

## PAC Study of Si with Fe Impurities Doped by Implantation or Diffusion

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## I. 11. PAC Study of Si with Fe Impurities Doped by Implantation or Diffusion

*Hanada, R*

*Institute for Materials Research, Tohoku University*

### **Introduction**

Fe impurity in Si has been a subject of Mössbauer spectroscopic study for a long time since  $^{57}\text{Fe}$  is the best nuclear probe for the spectroscopy. Also in Si industries, Fe has been known as one of the impurities to cause deterioration in electronic devices. It forms a deep trap to form a recombination center thus reducing the effective carrier concentrations. In this report a result of PAC spectroscopy for Si doped by Fe impurity will be described. Here, Si specimens were given either by Fe impurity implantation or by diffusion treatment. A part of the results has been reported in<sup>1)</sup>.

### **Experimental**

N-type Si specimens were implanted by Fe ions at a energy of 40keV to various doses. Since no high Fe ion beam current was obtained with a metallic Fe in the ion source (Dan-Fysik 910 type), an Fe chloride ( $\text{FeCl}_2$ ) was used as the source material to obtain a reasonably high  $^{56}\text{Fe}$  beam. This chloride method was found to work for several low vapor pressure elements as Cu, Sn, Zr, Ag and probably can be applied to others.

For the case of diffusion doping, Si specimens were annealed in a vacuum with a high purity Fe powder at 900°C for several hrs and cooled fast to RT by removing the furnace. It is not known, however, the cooling rate is high enough to freeze in the Fe atom in an isolated impurity in Si lattice.

Subsequently these specimens were implanted with 40keV  $^{111}\text{In}$  and PAC spectrum was measured at RT after the isochronal annealing in a vacuum. Since Fe impurity has been known to migrate at low temperature ( $E_M = 0.68\text{eV}$ )<sup>2)</sup>, the isochronal annealing was started from a low temperature.

### **Result**

Fig. 1 shows the PAC spectrum for Si to which Fe impurity was implanted. Fig. 2 shows the spectrum for Si given by the Fe diffusion treatment.

Although very small in magnitude, a PAC rotation pattern is noted in Fig. 1 after the annealing at 463-673°K which gradually fades out after the annealing above 773°K. A similar pattern with the almost same period with that in Fig. 1 is noted in Fig. 2 for the diffusion treated specimen.

One possible cause of the pattern is the formation of Fe-In pair although the formation of Fe precipitates with <sup>111</sup>In in them is another possibility. The latter will be discussed in terms of the reported results of <sup>57</sup>Fe Mössbauer spectroscopy in Si.

## Discussion

The CEMS for <sup>57</sup>Fe implanted Si have revealed that a doublet is observed near  $v=0$ mm/s in the as implanted state<sup>3</sup>. The doublet was interpreted as caused by a quadrupole interactions and the formation of Fe dimer (a pair of Fe atom) is responsible for the interaction. Namely the arrival of single Fe atom to the probe Fe atom breaks the cubic symmetry of Si lattice thus giving rise to a finite electric field gradient. Upon annealing above 600C the splitting is narrowed, which is interpreted as due to a formation of silicides (precipitates). So if one applies this model to our case of the implanted Si, no precipitates are present after the implantation and so the formation of the Fe-In pair upon the annealing may be concluded as the cause of the PAC rotation pattern below 673°K.

However a recent "in beam" Mössbauer spectroscopy for <sup>57</sup>Fe in Si<sup>4</sup>) has revealed a similar doublet. Since the <sup>57</sup>Fe concentration is extremely low in the "in beam" case, the formation of Fe dimer or precipitates is almost negligible in the experiment. So the doublet was interpreted as due to "a strongly disturbed environment", namely, a radiation damaged state which is created by the probe itself (correlated damage).

The values of the quadrupole splitting and the corresponding EFG's for these <sup>57</sup>Fe spectroscopy are summarized in Table 1 together with a <sup>57</sup>Co result<sup>5</sup>. Here  $V_{zz}$ 's are obtained using an expression for the quadrupole splitting,  $(1/4)eQV_{zz}$ , with a known quadrupole moment of  $I=3/2$  state of <sup>57</sup>Fe. If this value for <sup>57</sup>Fe is assumed to be felt by <sup>111</sup>In also, the frequency of PAC spectrum should become as high as 7 Grads<sup>-1</sup>, far above the observed value of 355 Mrads<sup>-1</sup>. So the EFG due to "a strongly disturbed environment" can not account for the present PAC result. This argument, however, assumes that the EFG felt by <sup>111</sup>In is the same with that felt by <sup>57</sup>Fe which, however, may not be justified.

A fast quenching experiment or the implantation at lower temperature will be necessary to obtain a clearer information on the state of Fe in Si.

## Acknowledgement

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Table 1. Quadrupole doublet after  $^{57}\text{Fe}$  Implantation in Si and the corresponding  $V_{zz}$  (EFG).

Probe	Q.S/mms <sup>-1</sup>	$V_{zz}/10^{16}\text{Vcm}^{-2}$	proposed species	Author
$^{57}\text{Fe}$	0.785	3.9	Fe-dimer	Sawicki et al
	0.43	2.1	$\beta$ - $\text{FeSi}_2$	Sawicki et al
$^{57}\text{Fe}$ (in beam)	0.84	4.2	disturbed environmt	Schwalbach et al
$^{57}\text{Co}$ ( $^{57}\text{Fe}$ )	3.16	15.7	$^{57}\text{Co}$ -dimer	Langouche
	0.465	2.3	disturbed environmt	Langouche et al

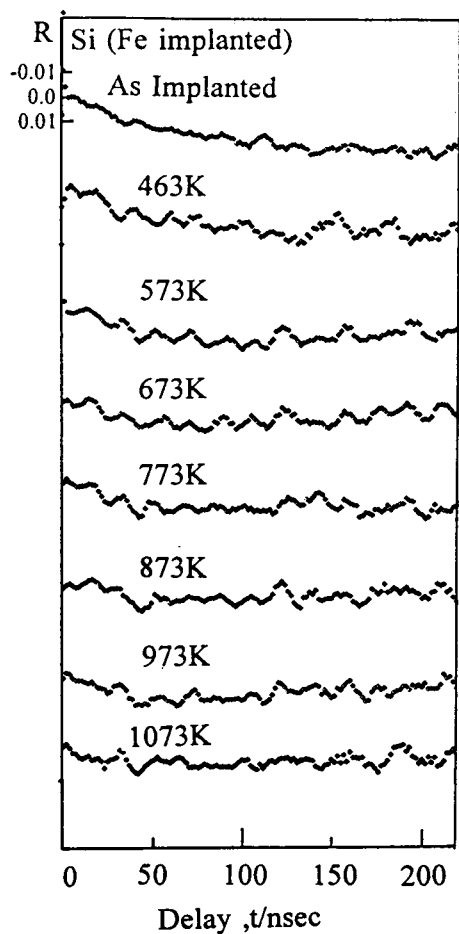


Fig. 1 PAC spectrum by  $^{111}\text{In}$  in Fe ions implanted Si.

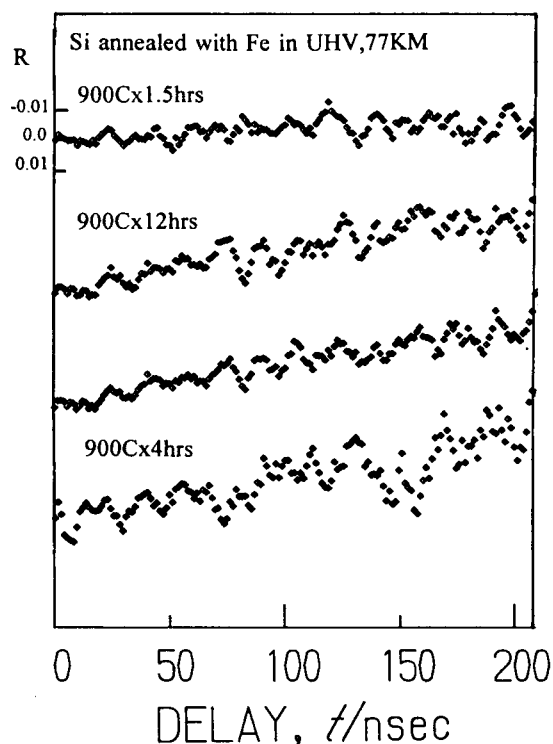


Fig. 2 PAC spectrum in Si annealed with Fe powder at 900°C. After the treatment,  $^{111}\text{In}$  was implanted.