Multiscale Modeling of Radiation Damage and Annealing in Si Samples Implanted with ^{57}Mn(^{57}Fe)

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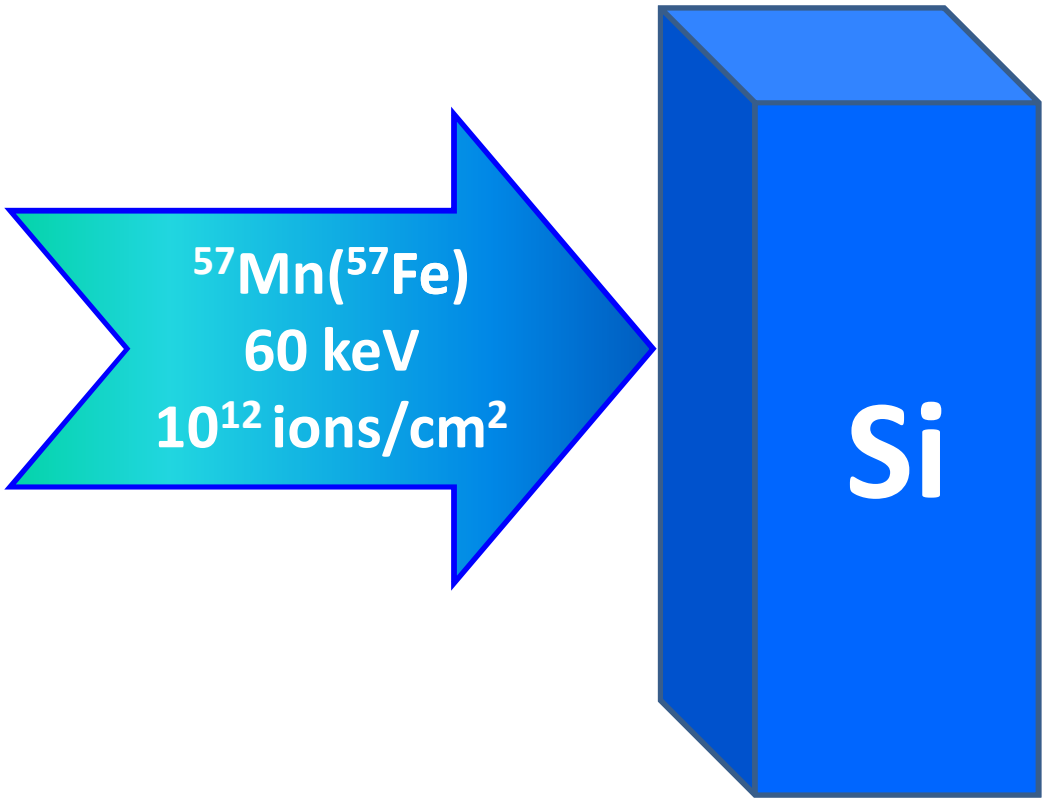
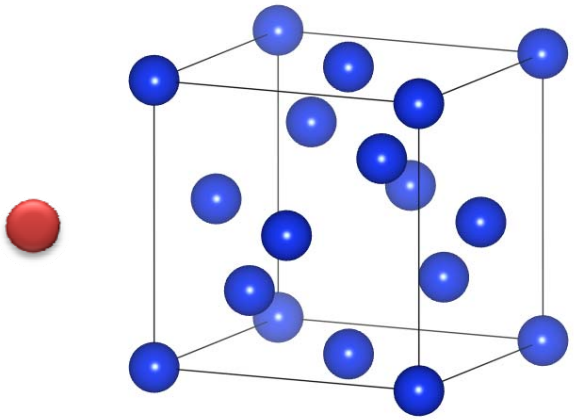
CENTRO DE APLICACIONES TECNOLÓGICAS Y DESARROLLO NUCLEAR

Universiteit Antwerpen

Experiment



Si Crystal Structure



Cubic fcc. a = 5.429 A

H. Gunnlaugsson, M. Fanciulli, M. Dietrich, K. Bharuth-Ram, R. Sielemann, G. Weyer, and I. Collaboration, *Nucl. Instr. and Meth. B*, vol. 186, p. 55, 2002.

Experiment

Isomer shifts ($\delta(mm/s)$) and quadrupole splitting ($\Delta(mm/s)$) of the lines assigned to interstitial (Fe-i), substitutional (Fe-s) and Fe in the damage sites (Fe-D and Fe-N)

Spectral Component	δ (mm/s)	Δ (mm/s)
Fe-s	-0.08(4)	–
Fe-i	0.76–0.81	–
Fe-D	0.33(3)	1.02(3)
Fe-N	0.24-0.31(5)	0.38-0.41(10)

H. Gunnlaugsson, M. Fanciulli, M. Dietrich, K. Bharuth-Ram, R. Sielemann, G. Weyer, and I. Collaboration, *Nucl. Instr. and Meth. B*, vol. 186, p. 55, 2002.

Experiment

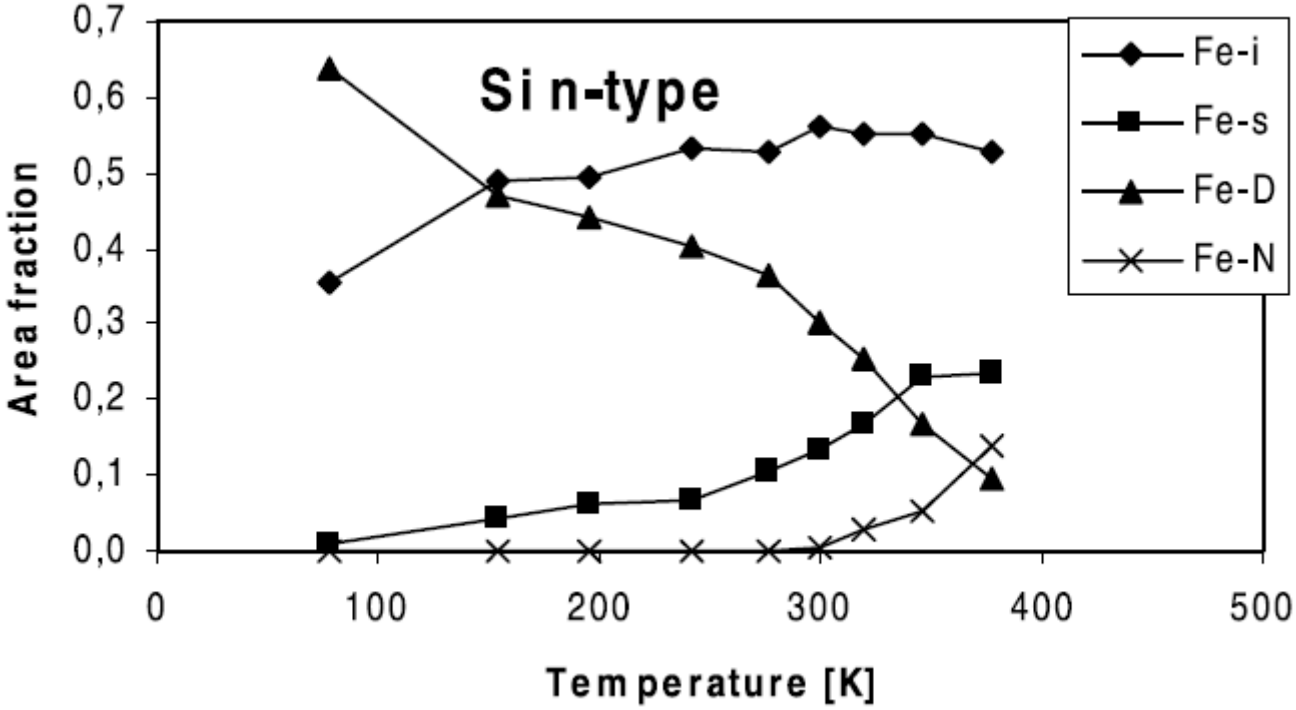


Fig. Site populations as a function of annealing temperature after implantation into n-type Si (P doped).

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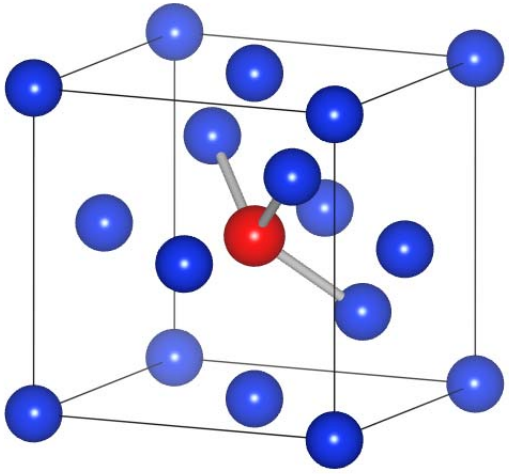
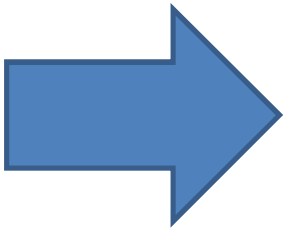
Multilscale Modeling

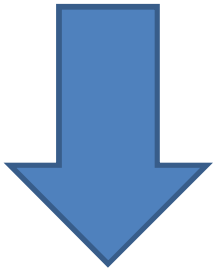
Possible Fe Implantations Sites and Coordination in the Si Crystal Structure

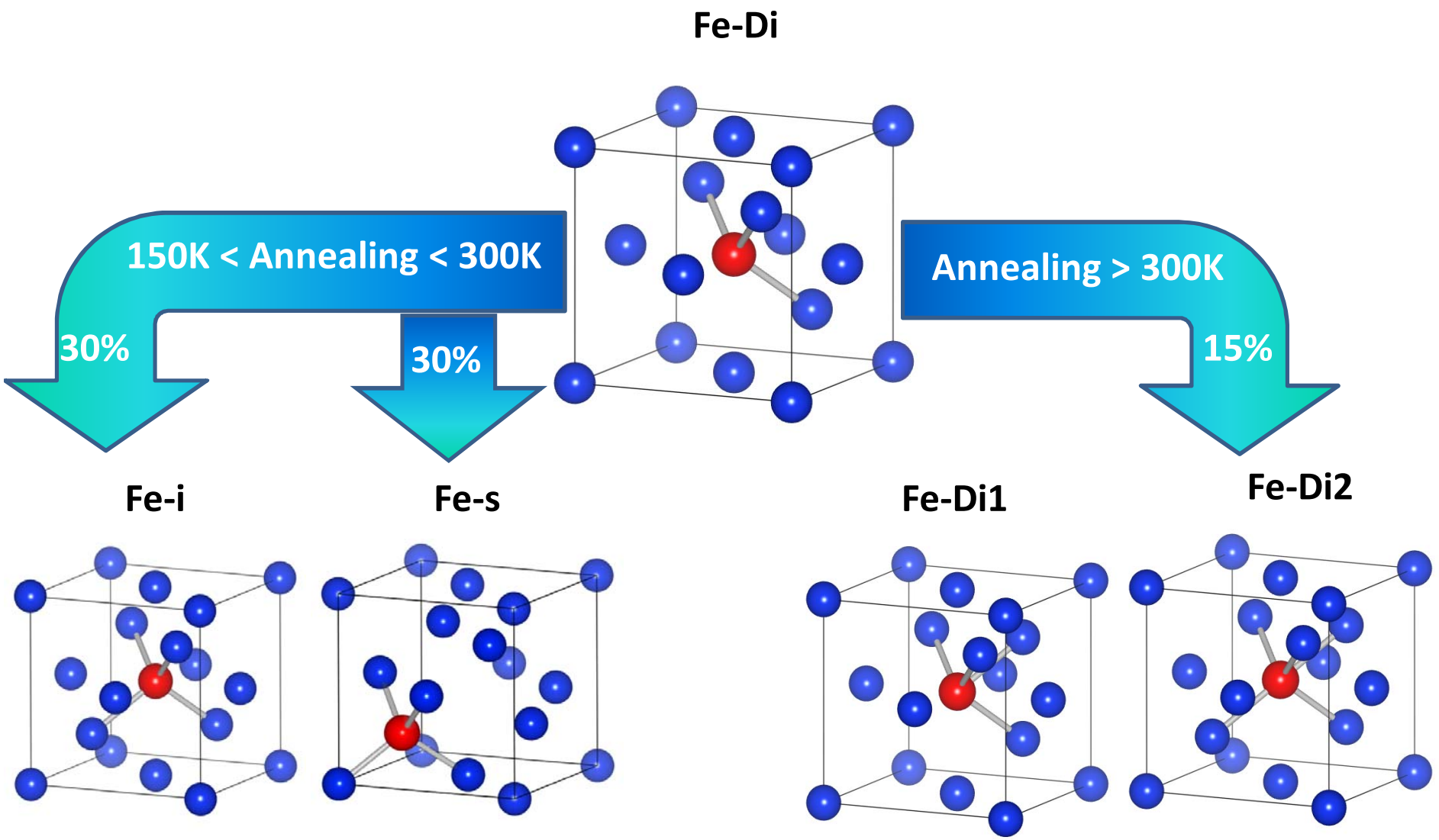
Fe-Di





DFT
&
SRIM

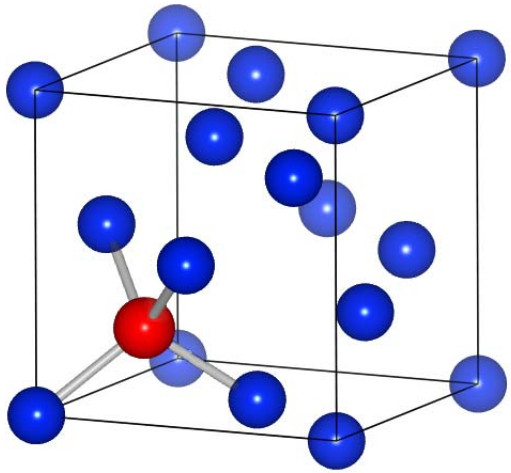



Fe-Di
150K < Annealing < 300K
30%
30%
Annealing > 300K
15%
Fe-i
Fe-s
Fe-Di1
Fe-Di2

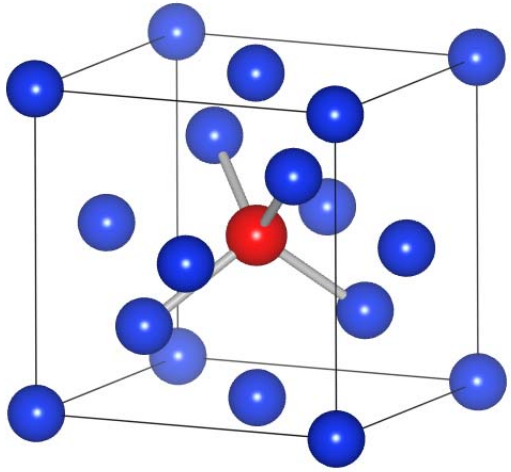
Thanks!!

Possible Fe Implantations Sites and Coordination in the Si Crystal Structure

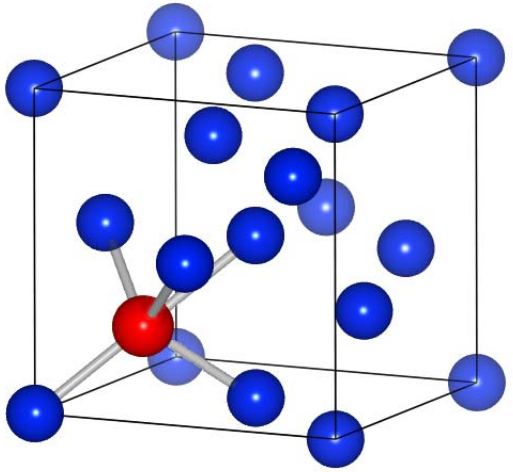
Fe-s



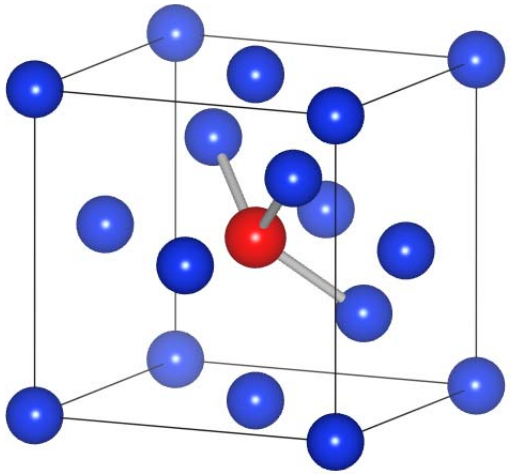
Fe-i



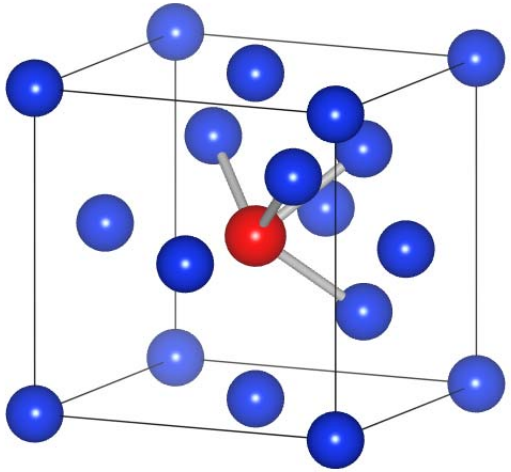
Fe-Ds



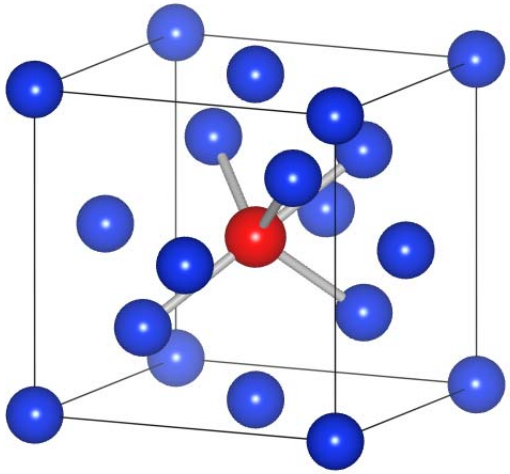
Fe-Di



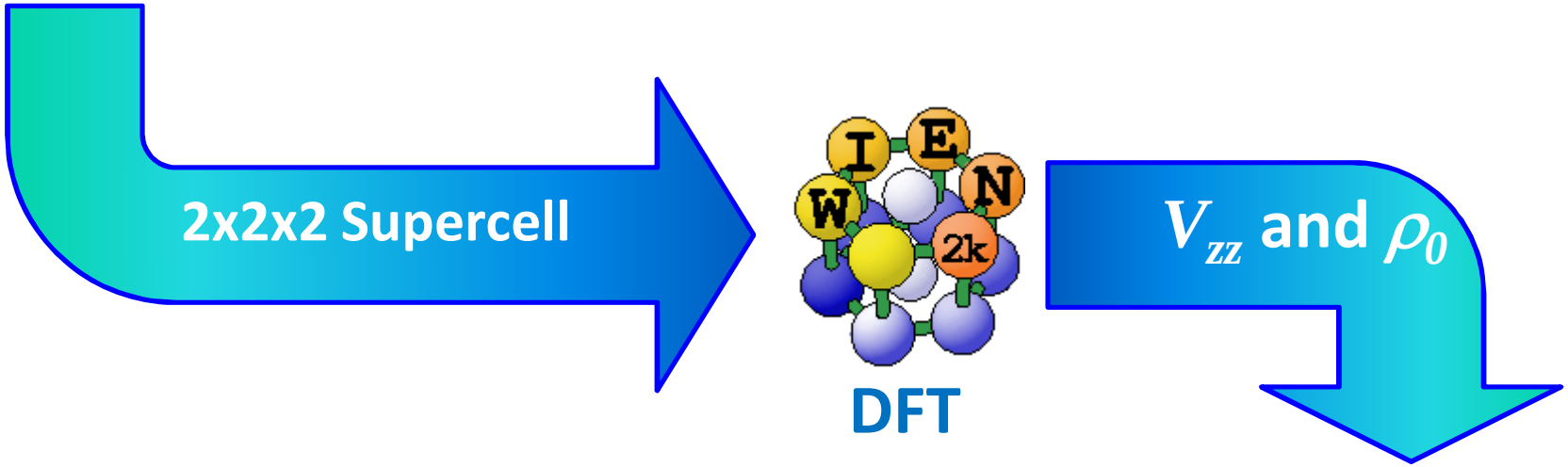
Fe-Di1



Fe-Di2



Hyperfine Electric Parameters Calculation



Isomer Shift

$$\delta = \alpha(\rho_0^{sample} - \rho_0^{reference}) \quad (1)$$

Quadrupole Splitting

$$\Delta = \frac{1}{2} eQV_{zz} \quad (2)$$

Hyperfine Electric Parameters Calculation

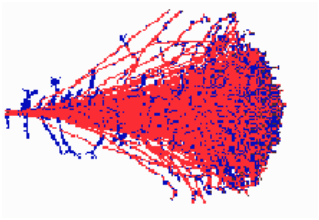
Experimental and calculated isomer shift ($\delta(mm/s)$) and quadrupole splitting ($\Delta(mm/s)$) values of Fe implanted in Si.

Site	Theory		Experiment	
	δ	Δ	δ	Δ
Fe-s	-0.12	-	-0.08	-
Fe-i	0.78	-	0.76 - 0.81	-
Fe-Ds	-0.08	-1.80	0.33(3)†	1.02(3)†
Fe-Di	0.49	1.11		
Fe-Di1	0.24	0.65	0.24-0.31(5)‡	0.38-0.41(10)‡
Fe-Di2	0.54	0.36		

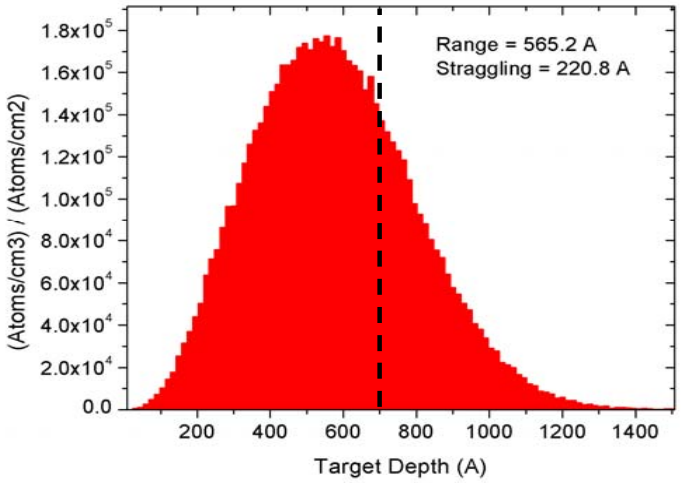
† Experimental designed as Fe-D line.

‡ Experimental designed as Fe-N line.

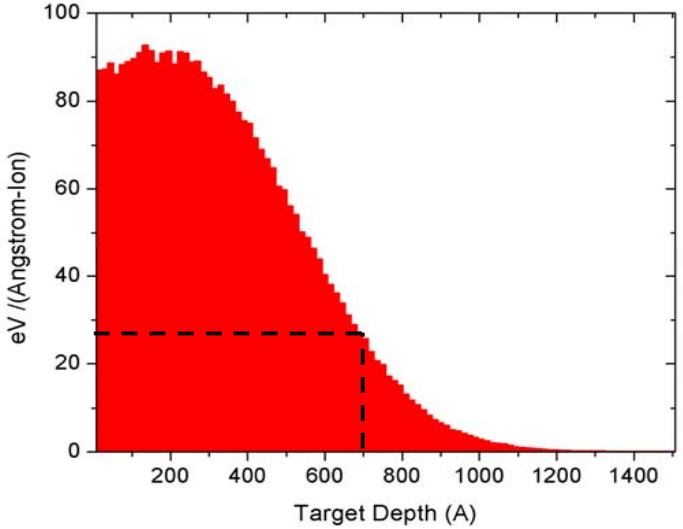
SRIM



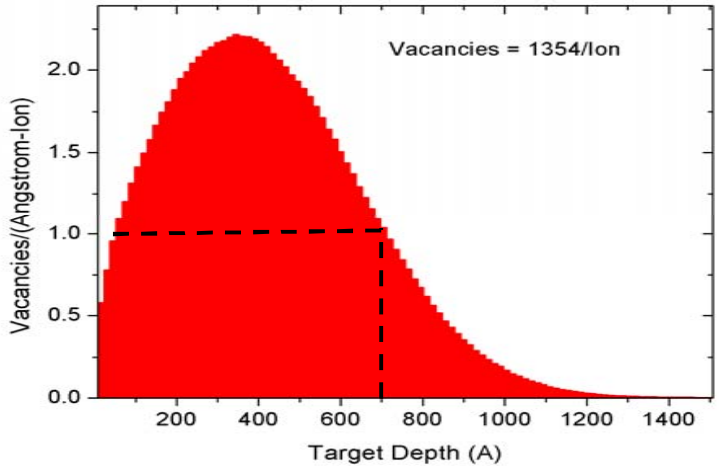
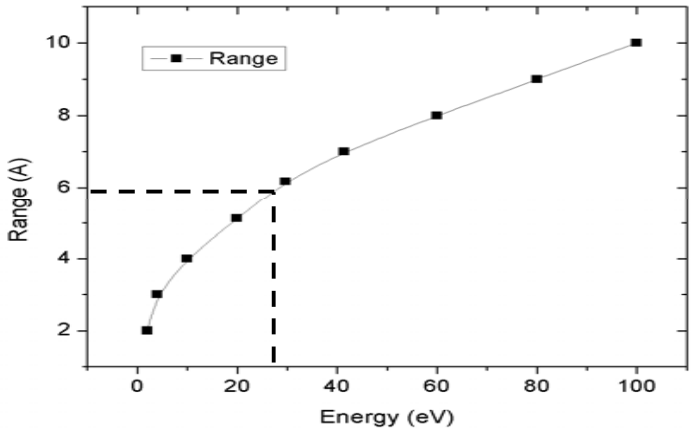
Ion Ranges



Energy to Si Recoils



Target Vacancies



Si Recoil Ranges