

Local structure analysis of metastable iron silicides formed in the Fe ion implanted Si

M. Naito and M. Ishimaru

*Institute of Scientific and Industrial Research, Osaka University, Mihogaoka, Ibaraki, Osaka
567-0047, Japan*

Iron silicides such as β -FeSi₂ and Fe₃Si have attracted much attention, because the compounds exhibit excellent optical or magnetic properties and are harmless to the environment. In addition to these stable phases, metastable iron silicides such as γ -FeSi₂ and *c*-FeSi have been observed in the epitaxially-grown Fe-Si thin films [1,2]. The metastable phases often appear as precursor or intermediate phases, prior to the formation of the stable phases. Therefore, understanding the crystallographic structure, morphology, and thermal stability of the metastable phases is of technological importance to control the microstructures and physical properties of the stable iron silicides. In this study, we investigated the crystal structure of metastable iron silicides observed in the early stage of crystallization of amorphous Fe-Si thin layers synthesized by ion implantation using transmission electron microscopy (TEM) and nano-beam electron diffraction (NBED).

Si(111) wafers were irradiated at cryogenic temperature with 120 keV Fe ions to a fluence of 1.0×10^{17} /cm², followed by thermal annealing at temperatures ranging from 350 to 550 °C in an Ar atmosphere. Microstructures of as-implanted and annealed samples were examined using a JEOL JEM-3000F electron microscope.

An amorphous Fe-Si layer embedded in an amorphous Si was formed in the as-irradiated sample. Plan-view TEM observations revealed that a part of the amorphous Fe-Si crystallized to metastable α -FeSi₂ after thermal annealing at 350°C for 8 h. The metastable α -FeSi₂ embedded in an amorphous phase has not been reported to date, because previous studies indicated that substrate constraint plays an important role in stabilizing the metastable iron silicides. NBED revealed that the metastable α -FeSi₂ consists of three types of domains whose *c*-axes are oriented 90° angles with respect to one another [3].

The α -phase changed to another metastable crystalline phase whose structure is close to the CsCl structure under high-energy electron beam irradiation. The phase transformation was caused mainly by displacement damage processes and suggest a low displacement energy for Fe atoms (< 9 eV). To explain these observations, it was considered that vacancies in α -FeSi₂ are responsible for the electron irradiation-induced phase transformation [4].

References

- [1] H. von Känel, R. Stalder, H. Sirringhaus, N. Onda, and J. Henz, *Appl. Surf. Sci.* **53**, 196 (1991).
- [2] H. von Känel, K. A. Mäder, E. Müller, N. Onda, and H. Sirringhaus, *Phys. Rev. B.* **45**, 13807 (1992).
- [3] M. Naito, M. Ishimaru, Y. Hirotsu, J. A. Valdez, and K. E. Sickafus, *Appl. Phys. A* **91**, 353 (2008).
- [4] M. Naito, M. Ishimaru, J. A. Valdez, and K. E. Sickafus, *J. Appl. Phys.* (submitted).