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The regularities of phase formation in $Fe_3Si(111)/Si(111)$ structure at vacuum annealing

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Abstract. The regularities of phase formation and thermal stability in $Fe_3Si(111)/Si(111)$ structure at stepped vacuum annealing (350, 450 and 550 °C) were investigated. The layer of 32 nm Fe_3Si was deposited onto Si(111) substrate by molecular beam epitaxy at 260 °C. Transmission electron microscopy (TEM) measurements demonstrated that the film thickness increases by ~19 % at 350 °C annealing without changing the phase composition. The polycrystalline ε-FeSi sublayer was formed on the interface at 450 °C annealing. Further annealing at 550 °C led to the ~ 80 nm polycrystalline film formation containing the crystallites of ε-FeSi, Fe_5Si_3, and β-$FeSi_2$ phases.

1. Introduction

Recently, one of the perspective directions in the field of electronics is the study of ferromagnetic/semiconductor heterostructures and the creation of integrated circuits based on them [1, 2]. The basic characteristics of the ferromagnetic layer in ferromagnetic/semiconductor heterostructures are high Currie temperature and high spin polarization level. The iron silicide Fe_3Si with DO_3 structure (Currie temperature is 840 K [3], spin polarization is about 40 % [4]) is an attractive ferromagnetic material for spintronic devices [5, 6]. There is a series of papers [7–10] discussing the growth conditions optimization, studying the structure and physical properties of epitaxial Fe_3Si films and Fe_3Si-based multilayer structures grown on various substrates (Si, Ge, GaAs).

However, the problem of phase formation and thermal stability in the $Fe_3Si(111)/Si(111)$ structure shown in the present study was not previously discussed.

2. Experiments

The Fe_3Si thin films were deposited by molecular beam epitaxy technique in ultrahigh vacuum ($1.3 \cdot 10^{-8}$ Pa) onto atomically pure *n*-type Si(111) substrate. The substrate preparation, growth and growth control technology is identical for the films studied in [6, 10], except that the growth temperature was raised to 260 °C. The thickness of as-grown films was 32 nm according to the ellipsometry data. When deposition was finished $Fe_3Si(111)/Si(111)$ structures were annealed at different temperatures: 350, 450 and 550 °C, respectively for 1 h at 10^{-7} Pa.

As-grown and annealed structures were characterized by transmission electron microscopy (Hitachi HT-7700 microscope operating at 100 kV) at "plan-view" and "cross-section" mode. The "plan-view" specimens were prepared by mechanical lapping and polishing, followed by Ar+ ion milling according to standard TEM techniques. The "cross-section" samples were prepared by Hitachi FB-2100 single-beam focused ion beam (FIB) system using FIB technique described in [10].

3. Results and discussion

Figure 1 shows the TEM study results of as-grown $Fe_3Si(111)/Si(111)$ specimen.

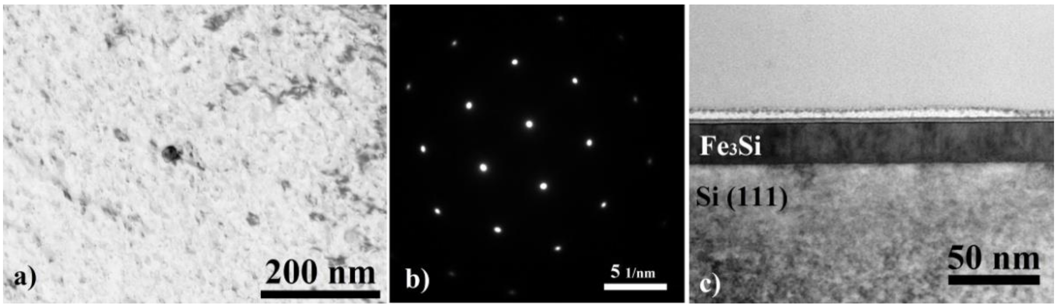

Figure 1. TEM images of as-grown $Fe_3Si(111)/Si(111)$ specimen: **(a)** – "plan-view" image; **(b)** – the SAED pattern corresponding to image (a); **(c)** – "cross-section" image.

The silicide film thickness is 32 nm. The "cross-section" image (figure 1(c)) demonstrates linear and sharp interface between Fe_3Si and Si(111) without a reaction sublayer, which indicates a high quality of the grown silicide film. The selected area electron diffraction (SAED) pattern corresponds to the Fe_3Si phase with the DO_3 structure.

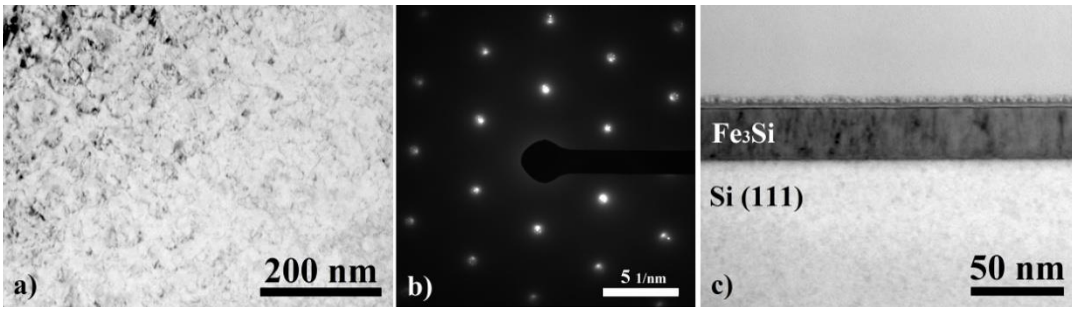

Figure 2. TEM images of 350 °C annealed $Fe_3Si(111)/Si(111)$ specimen: **(a)** – "plan-view" image; **(b)** – the SAED pattern corresponding to image (a); **(c)** – "cross-section" image.

The structure and phase composition of $Fe_3Si(111)/Si(111)$ specimens are not changed at 350 °C annealing (figure 2).

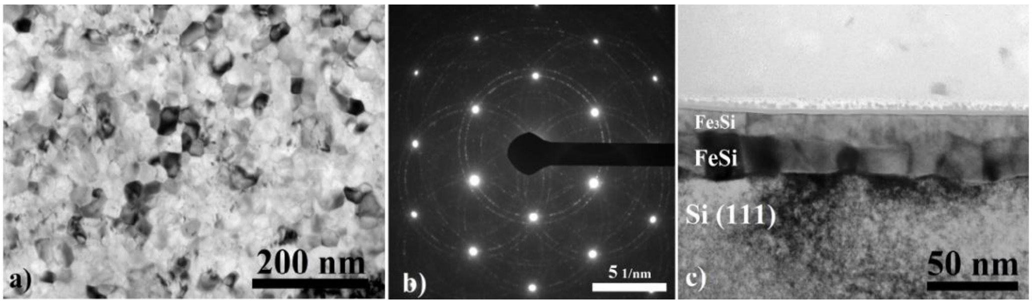

Figure 3. TEM images of 450 °C annealed $Fe_3Si(111)/Si(111)$ specimen: **(a)** – "plan-view" image; **(b)** – the SAED pattern corresponding to image (a); **(c)** – "cross-section" image.

The interface between the film and the substrate is still linear and sharp (figure 2(c)). However, the film thickness increased by 6 nm. This fact indicates the diffusion processes occurring on the interface. Figure 3 demonstrates the formation of polycrystalline sublayer at the $Fe_3Si(111)/Si(111)$ interface after 450 °C annealing. The SAED pattern (figure 3(b)) corresponds to single-crystal Fe_3Si and polycrystalline ε-FeSi phases. The ε-FeSi layer thickness varies from 10 to 45 nm, the average thickness is about 30 nm with linear crystallite sizes of 20 to 50 nm (figure 3(a), (c)).

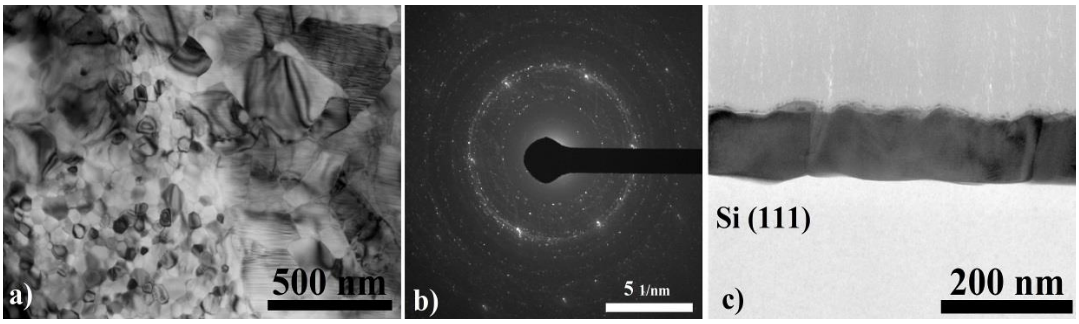

Figure 4. TEM images of 550 °C annealed $Fe_3Si(111)/Si(111)$ specimen: **(a)** – "plan-view" image; **(b)** – the SAED pattern corresponding to image (a); **(c)** – "cross-section" image.

At 550 °C annealing a polycrystalline film of iron silicides was formed (figure 4). The TEM studies results showed the presence of ε-FeSi phase "islands" with crystallite sizes from 30 to 100 nm surrounded by a matrix composed of the Fe_5Si_3 and β-$FeSi_2$ crystallites with crystallite sizes from 100 to 500 nm (figure 4(a), (b)). The average thickness of the film increased to 80 nm.

4. Conclusions

The regularities of phase formation in $Fe_3Si(111)/Si(111)$ structure at stepped vacuum annealing (350, 450 and 550 °C) were investigated. During the annealing at 350 °C the film thickness increased by ~19 % due to diffusion. The structure and phase composition not changed. The polycrystalline ε-FeSi phase sublayer with the thickness of 10 to 45 nm, and crystallite sizes from 20 to 50 nm was formed on $Fe_3Si(111)/Si(111)$ interface at 450 °C annealing. After annealing at 550 °C the polycrystalline film composed of β-$FeSi_2$ and Fe_5Si_3 phases crystallites with crystallite sizes from 100 to 500 nm and ε-FeSi phase "islands" with crystallite sizes from 30 to 100 nm was formed. The film thickness increased to ~80 nm.

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