

## Effects of Annealing on Atomic Interdiffusion and Microstructures in Fe/Si Systems\*

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**Abstract:** Pure metal Fe films with thickness of about 100nm were deposited on Si (100) substrates by DC magnetron sputtering. Annealing was subsequently performed in a vacuum furnace in the temperature range of 600~1000°C for 2h. The samples were characterized by means of Rutherford backscattering (RBS) with 3MeV carbon ions. The RBS data were fitted with SIMNRA 6.0, and the results show the atomic interdiffusion in Fe/Si systems. The microstructures and crystal structures were characterized by scanning electron microscope and X-ray diffraction. The effects of annealing on atomic interdiffusion, silicide formation, and microstructures in Fe/Si systems were analyzed.

**Key words:** magnetron sputtering; annealing; RBS; atomic interdiffusion; microstructure

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### 1 Introduction

Semiconducting iron disilicide  $\beta$ -FeSi<sub>2</sub> with orthorhombic structures in Fe/Si systems has attracted much attention as a novel optoelectronic material with potential for practical applications<sup>[1~4]</sup> in recent years.  $\beta$ -FeSi<sub>2</sub> is regarded as a quasi-direct band-gap semiconductor with a gap value in the range of 0.83~0.87eV<sup>[5~8]</sup>, which corresponds to an optical wavelength of 1.5 $\mu$ m close to the absorption minimum of silica optical fibers. Furthermore, this material has other favorable characteristics, such as high photo absorption in the infrared region, large thermoelectric coefficients, and high conversion efficiency for solar cells<sup>[9~11]</sup>, as well as the possibility of epitaxial growth on Si substrates<sup>[12,13]</sup> that is fully compatible with existing technology of silicon-based integrated circuits. Accordingly, it is expected to have practicable application in light-emitting diodes, infrared detectors, and solar cells<sup>[14~16]</sup>. Moreover,  $\beta$ -FeSi<sub>2</sub> is also nontoxic and an 'ecologically friendly' material<sup>[17]</sup> abundantly available in the

Earth's crust.

Various techniques for producing semiconducting  $\beta$ -FeSi<sub>2</sub> thin film or precipitates on Si substrate have been investigated. Usually, metal Fe films or (Fe/Si)<sub>n</sub> multilayer films are pre-deposited on Si substrates by ion beams implantation<sup>[18]</sup>, molecular beam epitaxy<sup>[19]</sup>, electron-gun evaporation<sup>[20]</sup>, chemical vapor deposition<sup>[21]</sup>, laser assistant deposition<sup>[22]</sup>, ion beam sputtering, or magnetron sputtering (MS) deposition<sup>[23,24]</sup>. Then  $\beta$ -FeSi<sub>2</sub> thin film or precipitates are produced by solid phase synthesized via one or two thermal process steps, such as annealed in a conventional furnace flowing with some kind of protective atmosphere<sup>[25]</sup>, annealed in a vacuum furnace<sup>[26]</sup>, ion beam mixing (or irradiation)<sup>[27]</sup>, laser scanning (or irradiation)<sup>[28]</sup>, rapid thermal annealing (RTA)<sup>[29]</sup>, RTA then common annealing<sup>[30]</sup>, or irradiating by ion beams or laser then common annealing<sup>[31,32]</sup>. It can also be synthesized directly by reaction deposition Fe films on heating Si substrates<sup>[33]</sup>, or synthesized by co-deposited Fe and Si with certain ratios on Si or non-Si substrates and subsequently thermally processed<sup>[34,35]</sup>. In or-

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der to obtain large area, homogeneous, single phase  $\beta$ -FeSi<sub>2</sub> film, the MS method is good because it is the most economical technique and is widely used in the micro-electronic industry.

According to the phase diagram<sup>[3]</sup>, there are at least three stable phases in a Fe/Si system. They are metal-rich silicide Fe<sub>3</sub>Si, intermediate phase FeSi, and silicon-rich disilicide FeSi<sub>2</sub>. In the region of the disilicide composition three phases are distinguished: high temperature phase  $\alpha$ -FeSi<sub>2</sub> with tetragonal structure, low temperature stable phase  $\beta$ -FeSi<sub>2</sub> with orthorhombic structure, and metastable phase  $\gamma$ -FeSi<sub>2</sub> with cubic structure. The formation temperatures of different phases depend on not only the deposition condition but also the thickness of the film. Among the iron silicides, intermediate phase FeSi is also a semiconductor<sup>[36]</sup> except  $\beta$ -FeSi<sub>2</sub>. FeSi is a magnetic semiconductor with an extremely narrow band gap and it is expected to have applications in spintronics. It is difficult to get a single phase of  $\beta$ -FeSi<sub>2</sub> because Fe<sub>3</sub>Si, FeSi and FeSi<sub>2</sub> can usually coexist in the same temperature range during the process of silicides film growth in a Fe/Si system. In spite of the fact that the silicidation of the Fe/Si system has been investigated previously<sup>[37~39]</sup>, atomic diffusion and the sequence of phase formation in a Fe/Si system is still not clear. In order to obtain large area, high quality, single phase  $\beta$ -FeSi<sub>2</sub> film, some details need to be clarified. In this work, a group of Fe/Si samples was prepared by the DC MS method under the same condition; subsequently these samples were annealed at various temperatures for 2h. The effects of annealing on atomic interdiffusion, silicide formation, and microstructure in Fe/Si systems were investigated by means of Rutherford backscattering (RBS), scanning electron microscope (SEM), and X-ray diffraction (XRD).

## 2 Experiment

The 100nm thin Fe films were deposited by a JGP 560 magnetron sputtering system onto Si (100) substrates (p-type,  $7 \sim 13\Omega \cdot \text{cm}$ ) at Guizhou University, China. The Si wafers were ultrasonically cleaned for 10min in acetone, ethanol, and deionized water one after another before mounting in the chamber. The target for the puri-

ty of the Fe was 99.95%. The base pressure was  $2 \times 10^{-5}$  Pa and the Ar pressure was 2.0 Pa during the sputtering process. The sputtering power was 100W, the Ar flux was 20sccm, and a 50V minus bias was put on substrates. The deposition rate was 10nm/min, deposition time was 10min, and the substrates were held at room temperature. The Fe film thickness was confirmed by a Ambio XP-II Stylus Profiler to be 100nm. Subsequently, the samples were annealed in a vacuum furnace in the temperature range of 600~1000°C for 2h, respectively. The samples were put into a small molybdenum box in case of pollution and the pressure was controlled under  $2 \times 10^{-3}$  Pa during the process.

A RBS test was performed at the Rudjer Bošković EN Tandem Van de Graff Accelerator, Croatia at perpendicular incidence with 3.0MeV carbon ions and with a silicon solid state surface barrier detector positioned at a scattering angle of 165° in the IBM geometry. The analysis of the RBS spectra was done with SIMNRA 6.0<sup>[40]</sup>. The SEM observations were performed to characterize the microstructure of the Fe/Si systems by a JSM-7401F SEM at the International Technology Center, USA. XRD was performed to verify the phase formation of silicide using a Philips MPD 1880 counter diffractometer with monochromatic CuK $\alpha$  radiation at the Rudjer Boskovic Institute, Croatia.

## 3 Results and discussion

### 3.1 Atomic interdiffusion in Fe/Si systems

Figure 1 shows the RBS spectra and the depth profiles of the element concentration simulated with SIMNRA 6.0. Figure 1 (a) shows a clear interface and there is almost no atomic mixing for the as-deposited sample. After annealing at various temperatures for 2h, the diffusion of Fe and Si atoms at the interface is clearly seen and the width of the interface increases as the annealing temperature increases. After annealing at 600°C, there is only a few atoms to diffuse near the interface, and the interface is slightly broader but the surface keeps a continuous Fe film. After annealing at 700°C, the interface broadening is enhanced and the concentration depth profile of Fe and Si atoms forms a graded distribution. Further-

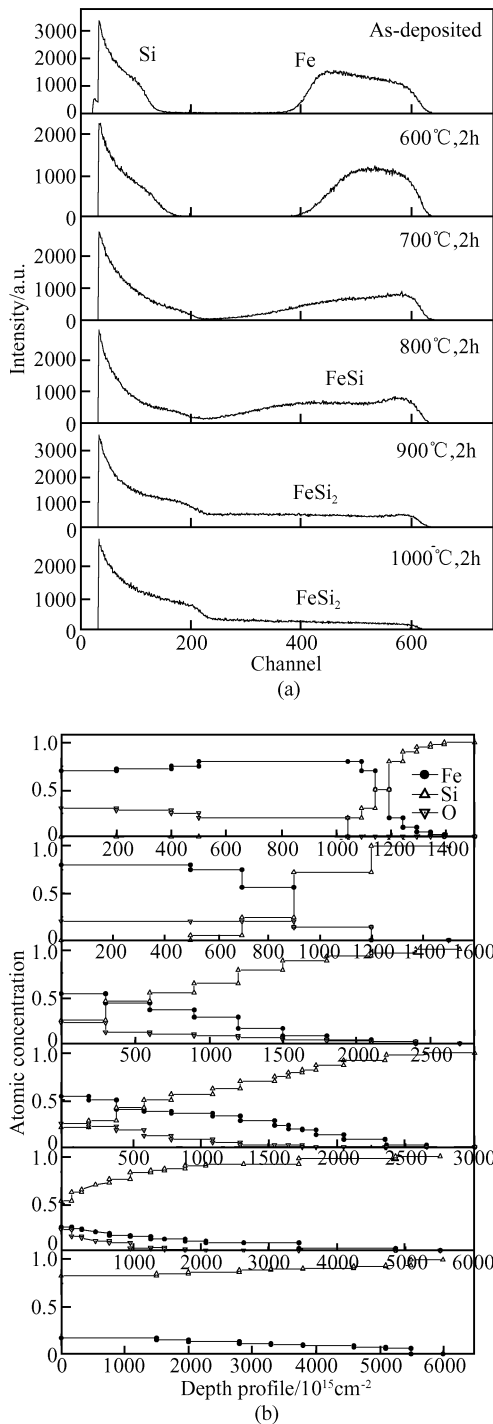
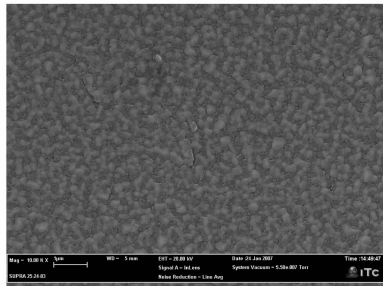


Fig.1 Results of RBS with 3.0MeV carbon ions and elements distribution simulated by SIMNRA 6.0 for the Fe/Si systems annealed at 600~1000°C for 2h  
(a) RBS results; (b) Element distribution

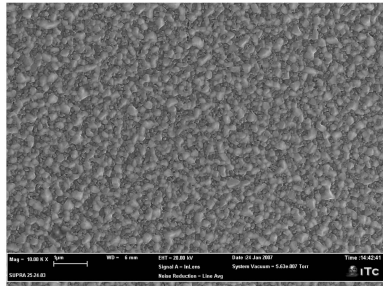
more, though the surface remains a continuous Fe film, the Fe and Si atoms start to react, and the intermediate phase FeSi starts to nucleate and grow near the Fe/Si interface. For the sample annealed at 800°C, the atomic diffusion is enhanced

significantly, more atoms join the silicidation, and a ratio of Fe and Si close to  $Fe : Si \approx 1 : 1$  is achieved. From the simulation results, as shown in Fig. 1 (b), after annealing at 600~800°C for 2h, some unreacted Fe atoms remain on the surface because of low annealing temperature, and the amount of Si atoms diffused from the substrate is limited by diffusion-control so that it is not enough to make all Fe atoms join the silicidation and form silicides. However, the RBS results indicate that the enhancement of atomic interdiffusion is significant as the annealing temperature increases. The original Fe/Si interface has disappeared gradually and the new interface of silicides/Si starts to form.

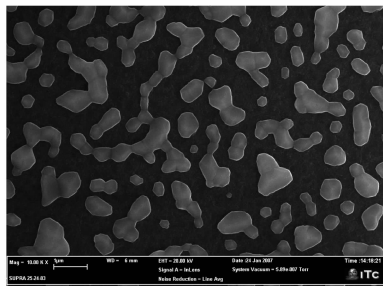
When the temperature increases to 900°C, more Si atoms diffuse from the substrate and react with FeSi, and intermediate FeSi gradually transforms into stable phase  $\beta$ -FeSi<sub>2</sub>. The position of the interface shifts slightly more toward the surface than that annealed at 800°C due to the FeSi<sub>2</sub> growth by consuming FeSi. The elements distribution indicates that most of the region has formed FeSi<sub>2</sub> with the stoichiometric  $Fe : Si = 1 : 2$  in the Fe/Si system, as shown in Fig. 1 (b). However, the ratio of Fe and Si is still close to  $Fe : Si = 1 : 1$  on the surface, indicating that, on the one hand, the transformation from FeSi into FeSi<sub>2</sub> has not finished and, on the other hand, the silicidation has not finished in big islands on the surface and some unreacted Fe atoms remained. When the temperature increases to 1000°C, the amount of Si atoms exceed the ratio of  $Fe : Si = 1 : 2$  due to the increased diffusion ability of Si atoms with the increase of the temperature. The transformation from FeSi into FeSi<sub>2</sub> has been going on in the big islands. However, because the rate of crystalline for FeSi<sub>2</sub> is slow, the film should be crystalline FeSi<sub>2</sub> and amorphous of Si and silicides coexisted. According to the density of Fe and FeSi<sub>2</sub> the thickness of the silicides film should be three times as that of the Fe film if all Fe atoms transformed into FeSi<sub>2</sub> completely, but from the results of RBS, the thickness of forming silicides is just as two times greater than that of the Fe films after annealing at 1000°C for 2h. This difference indicates that the phase transformation has not finished completely. As the high temperature phase  $\alpha$ -FeSi<sub>2</sub> forms above 950°C, it is necessary to con-



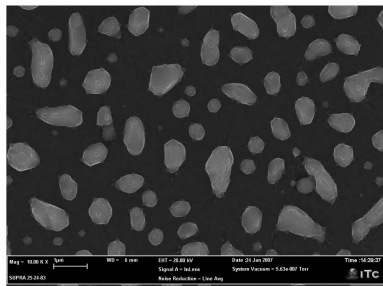
(a)



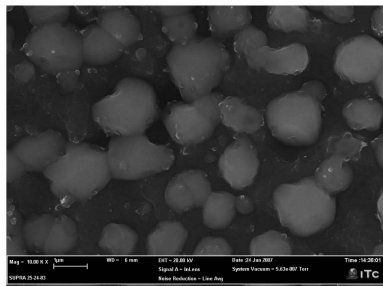
(b)



(c)



(d)



(e)

Fig.2 SEM images of Fe/Si systems annealed in the temperature range of 600 ~ 1000°C for 2h (a) 600°C ;(b) 700°C ;(c) 800°C ;(d) 900°C ;(e) 1000°C

trol the anneal temperature at 900°C and prolong the time duration to get the single phase  $\beta$ -FeSi<sub>2</sub>.

### 3.2 Characterization of microstructures and crystal structures for Fe/Si systems

Figure 2 (a) shows the SEM images for the Fe/Si systems annealed at various temperatures for 2h. The effects of annealing on microstructures is obvious, because silicides with different compositions and structures form with increasing annealing temperatures. The results are correlated with the RBS analyses. The film deposited by MS is usually amorphous, but to thick metal Fe film, it may be polycrystalline with fine grains. For the sample annealed at 600 and 700°C, though the grain sizes of Fe vary from tens to hundreds of nanometers, the whole surface seems to form a continuous and homogeneous Fe film. After annealed at 800°C, the grains of Fe on the surface grow larger than that of those annealed at 600 and 700°C and are no longer continuous. They aggregate into separate islands and form intermediate phase FeSi by reacting with Si atoms diffused from the substrate. The sizes of most islands are in the range of 300 to 500nm. Energy dispersion X-ray spectra confirms the composition of islands to be Fe : Si = 1 : 1, and the XRD results indicates that the crystal structures of the islands is  $\epsilon$ -FeSi, as shown in Fig. 3 (b). When the temperature increases to 900°C, the grains separate further, from the surface to inside the islands and the intermediate phase FeSi transforms into stable phase  $\beta$ -FeSi<sub>2</sub>. From Fig. 2 (d), the surface of the islands seems to have the tendency of melting and some fine grains of  $\beta$ -FeSi<sub>2</sub> appear on the surface of the islands. However, the peak of  $\beta$ -FeSi<sub>2</sub> is not observed as its contents are too low due to its high formation energy and low rate of crystalline. When the annealing temperature is 1000°C, many of the Si atoms diffuse from substrates and they are far in excess of the demands of stoichiometric Fe : Si = 1 : 2. These Si atoms cannot form crystalline in time, so they can only exist in the form of amorphous. Similarly  $\alpha$ -FeSi<sub>2</sub> grows very slowly due to its high formation energy and low rate of crystalline; two hours is too short to form crystalline completely. Accordingly, the island grains seem to embed themselves into the amorphous matrix, the film becomes a mixture of the  $\alpha$ -FeSi<sub>2</sub>

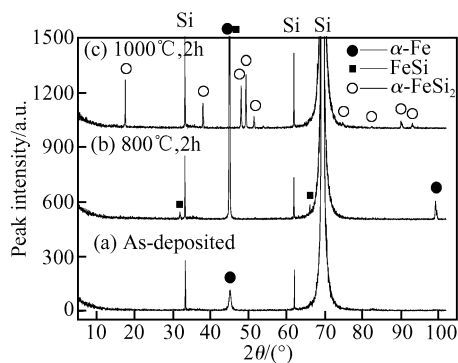


Fig. 3 XRD patterns for Fe/Si systems prepared by magnetron sputtering

and amorphous Si and silicides, as shown in Fig. 3 (c). Figure 3 shows the XRD patterns for the samples of as-deposited, annealed at 800 and 1000°C. From the result of the as-deposited sample shown in Fig. 3 (a), only one broad peak of Fe (110) at  $2\theta = 44.998^\circ$  is observed, except the peaks of Si from the substrate, indicating that the Fe film deposited by magnetron sputtering is crystalline with fine grains. The grain size was estimated using Scherrer formula<sup>[31]</sup> to be about 20~30nm. The size of grains becomes tens to hundreds of nanometers from the SEM observation after annealing at 800°C for 2h, so the peak intensity of Fe (110) enhances and the full width at half maximum decreases significantly. Another peak of Fe (220) appears at  $2\theta = 99.2^\circ$ , and some small peaks of FeSi also appear at the same time. Actually, the peak at  $2\theta = 44.998^\circ$  cannot exclude the contribution of FeSi, according to the data existing in the ICDD powder diffraction file; card number 65-4899 for  $\alpha$ -Fe (110);  $2\theta = 44.663^\circ$  and card number 38-1397 for  $\epsilon$ -FeSi (210);  $2\theta = 45.124^\circ$ . They almost overlap and are difficult to distinguish. After annealing at 1000°C for 2h, only peaks of  $\alpha$ -FeSi<sub>2</sub> are observed, except the peaks of substrates Si, as shown in Fig. 3 (c). All silicides transform into  $\alpha$ -FeSi<sub>2</sub> completely. The results given here were collected over a long time as the signal is very weak due to the short annealing time. Actually, from the SEM observation in Fig. 2 (e), the film is a mixture of  $\alpha$ -FeSi<sub>2</sub>, amorphous Si, and silicides. To improve the quality of crystalline, it is necessary to prolong the annealing time.

## 4 Conclusions

Pure metal Fe films of about 100 nm were de-

posited on Si (100) substrates by DC MS. Subsequent annealing in a vacuum furnace was performed in the temperature range of 600~1000°C for 2h. The effects of annealing on atomic interdiffusion and silicide formation in Fe/Si system were analyzed by means of RBS with 3MeV carbon ions. The microstructures and crystal structures were characterized by SEM and XRD.

The results indicate that as the annealing temperature increases from 600 to 800°C, atomic interdiffusion starts at the Fe/Si interface, gradually extends to the surface, the interface continues to broaden, and yields a graded concentration distribution of Fe and Si. At the same time, the Fe and Si atoms near the interface react and form the intermediate phase FeSi. When the anneal temperature reaches 800°C, the film is no longer continuous and it aggregates into separate islands. As the annealing temperature increases further, the atomic interdiffusion enhances further and more silicides form. Then the interface is no longer broad but shifts forward to the substrate, a new interface of silicides/Si forms, and Si atoms cross through the interface, react with FeSi, and transform into FeSi<sub>2</sub>. When the temperature reaches 1000°C, the ratio of Fe and Si in the whole film is in excess of Fe : Si = 1 : 2, and the results of XRD confirm that high temperature phase  $\alpha$ -FeSi<sub>2</sub> is formed and the island grains embed themselves into the continuous, homogeneous, and softly amorphous Si matrix. The film becomes a mixture of  $\alpha$ -FeSi<sub>2</sub>, amorphous Si, and silicides for the short duration of the annealing time. To improve the quality of crystalline, prolonging the duration of the annealing time is necessary.

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## 退火对 Fe/Si 结构原子间互扩散及显微结构的影响\*

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**摘要:** 在 Si(100)衬底上,用直流磁控溅射沉积约 100nm 的纯金属 Fe 膜,然后在 600~1000℃ 真空退火 2h.用能量为 3MeV 的 C 离子进行了卢瑟福背散射(RBS)测量,并用 SIMNRA 6.0 程序分析了测量结果,给出了界面附近 Fe 原子与 Si 原子间互扩散的完整图像.扫描电镜(SEM)观察和 X 射线衍射(XRD)测量表征了不同温度退火 2h 后 Fe/Si 系统表面的显微结构和晶体结构.由 RBS、XRD 测量与 SEM 观察结果,分析了退火过程对磁控溅射制备的 Fe/Si 双层膜结构原子间的互扩散行为、硅化物形成及显微结构的影响.

**关键词:** 磁控溅射; 退火; RBS; 互扩散; 显微结构

**PACC:** 8115; 8140E; 2940

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