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Citation: [AIP Conference Proceedings](#) **1321**, 278 (2011); doi: 10.1063/1.3548379

View online: <http://dx.doi.org/10.1063/1.3548379>

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Optimization and Characterisation of Amorphous Iron Disilicide formed by Ion Beam Mixing of Fe/Si Multilayer Structures for Photovoltaic Applications

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Abstract. This study presents an optimization and characterization of amorphous Iron Disilicide (α -FeSi₂) synthesized using Ion Beam Mixing (IBM) of Fe/Si multilayer structures. The layers were deposited using RF magnetron sputtering, and subsequently irradiated with Ar⁺ and Fe⁺ beams of 150 and 200keV. Rutherford Back Scattering (RBS) analysis was used to determine the structure and level of silicidation of the samples. The nature of the band-gap and the optical absorption coefficients were determined by optical transmission analysis. The results demonstrate that the synthesis of α -FeSi₂ can be achieved using this technique, with the total level of silicidation being highly dependant upon the initial structure configuration and beam parameters. Direct band-gap energies of $\sim 0.90\text{eV}$ have been observed for those samples with the highest levels of silicidation, with optical absorption coefficients of $\sim 10^4\text{ cm}^{-1}$. Therefore this method of fabrication has been shown to produce α -FeSi₂ layers without the need for post-synthesis treatment, using established technologies without compromising the optical properties that make this material such a promising semiconductor for the photovoltaics market.

Keywords: Ion Beam Mixing, Iron Disilicide, Multilayer Deposition, Photovoltaics

PACS: 68.35.bj; 68.35.fx; 78.20.Ci

INTRODUCTION

With the ever increasing global demand for energy, the solar sector has enjoyed unparalleled growth over the last decade in excess of 30% per year [1]. To continue this growth trend, certain long-term requirements have been identified that any photovoltaic (PV) technology will have to satisfy. These requirements are that the technology must be

- [1]:1) Highly efficient
- 2) Non-toxic
- 3) Based upon highly abundant materials
- 4) Durable
- 5) Thin-film

Iron disilicide, in its semiconducting β -phase, has been thoroughly investigated with a view to its optoelectronic potential due to its direct band-gap and high optical absorption coefficient [2]. However, most formation processes for this phase of the material require epitaxial growth off expensive silicon substrates requiring high thermal budgets for their production and for the post deposition treatment of the silicide. The recently discovered semiconducting amorphous phase of the material (α -FeSi₂) has shown similar band-gap energies and optical absorption coefficients to that of the β -phase [3]. The amorphous phase has the distinct advantage that the material can be synthesized using more economical techniques on large area substrates with little thermal processing

required. Furthermore, it satisfies all of the aforementioned technology requirements, making it a significant candidate as a potential low cost, high efficiency photovoltaic material.

This study examines the formation of α -FeSi₂ using the Ion Beam Mixing (IBM) technique. Previous studies into this process have focused on the mixing of a single layer of Fe deposited on an Si substrate using 120keV Ar⁸⁺ ions with a substrate temperature of 300°C [4]. This study will investigate the mixing of Fe/Si multi-layered structures, with particular emphasis on the level of silicidation achieved within the structures.

EXPERIMENTAL DETAILS

The multi-layered structures were deposited on quartz substrates with a Nordiko 2000 RF magnetron deposition system, using argon as the sputter gas. The structures were of a constant total thickness of 130nm, with the number of discrete layers comprising each structure varied from 6 to 12. The samples were subsequently mounted within a DF 1090 200keV ion implanter, and irradiated with Ar⁺ and Fe⁺ beams. The samples were held at room temperature during the irradiation process. The complete beam parameters are shown in table 1. The samples are forthwith labeled

with the format nPx , where n is the number of layers, and Px is the mixing process employed.

TABLE 1. Beam parameters used for the mixing process

Process	Specie	Energy (keV)	Fluence (ions/cm ²)
P1	Fe ⁺	150	1x10 ¹⁵
P2	Fe ⁺	200	1x10 ¹⁵
P3	Ar ⁺	150	1x10 ¹⁵
P4	Ar ⁺	200	1x10 ¹⁵

Rutherford Back Scattering (RBS) analysis was carried out using a 1.1MeV He⁺ beam on the Surrey University Ion Beam Centre tandem accelerator. The beam current was approximately 30nA, and the nominal beam spot size had a 2mm diameter. Two particle detectors were placed at angles of 172.8° and 148.2° with respect to the beam propagation axis to detect the backscattered He⁺ ions. The RBS spectrum consists of a plot of counts vs. energy, from which structural information can be extracted using the IBA DataFurnace NDFv9.3b code [5].

Optical transmission analysis was carried out using a Varian Cary 5000 spectrophotometer, with a wavelength range of 865 to 1360nm, equating to a photon energy range of 0.7 to 1.1eV. The transmission data for each sample was normalized against a spectrum taken for the corresponding unmixed sample. It was then processed to determine the absorption as a function of photon energy, and extrapolation from the linear region to the x-axis yielded the band-gap energy.

RESULTS AND DISCUSSION

RBS RESULTS

For each sample, the ‘level of mixing’ was calculated as the percentage volume of the sample that contains Fe and Si in FeSi₂ stoichiometric atomic ratios. This level of mixing for each of the samples and processes is shown graphically in figure 1. It is important to note here that the RBS results will yield the atomic ratios, but do not confirm that ‘silicidation’ has taken place, ie, that the compound FeSi₂ has been formed. The mixing levels are highest for the 8-layered structure, particularly for processes P1 and 2. Furthermore, simulation suggests that the levels of inter-mixing due to ballistic transport of the target atoms alone is considerably lower than those achieved in these samples [6], suggesting that diffusion plays a major and dominant role in the mixing process. Examination of the elemental depth profiles of the samples, an example of which is shown in figure 2,

FIGURE 1. Silicidation levels achieved for all samples and processes.

indicate thin residual layers of Fe left within the structures positioned approximately at the centre of where the initial Fe layers were deposited. This suggests that the mixing mechanism is dominated by a movement of Si atoms into the Fe layers. This mechanism has been found in previous studies [4].

FIGURE 2. RBS elemental depth profiles of sample 6P1 before (top) and after (bottom) irradiation

A further result determined from the RBS data suggests that the presence of residual argon in the initial structures, embedded during the sputter deposition process, has a possible inhibition effect upon the Si diffusion. This effect is illustrated in figure 3. The trend suggests that a doubling of the latent Ar concentration reduces the mixing levels by ~10-15%.

FIGURE 3. The apparent trend between silicidation efficiency and latent Ar concentration for the Fe^+ irradiated samples. The line is a guide for the eye only.

However, it should be noted that this trend was only observed for the Fe^+ irradiated samples, and not for the Ar^+ irradiated samples. Therefore, while argon is known to inhibit the diffusion and growth of silicon [7,8], further work is still required to establish the exact mechanism, if any exists, by which argon inhibits the inter-diffusion of Fe and Si layers.

Optical Absorption Results

The results of the optical absorption analysis indicated that the band-gap for all of the samples was direct in nature. The band-gap energies for all samples are shown in figure 4.

FIGURE 4. Band-gap energies for all samples and processes.

As can be seen, the band-gap energy for all samples was found to be $\sim 0.9\text{eV}$, a figure that is in good agreement with previous studies [3,4], suggesting that the material has indeed undergone 'silicidation' to form FeSi_2 . The energies varied little as a function of the initial structure or the mixing process employed, or with the level of silicidation achieved, with the lowest energy of 0.86eV being found for the 6P2 sample, and the highest of 0.92eV being found for samples 8P1 and 8P4.

Figure 5 illustrates the absorption coefficients, taken at the band-gap energy (0.9eV) for all of the samples.

FIGURE 5. Absorption at the band-gap for all samples and processes.

As with the band-gap energies shown in figure 3, there is little variation as a function of initial structure and mixing process, with all of the values found to be $\sim 2.5 \times 10^4 \text{ cm}^{-1}$. Again, this is in good agreement with previous studies [3,4].

When the absorption coefficients are plotted as a function of the level of silicidation, as shown in figure 6, it becomes apparent that the level of absorption varies with the level of silicidation achieved within the samples.

FIGURE 6. Absorption coefficients plotted as a function of levels of silicidation for the Fe^+ irradiations (top) and Ar^+ irradiations (bottom). The line is a guide for the eye only.

SUMMARY

In summary, it has been demonstrated that a-FeSi₂ can be synthesized using both Fe⁺ and Ar⁺ beams in an Ion Beam Mixing process with Fe/Si multi-layered structures. RBS results indicate that the level of mixing achieved within the samples is dominated by a diffusion process, particularly the diffusion of Si into the Fe layers. Optical analysis indicated a direct band-gap semiconductor with a band-gap energy of ~0.9eV and an absorption coefficient at the band-gap energy of ~2.5x10⁴ cm⁻¹. The absorption coefficient appears to vary with the level of silicidation achieved within each sample. It is postulated that residual Ar, embedded within the initial structures during the deposition process, may be inhibiting the Si diffusion into the Fe layers, thus reducing the overall level of silicidation achieved. To further this study, an enhancement of the mixing process is necessary in order to achieve 100% silicidation of the structures

ACKNOWLEDGMENTS

This work was funded and supported by the UK Engineering and Physical Sciences Research Council (EPSRC).

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