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Phase study of Fe-Si alloys at 3.5 GPa

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Introduction

Silicon has been proposed as a probable candidate to solve the density deficit between seismic observa-tions of the Earth Core and high pressure, temperature iron [1]. Besides, Fe-Si alloy is also a quite good soft-magnetic material and its phases and properties are quite complex as Si content, pressure and temperature varying. Our study focused on the Fe-Si system at 3.5GPa, trying to realize its phase changes and order variation as Si content and temperature changing.

Experimental

Synthetic Fe-Si alloy with different stoichiometric compounds at different temperatures (2041, 1423 and 1173K) annealing by piston-cylinder at 3.5GPa were observed by Scanning Electron Microscopy and Elec-tron Microprobe to determine the structures and com-positions. Phase determinations were conducted by both X-Ray Powder Diffraction Spectrometry and Transmission Electron Microscopy. Lattice parameters were calculated using GSAS software from the angular position of main XRD peaks.

Local atomic orders of Fe?Si alloys were studied by 57Fe Mossbauer Spectrometry. The spectra exhib-iting magnetic sextets were described by means of a discrete number of magnetic components, values of the isomer shift, quadrupolar shift and hyperfine field independently refined by Normos software.

Fe3Si containing 25wt% 57Fe prepared for Dia-mond Anvil Cell experiments synthetized at 2041K, 3.5GPa by piston-cylinder was polished to the foil (~20 micros thickness, ~150 micros diameter). We chose 400 micros diameter diamond cell and Re gasket as sample holder. Two rubies were added to measure pressure and noble gas Neon was inflated into cell as pressure medium. In-situ magnetization order meas-urements in DAC were carried out by Mossbauer spec-trometry at 300K with increasing 3~4GPa every time by step from room pressure.

Results and Discussion

Fe-Si alloys containing >26at% Si will decompose into DO3 Fe3Si and some other phases at room pres-sure [2]. But in our sample of low temperature, the decomposition did not happen until the sample Fe2Si. We found the sample Fe5Si2 at 1173K was still one phase while Fe2Si at 1173K decomposed into three phases. I think decomposition nearly begins at the composition of Fe2Si because of very little fraction of epsilon-FeSi and eta-Fe5Si3. The microprobe data supported this opinion because of Si contents of al-pha-phase in the decomposed samples were all in the range of 29-32at%, which is also different from the room pressure. The phenomenon may represent higher stability of alpha-phase as pressure increasing and that is why s?Fe2Si found at room pressure cannot be found at 3.5GPa instead by DO3 Fe2Si and B2 phase FeSi appears in very high pressure.

Mossbauer evolutions clearly demonstrated mean hyperfine field of the Fe-Si alloy at 3.5GPa decreased as the Si content increasing like room pressure. It is interesting that the spectrum of Fe3Si (exact composi-tion is 24.73at% Si content) is quite different from room pressure. The DO3 Fe3Si in room pressure can be emphasized by only two Fe sites: A4 and D6 [2]. But our sample showed there were at least four sites Fe. Except the normal D6 (36%), A4 (31%), there are a site (17%) between A4 and D6 and a site (16%) of which hyperfine field is smaller than D6. More than two Fe sites mean not completely order because of replacement of Si atoms and quench at high pressure.

Because of weakening signal in DAC, we just use two Fe sites, D6 and A4 to fit the Mossbauer spectra. The mean hyperfine fields of Fe-Si alloys decrease as pressure increasing. Because of broken of diamond at 17GPa, we have not got the nonmagnetic pressure of Fe3Si but hyperfine field still showed a good decrease trend. At >10GPa pure Fe will become nonmagnetic but our sample Fe3Si at 17GPa still have clear mag-netic feature.

References

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[2] K Varga, F Mazaleyrat and J Kovac(2002)J. Phys. Condens. Matter 14(2002)1985-2000

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