hyperfine magnetic properties of thin Fe_3Si films grown by codeposition in ultrahigh vacuum (UHV) on various substrates at low temperature. The results were obtained by X-ray diffraction (XRD), transmission electron microscopy (TEM) and ^{57}Fe conversion electron Mössbauer spectroscopy (CEMS).

2. Experimental details

The Fe_3Si films were synthesized on various substrates in a molecular beam epitaxy system (base pressure: 5×10^{-10} mbar). The NaCl(100)-, KCl(100)- and Si(100)-substrate surfaces were first cleaned by using isopropanol. Additionally the Si(100)-wafer was cleaned with 50% HF solution. After insertion into the ultrahigh vacuum system, the NaCl(100)- and KCl(100)-substrates were heated at 150 °C, while the Si(100)-substrate was heated at 900 °C to remove surface contaminants. On KCl (100)- andSi(100)-substrates nominally 10-nm thick $^{57}Fe_3Si$ films were grown at 130 K by co-deposition of ^{57}Fe and Si. Nominally 40-nm thick natural Fe_3Si films on NaCl(100) were prepared at 130 K by alternate deposition of 0.04-nm thick ^{nat}Fe- and 0.0288-nm thick Si-layers (digital alloys). In each case the pressure during growth was 5×10^{-9} mbar and the deposition rates were 0.002 nm/s (^{57}Fe and natural Fe) and 0.0029 nm/s (Si). High-purity materials (^{57}Fe: 99.95 at.% with isotopical enrichment of 95%; ^{nat}Fe (natural Fe): 99.9985 at.%; and Si: 99.999 at.%) were evaporated from resistively heated Knudsen cells (^{57}Fe and natural Fe) or from an electron gun (Si). The deposition rates and the film thicknesses were measured by two independent calibrated quartz crystal oscillators. The composition given for the samples is the nominal composition as determined from the ^{57}Fe (or ^{nat}Fe) and Si deposition rates.

CEM spectra were measured at RT by mounting the sample in a He/CH_4^- proportional counter, and by using a ^{57}Co source (Rh matrix). For the least-squares fitting of the CEM spectra, the NORMOS computer program by Brand [12] was used. Θ–2θ X-ray diffraction was performed ex-situ at RT by using a Cu anode and a graphite monochromator ($\lambda_{K\alpha}=0.154178$ nm). For TEM, a commercial electron microscope (Philips Tecnai F20 Super Twin with 200 kV) was used.

3. Results and discussion

3.1. Structural investigations

In the XRD pattern of the 10-nm thick Fe_3Si film on KCl (100) (Fig. 1(a)), at a first glance only the strong reflections of the KCl substrate (and no other Bragg peaks from Fe_3Si) seem to exist, demonstrating the predominance of the amorphous structure of this Fe_3Si film. However, closer inspection shows that a weak peak in the harrow-like XRD pattern exists near about 41°. Undistorted Fe_3Si has no Bragg reflection at 41°. However, we cannot completely exclude that the weak Bragg peak at about 41° results from the $Fe_3Si(220)$ reflection of a small fraction of possibly strongly distorted (epitaxial) crystalline Fe_3Si in the Fe_3Si/KCl(100) film due to the large lattice

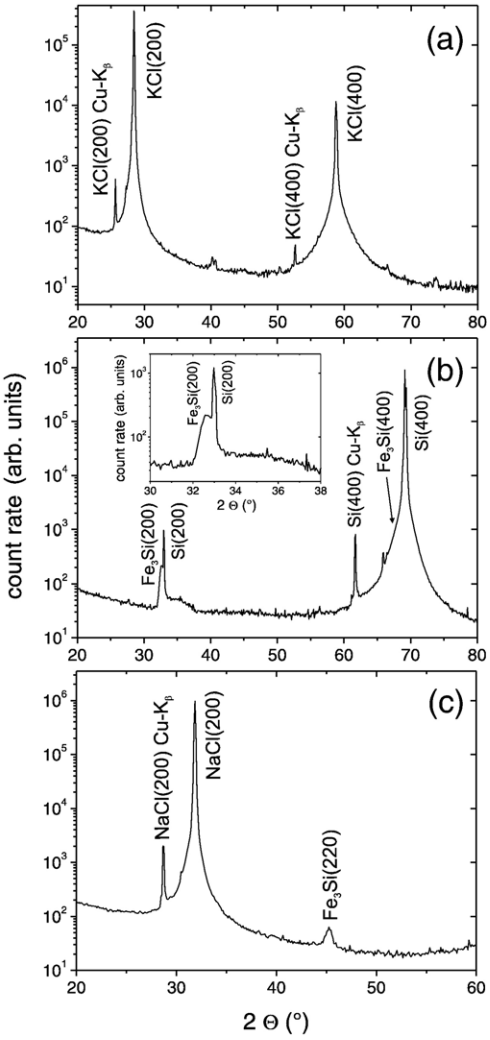

Fig. 1. θ–2θ X-ray diffraction diagrams at RT of the various Fe_3Si films grown on KCl(100) (a), Si(100) (b) and NaCl(100) (c). The insert in (b) shows a magnification of the range between $2\theta=30$ and 38°.

mismatch (− 10.2%) between the KCl(100) substrate and the film. We conclude that the Fe_3Si/KCl(100) film consists predominantly of the amorphous structure, but a small fraction of heavily strained crystalline Fe_3Si cannot be excluded. We have checked the latter possibility by TEM (see below).

Fig. 1(b) displays the XRD pattern of the 10-nm thick $^{57}Fe_3Si$ film on Si(100). We clearly observe a Bragg peak at 32.62° corresponding to the $Fe_3Si(200)$ reflection of the B2 structure, while at 68.34° the fundamental $Fe_3Si(400)$ reflection is barely visible as a weak shoulder of the Si(400) peak. The (n00) peaks are the only observable reflections due to the epitaxial relation $Fe_3Si(100)$ || Si(100) of the film. (The peak at $2\theta=33.05°$ is a Si(200) reflection which is theoretically forbidden but appears experimentally; it originates from the Si (400) Bragg reflection of half the wavelength of the Cu-K_α radiation, the half wavelength being present in the white radiation background and passing the graphite monochromator.) For the lattice spacing perpendicular to the surface a value of 0.549(5) nm at RT was deduced by XRD. This value is slightly smaller than the corresponding value of 0.5653 nm for bulk-