Positron beam study on the ion-implated Si

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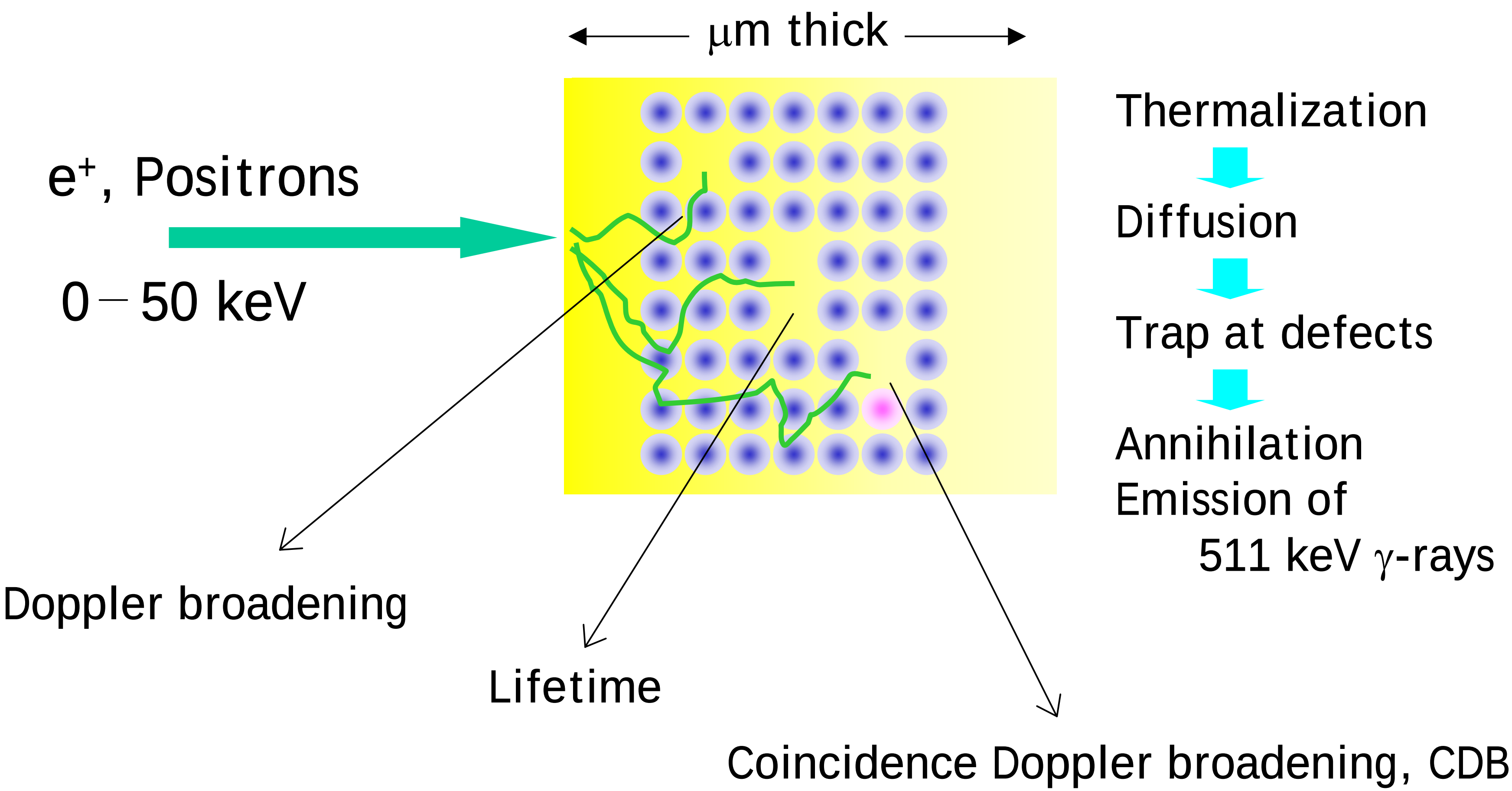
1. Depth resolution-enhanced VEPAS
2. O ion implanted Si
3. Noble-gas ion implanted Si (He^+ & Ar^+)
4. Summary

Acknowledgments

T. Miyagoe (Univ. of Tokyo)
T. Akahane (NIMS)
R. Suzuki (AIST)
T. Ohdaira (AIST)

1. Depth resolution-enhanced VEPAS

VEPAS: Variable-energy positron annihilation spectroscopy

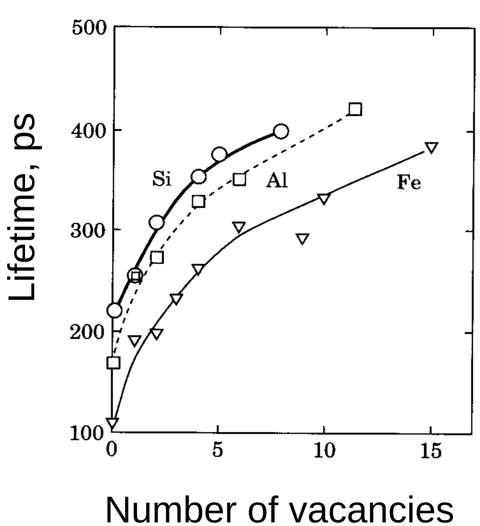


Information from positron data

Lifetime

Electron density

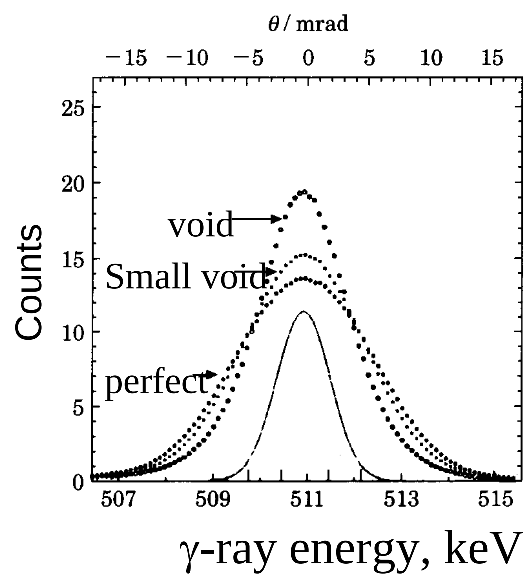
Defect size

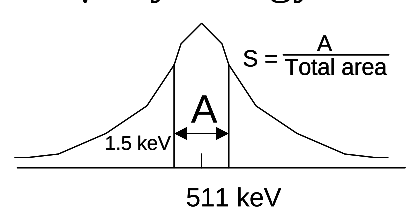


Doppler broadening

Low electron momentum

Amount of defects

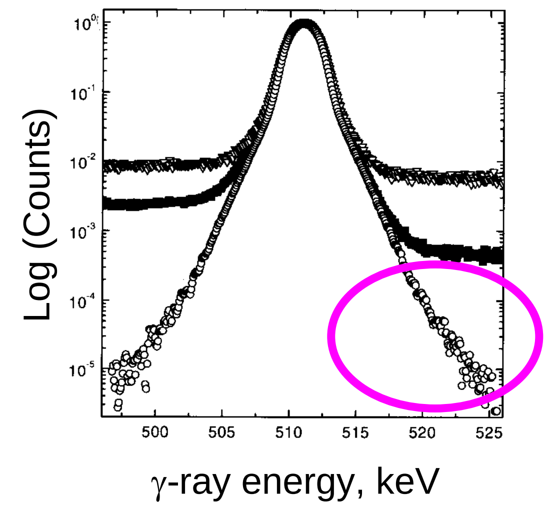




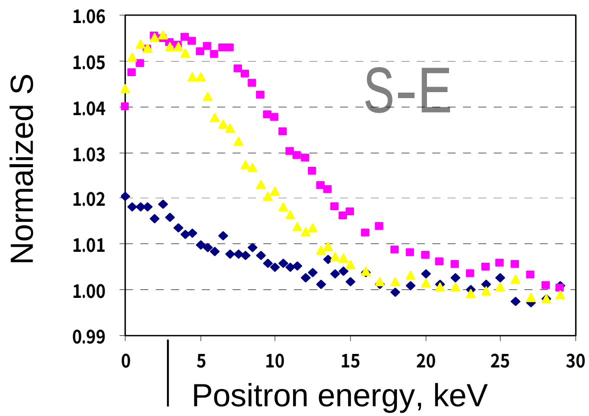
CDB

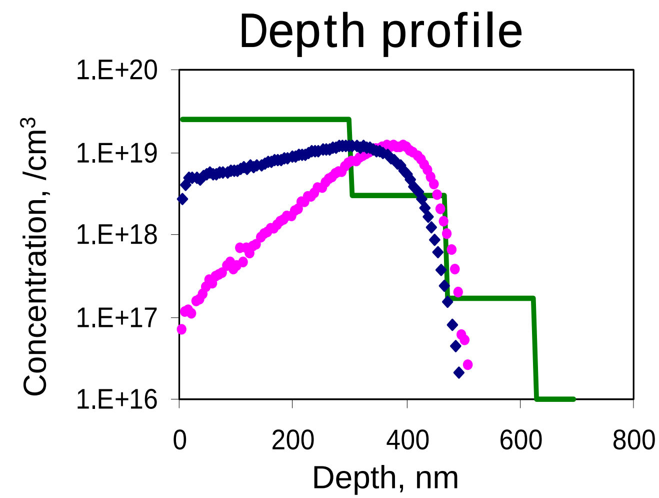
High electron momentum

Chemical analysis of defects

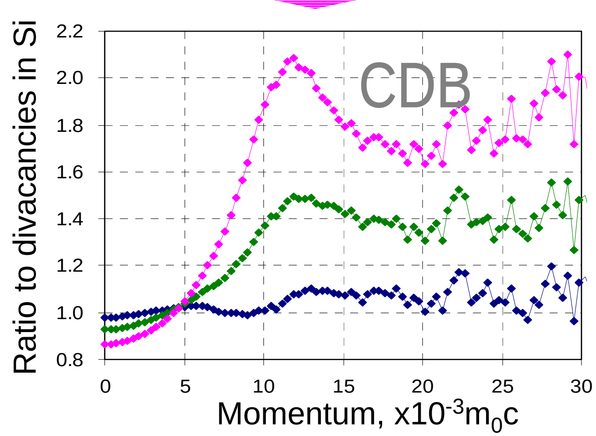


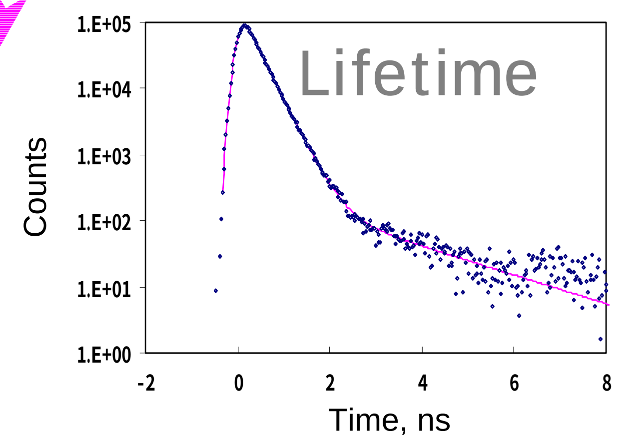
S-E, CDB and lifetime measurements using e^+ beam





Determine the depth; the fixed e^+ energy





Chemical information

Size information

AIM

Interaction of vacancy-impurity complexes in Si with positrons

Introduction of impurity and vacancies

Suitable specimens: Ion irradiated Si

V-oxygen: One of the most important impurities in Si
$1x10^{18}$ O/cm^3 in CZ-Si, SIMOX wafers

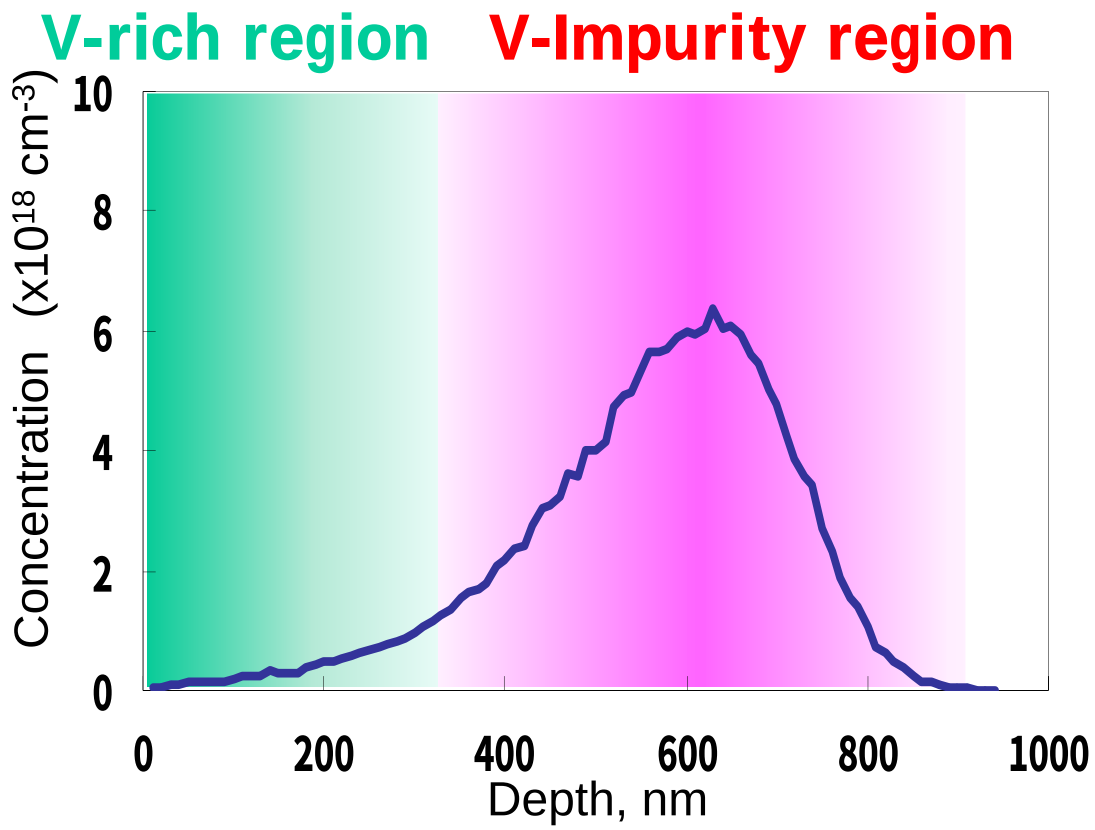
V-helium: Bubble formation

V-argon: Bubble formation

Methodology

- Enhanced depth resolution ➡ layer-by-layer analysis
- V-impurity complexes ➡ CDB ratio curves

Depth dependence of the induced defects



The induced defects and their anneal behavior are strongly influenced with the content of impurities as well as the element.

⇒ Resolution enhanced VEPAS is required.

Positron implantation profile

Mean implantation depth

$$P(z,E)=\frac{mz^{m-1}}{z_0^m}\exp\left[-\left(\frac{z}{z_0}\right)^m\right]$$

$$\overline{Z}=\frac{A}{\rho}E^{1.6}$$

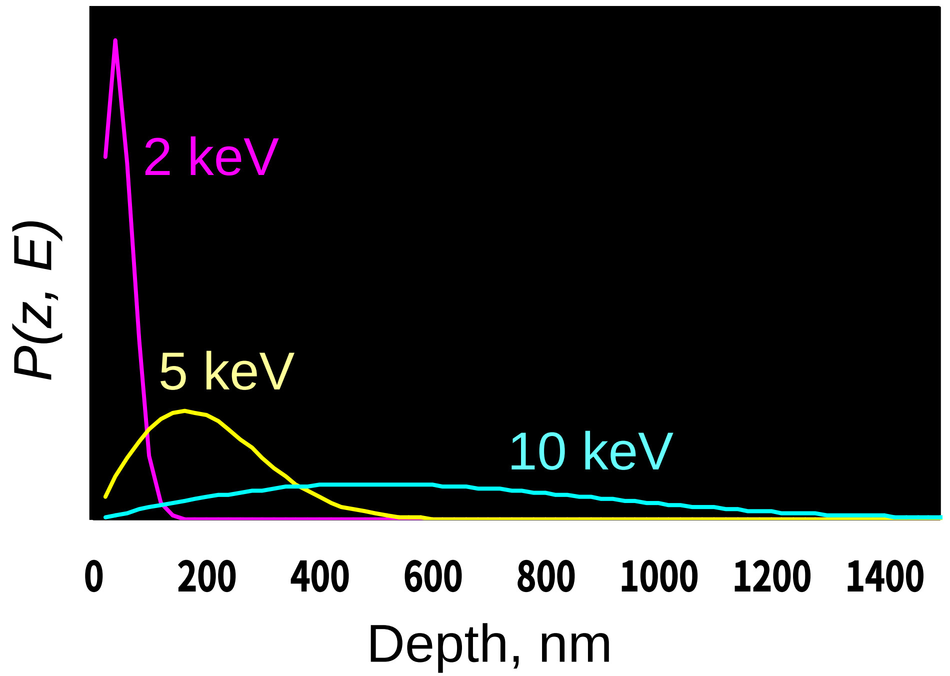
ρ = 2.3 g/cm^3

A = 3.6 mg/cm^{2}keV$^{-1.6}$

$$Z_0=\frac{\overline{z}}{\Gamma\left(1+\frac{1}{m}\right)}$$

m = 2

Positron implantation profile in Si



> 5 keV

Diffusion length of e$^+$ in Si = FWHM of incident e$^+$ profile

Usual analysis has a limited on depth resolution.

Combination of e^+ measurement and etching of the surface layer

Fujinami *et al.*

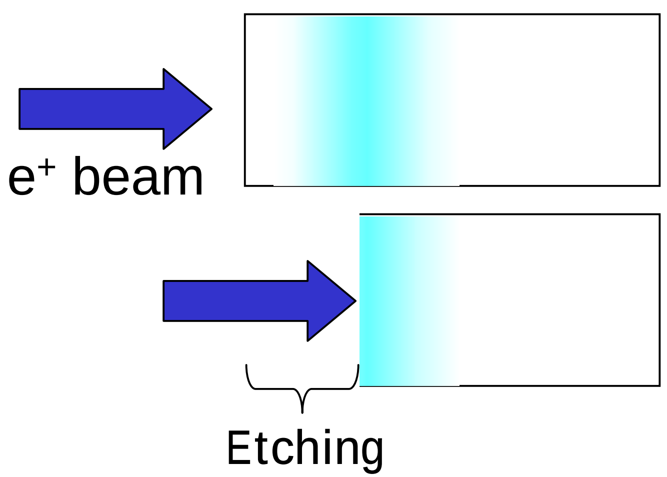
Chemical etch in Si (1993, JAP)

Coleman *et al.*

Anodic oxidation + etch in Si (1998, SLOPOS-8)

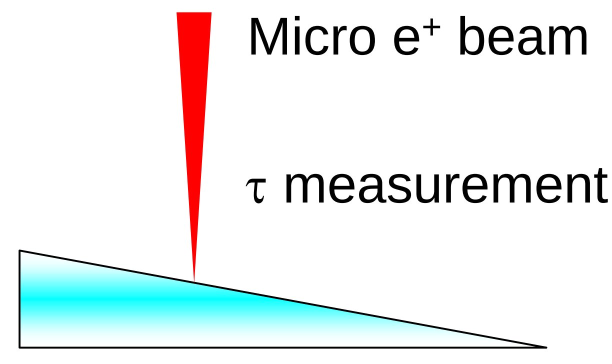
Krause-Rehberg *et al.*

Ar^+ sputtering at 2 keV in Si (2000, APL)



Krause-Rehberg *et al.*

Wedge-shaped polished sample & micro positron beam (1-2 $\mu m\phi$) (2001, SLOPOS-9)



To determine the precise defect depth profile.

Analysis of CDB

The reference specimen for the CDB ratio curve

Most of previous reports: Bulk Si

Every sample has a peak at 10×10^{-3} m_0c in Si.

Difficult to analysis

Problem:

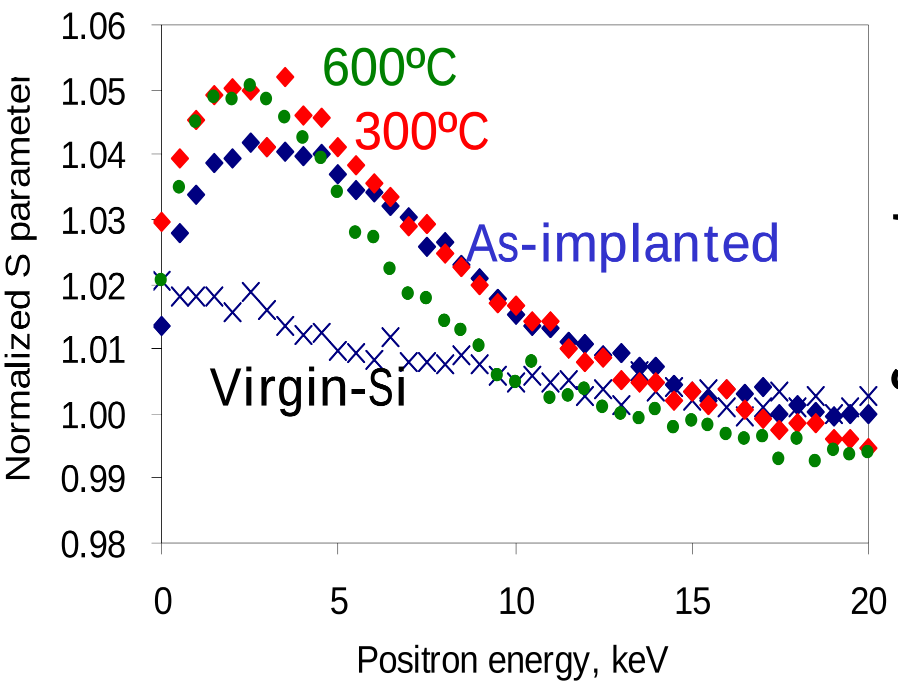
- ✓ The boundary of Jones zone around 10×10^{-3} m_0c
- ✓ The effect of the positrons trapped at the surface
- ✓ The different fraction of the annihilation rate with electrons of core shells

Proposal:

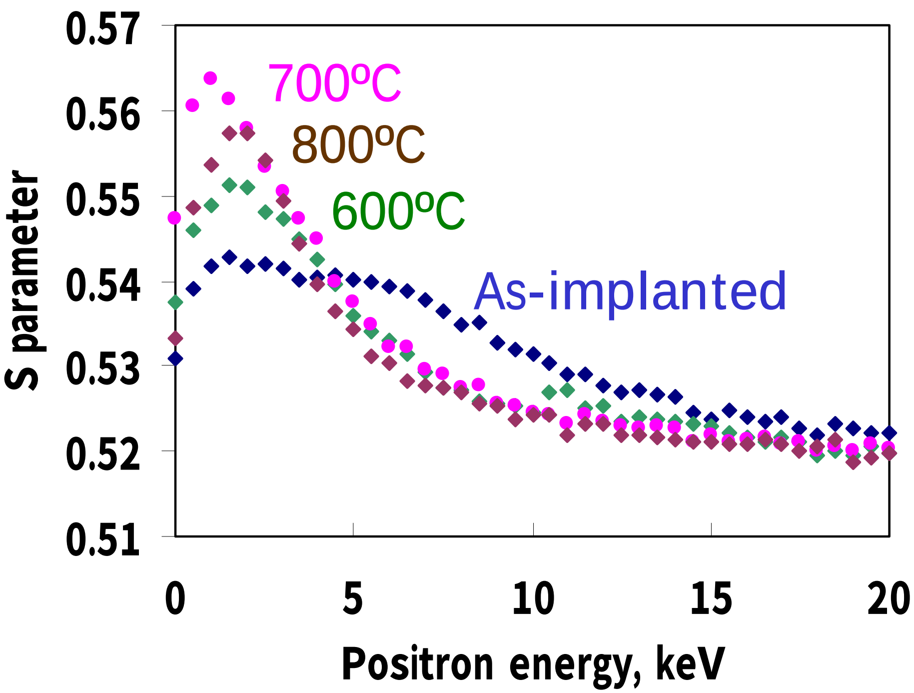
Divacancies, V_2: self-ion implanted FZ-Si

S-E curves in self-ion implanted Si

$2x10^{14}$ Si^+/cm^2 at 100 keV



$2x10^{15}$ Si^+/cm^2 at 100 keV

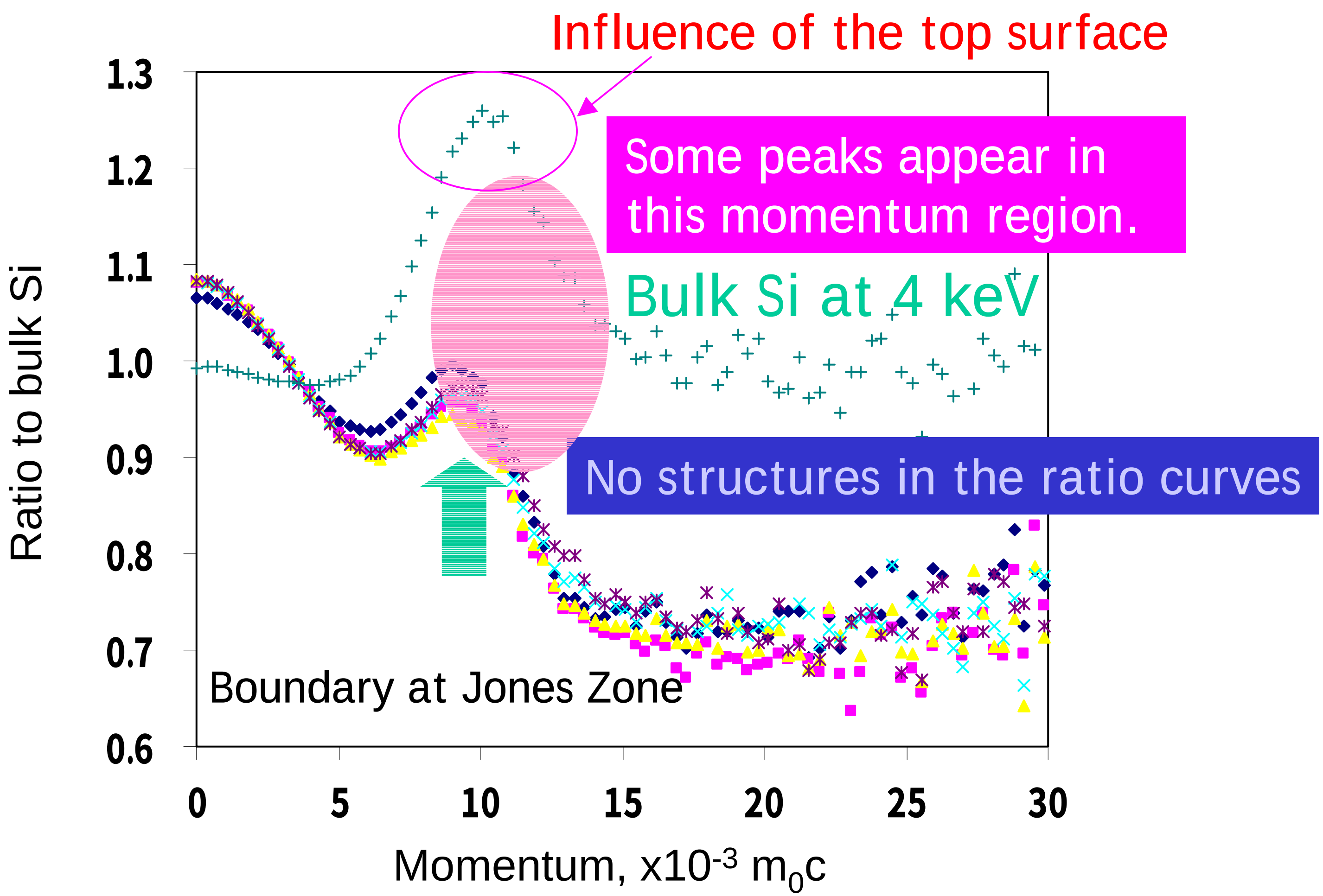


V_2 in crystalline phase → Larger vacancy clusters above 300ºC

Amorphous phase → Larger vacancy clusters above 600ºC

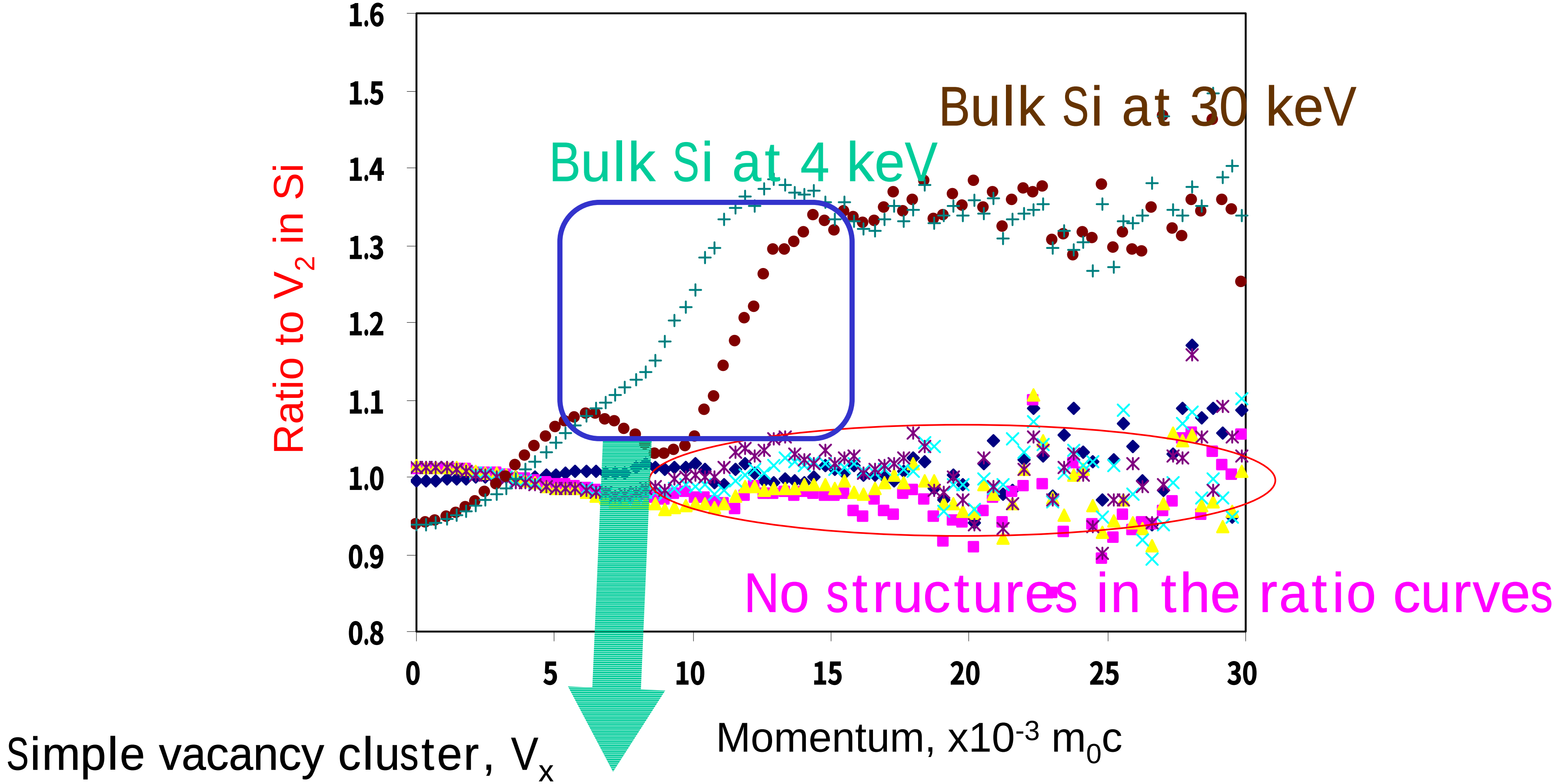
The dominant defects are simple vacancy clusters.

CDB ratio curves in self-ion implanted Si
Normalized by bulk Si



CDB ratio curves in self-ion implanted Si

Normalized by V_2 in Si



A linear combination of bulk Si and V_2 in CDB at the fixed e^+ energy.

It is easy to distinguish a slight change around $10 \times 10^{-3}\ m_0c$.

Experiment

- The ion implanted Cz-Si: O ion $2x10^{15}$ /cm^2, 180 keV
  He ion $1x10^{15}$ /cm^2, 60 keV
  Ar ion $1x10^{15}$ /cm^2, 100 keV

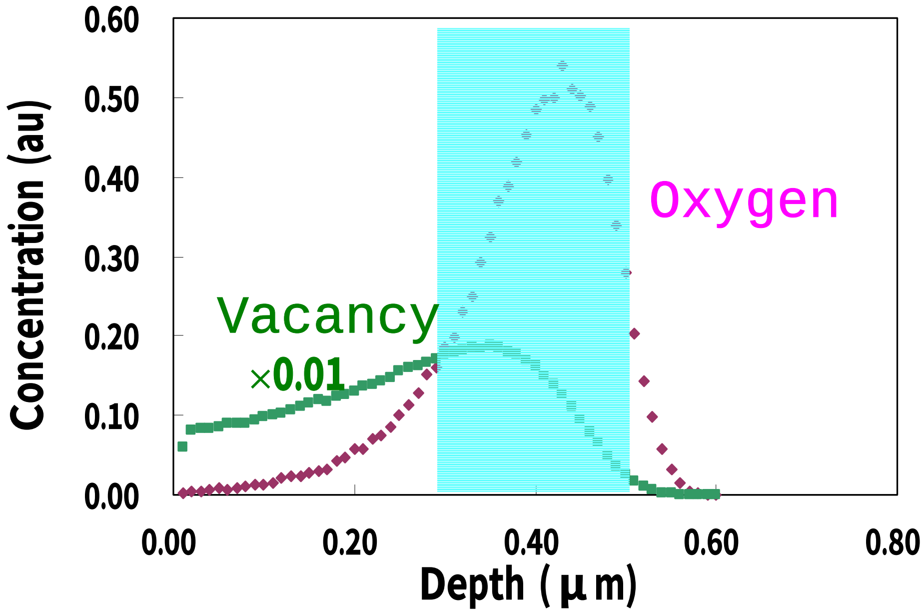
- Chemical etch: KOH solution
  The thickness of a removal was estimated by a weight change.

- Positron measurements: S-E curves
  CDB ratio curves
  Lifetime

2. Vacancy-oxygen complexes in Si

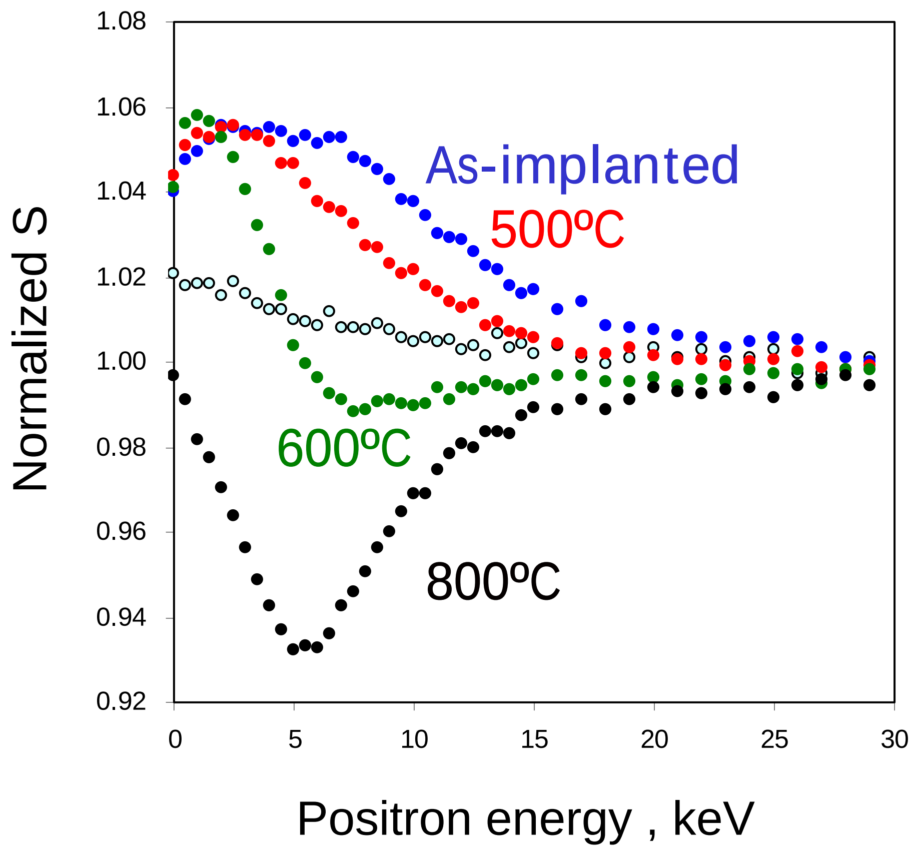
Si implanted with $2x10^{15}$ O^{+}/cm^{2} at 180 keV

O and Vacancy profiles in depth



S-E curves and lifetime for Si implanted with $2x10^{15}$ O^+/cm^2

S-E curves



Lifetime at 6.5 keV, ps

Virgin Si	220
As-implanted	294
600º C	330
800º C	322

@8 keV
275 ps

Lifetime in Si

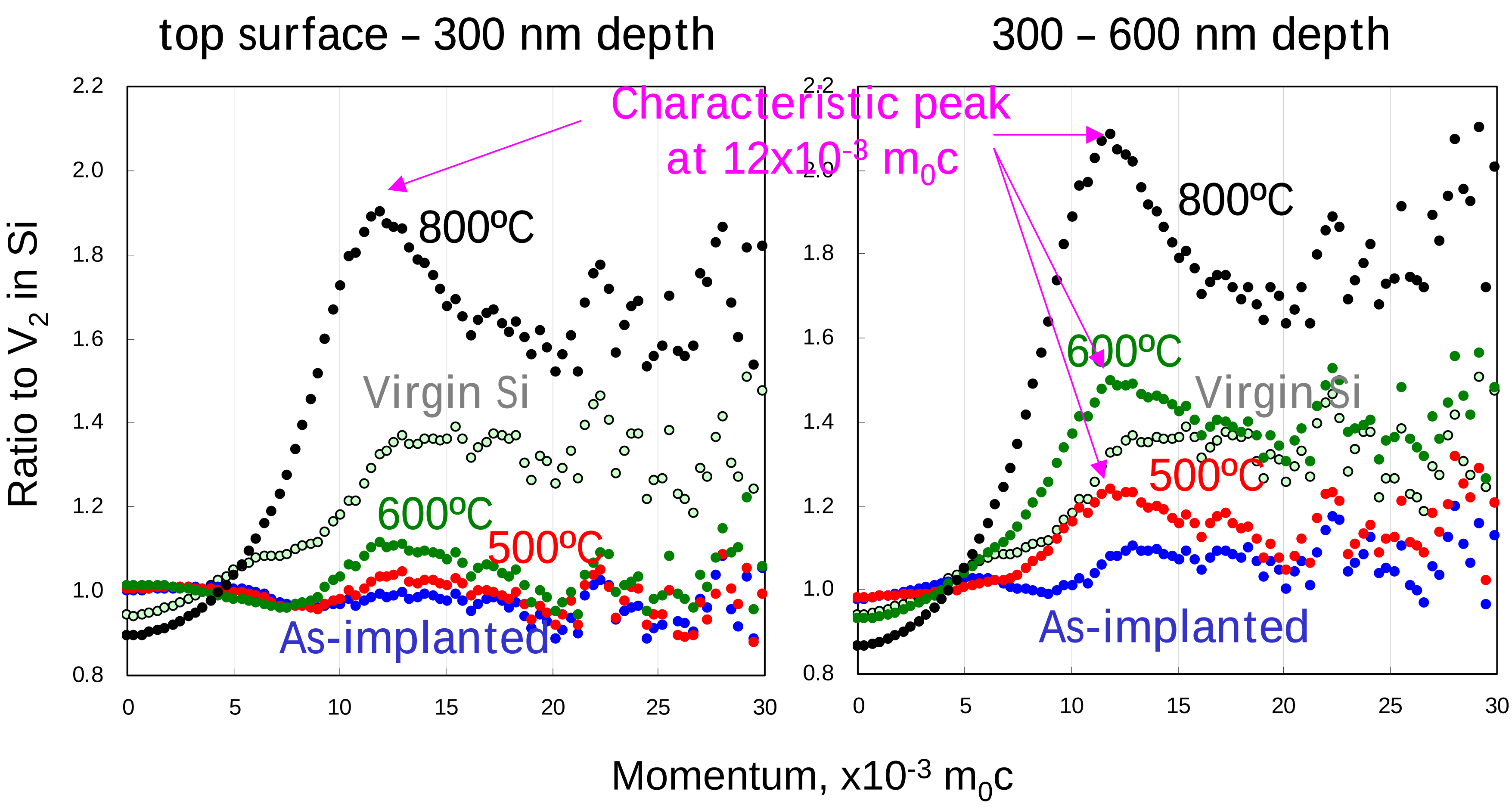
Bulk 220 ps

V_2 300 ps

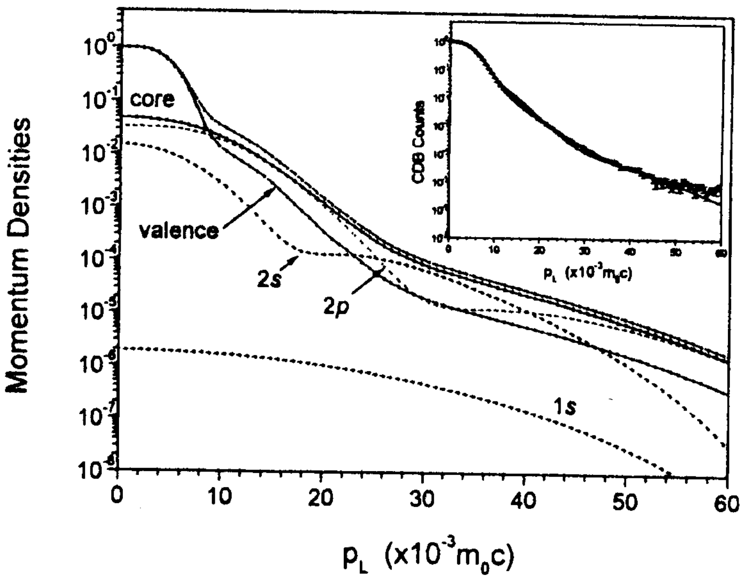
V_4 330 ps

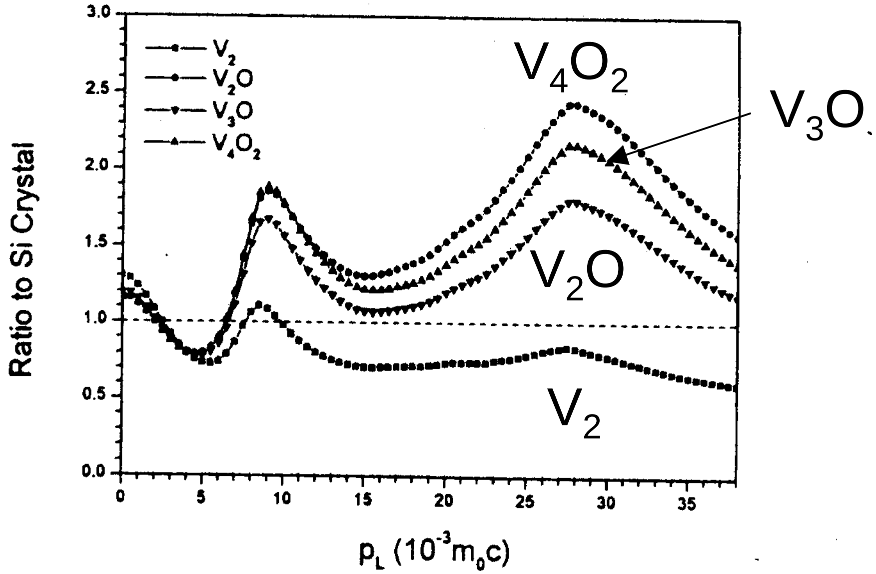
CDB ratio curves for O-implanted Si

3 keV positron energy = top surface – 300 nm depth



First-principles calculation for V-O in Si





Tang et al., ICPA-12, Mater. Sci. Forum 363-365, 67 (2001)

Behavior of V-O complexes in Si

	top surface – 300 nm	300 – 600 nm depth	
As-implanted	V_2	V_2	300 ps lifetime No structure in CDB
500ºC	V_4	V_xO_y (x-y=1)	275 ps lifetime weak structure in CDB
600ºC	V_4		275 ps lifetime strong structure in CDB
800ºC	V_xO_y (x-y=4)	V_xO_y (x-y=4)	322 ps lifetime strong structure in CDB

O diffusion takes place.

3. Vacancy-noble gas atoms complexes in Si

Vacancy-noble gas atom complexes

Initial stage of bubble formation in Si

A positron is suitable probe in the initial stage of defect evolution.

He ions Ar ions

- ✓Can a positron detect noble gas atoms in vacancies?
- ✓Is a positron sensitive to passivate vacancies?

For example: V-H defects in Si → Low S

Positron is not sensitive to H-passivated defects.

3. Vacancy-noble gas atoms complexes in Si

Vacancy-noble gas atom complexes

Initial stage of bubble formation in Si

A positron is suitable probe in the initial stage of defect evolution.

He ions   Ar ions

- ✓Can a positron detect noble gas atoms in vacancies?
- ✓Is a positron sensitive to passivate vacancies?

PRB 58, 12559 (1998)

For example: V-H defects in Si ➡ Long lifetime 280 ps

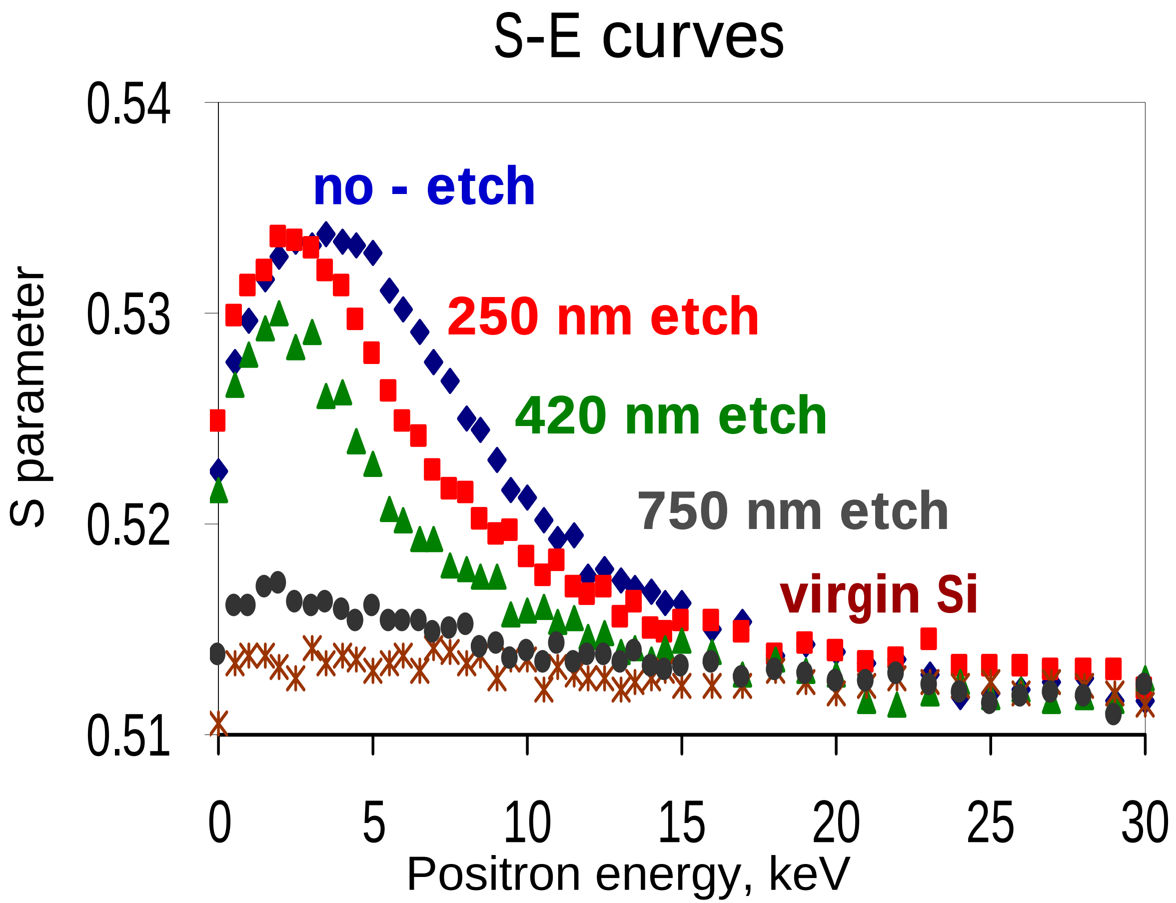
Positron is sensitive to H-passivated defects.

Lifetime & CDB measurements is necessary.

S-E curves for He implanted Si

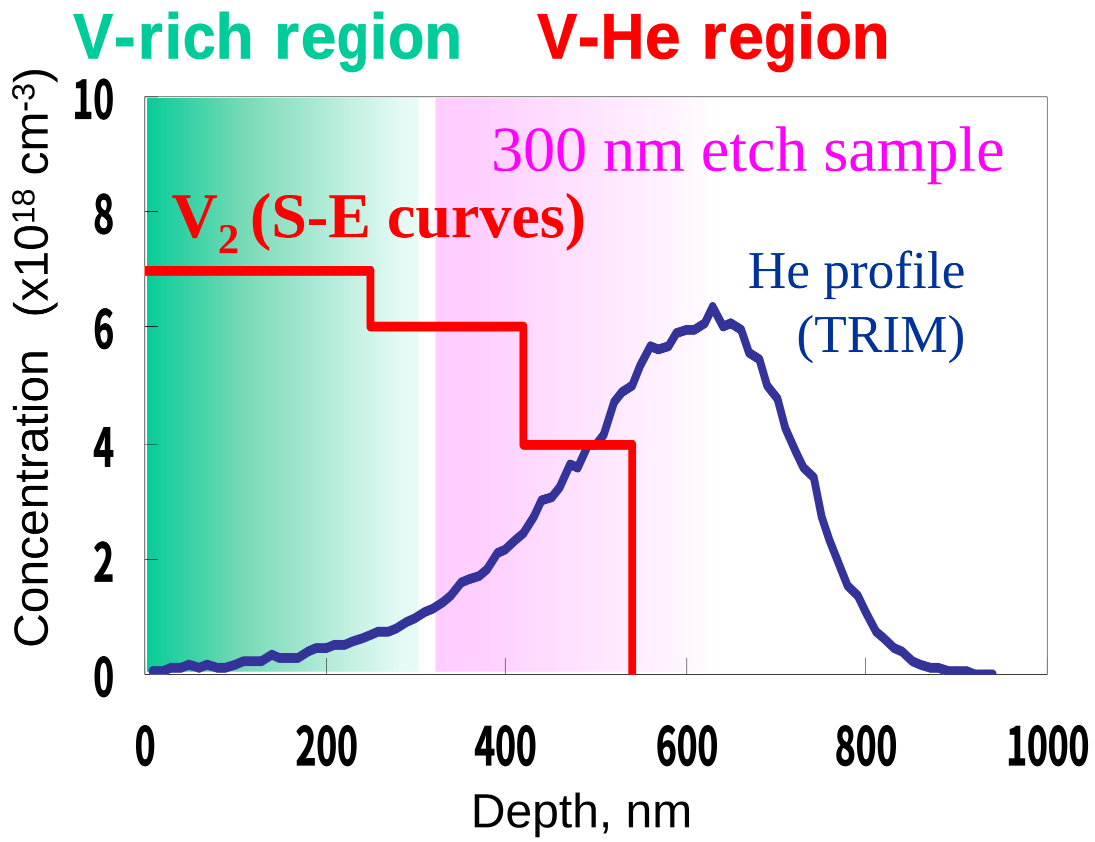
He: 1×10^{15} /cm^2 at 60 keV

Mean projected range: 560 nm
Straggling range: 140 nm



The defect, V_2, profile for He implanted Si

He: $1x10^{15}$ /cm^2 at 60 keV



Layer-by-layer analysis: Lifetime & CDB

Positron lifetime for He implanted Si

	lifetime	size
V-rich region (Top surface〜300 nm)	302 ps	V_2
V-He region (300 nm〜600 nm)	285 ps	V

Positron energy: 4 keV

Positron lifetime in Si

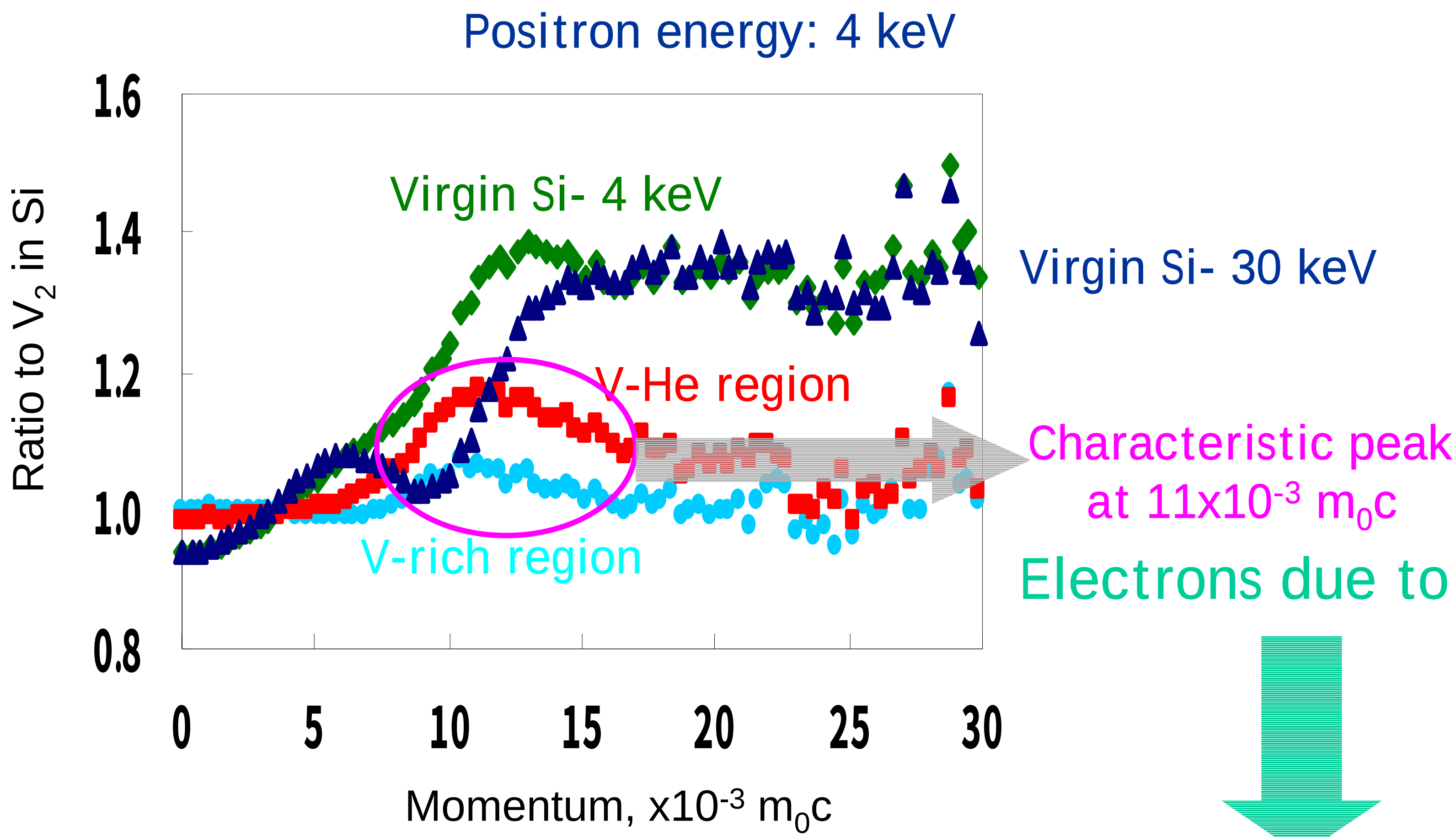
Defect	lifetime
Bulk	218 ps
V	275 ps
V_2	300 ps
V_4	330 ps

V-He region Positron trap site with one vacant

↓

Speculation: V-He complexes such as V_2He

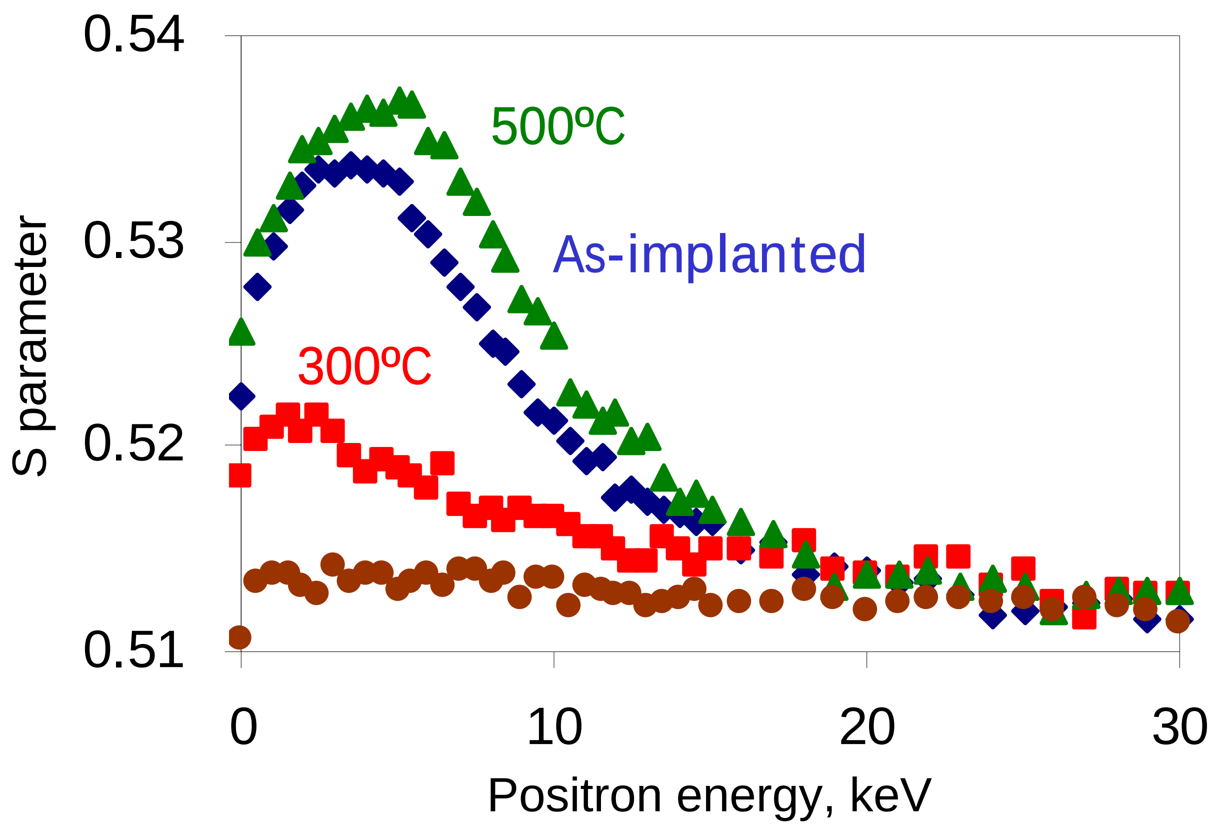
CDB ratio curve for He implanted Si



Electrons due to He ?

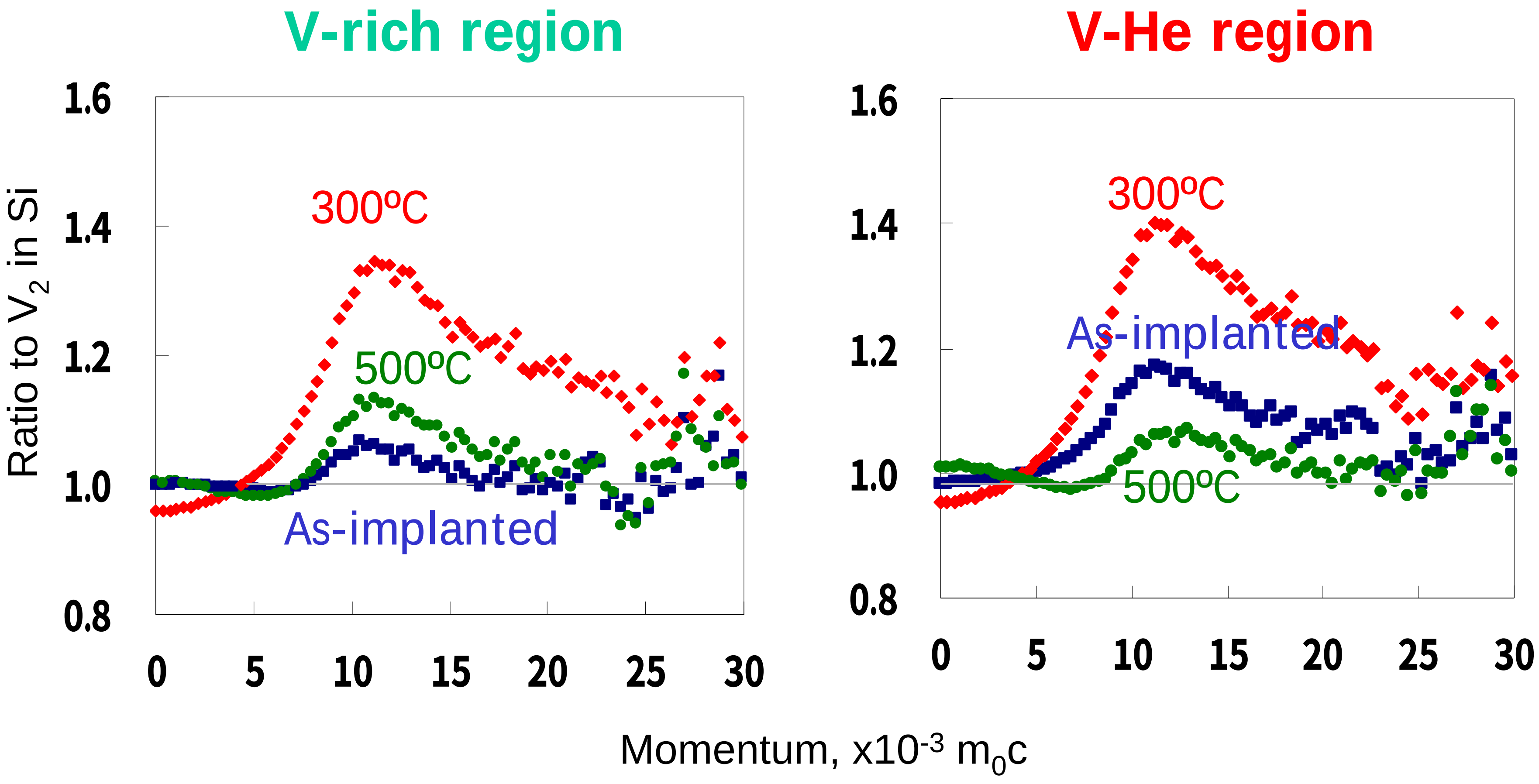
The theoretical calculations are needed.

S-E curves for He implanted Si after annealing

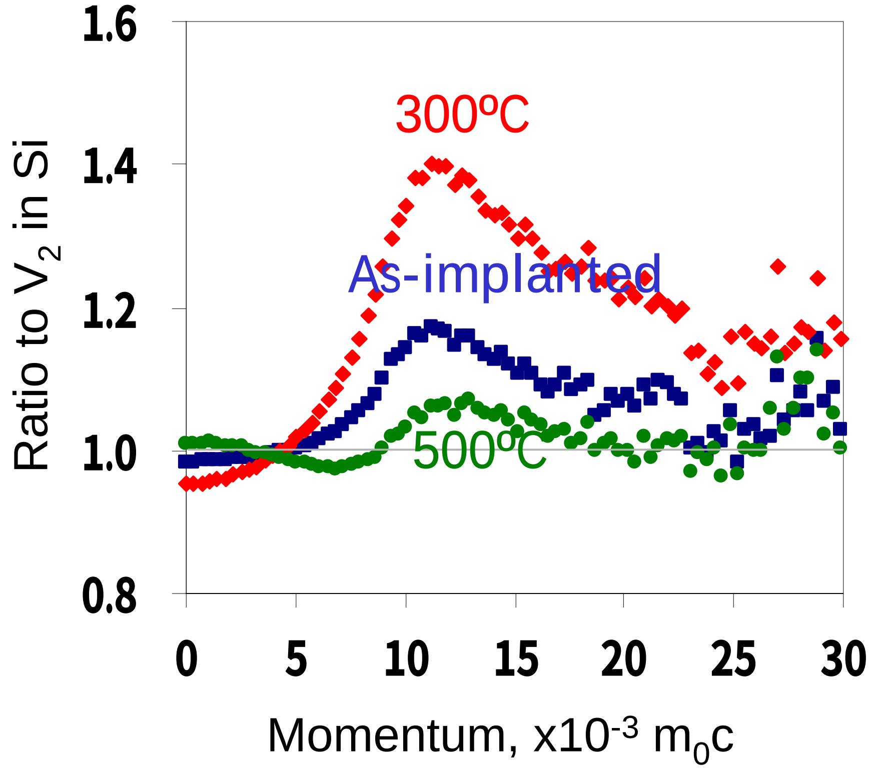


Low S at 300ºC and high S at 500ºC.

CDB ratio curve for the annealed samples



CDB ratio curve & lifetime in V-He region



As-implanted

→ V_2He

He diffusion

300ºC

- Single vacant
- Large He fraction

→ V_4He_3?

He release

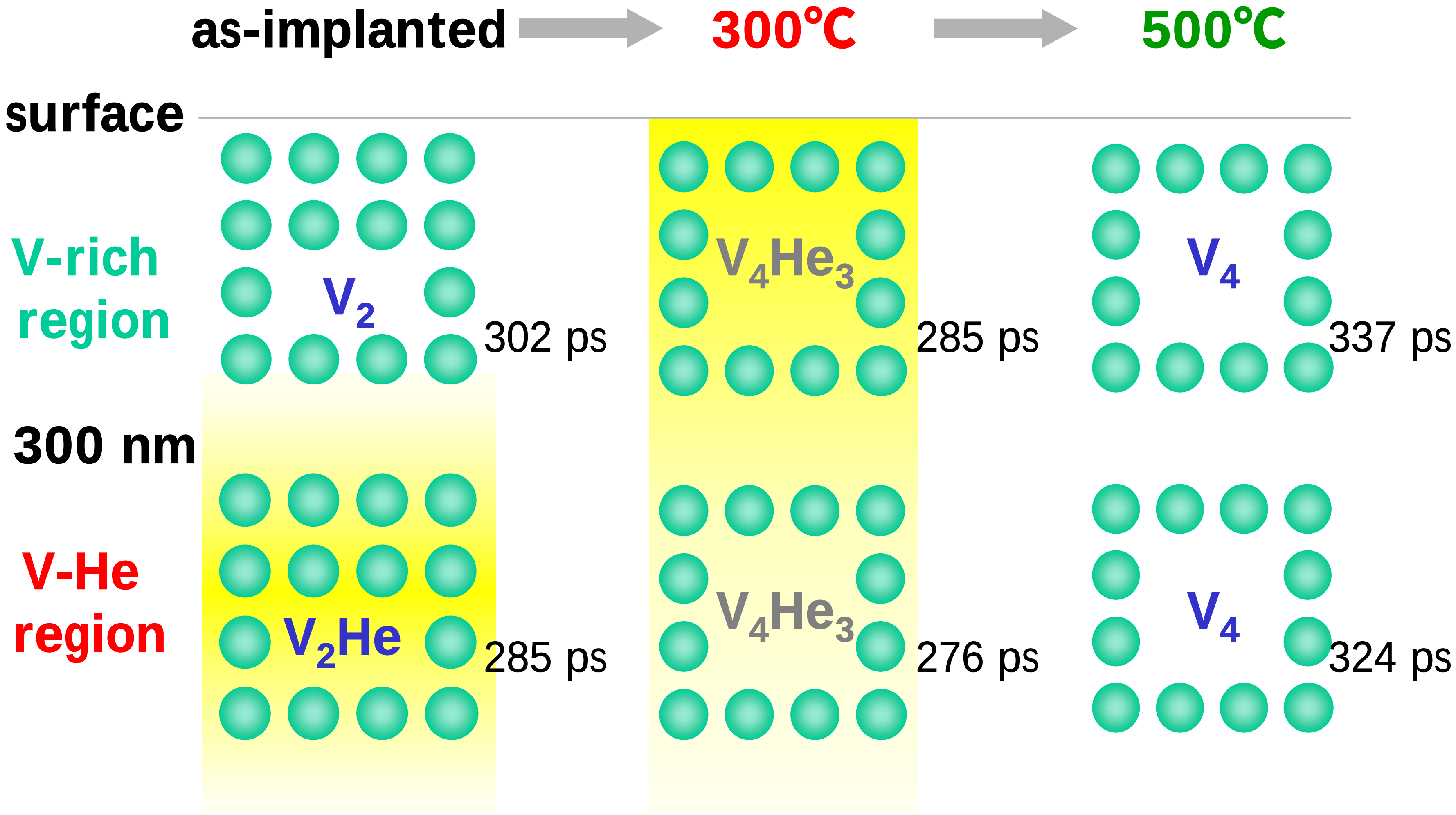
500ºC

- Four vacant
- No He fraction

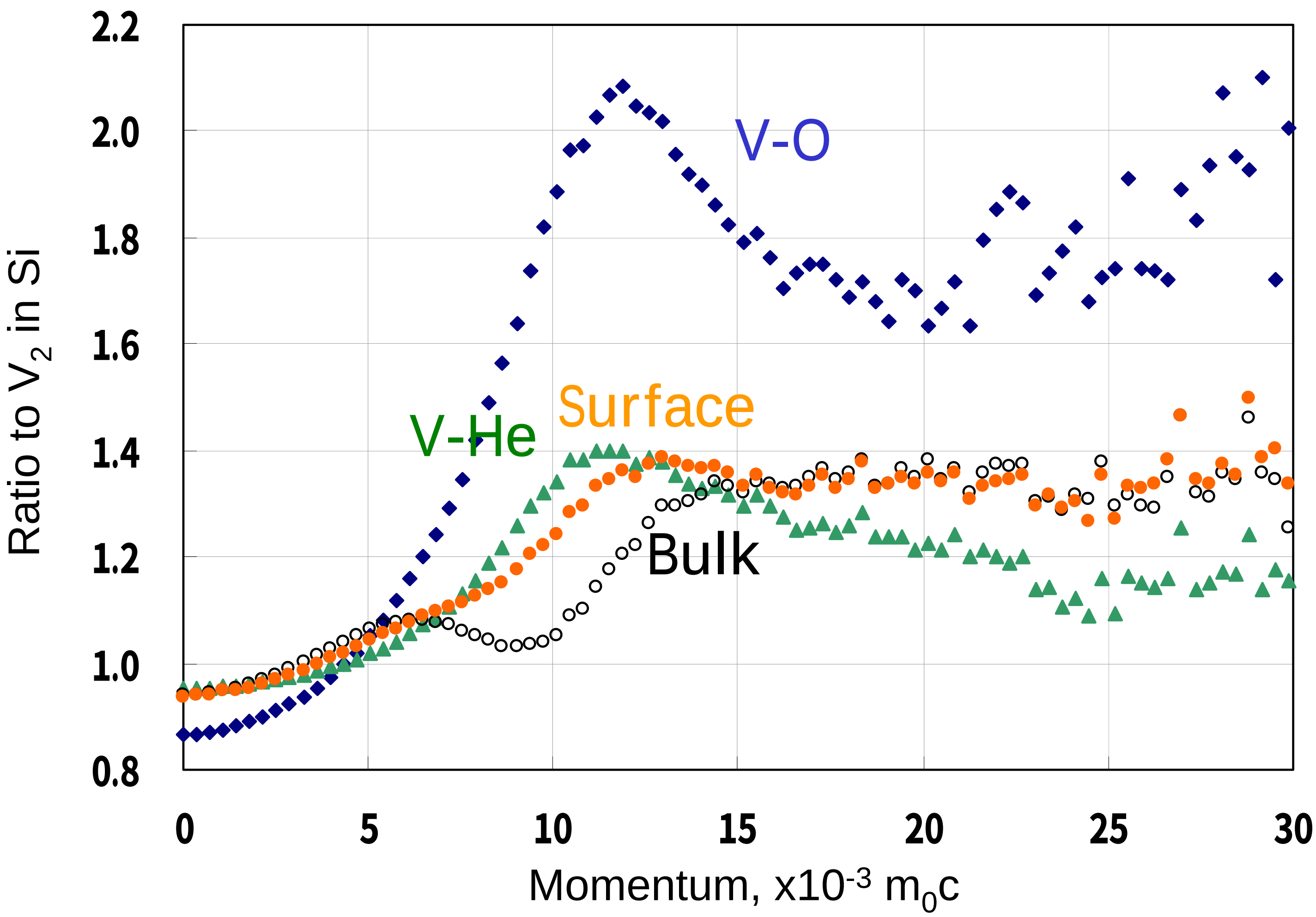
→ V_4

	as-implanted	300ºC	500ºC
Lifetime	285 ps(98%)	276 ps(98%)	324 ps(98%)

V-He complexes behavior in Si



CDB ratio curves for V-O and V-He in Si

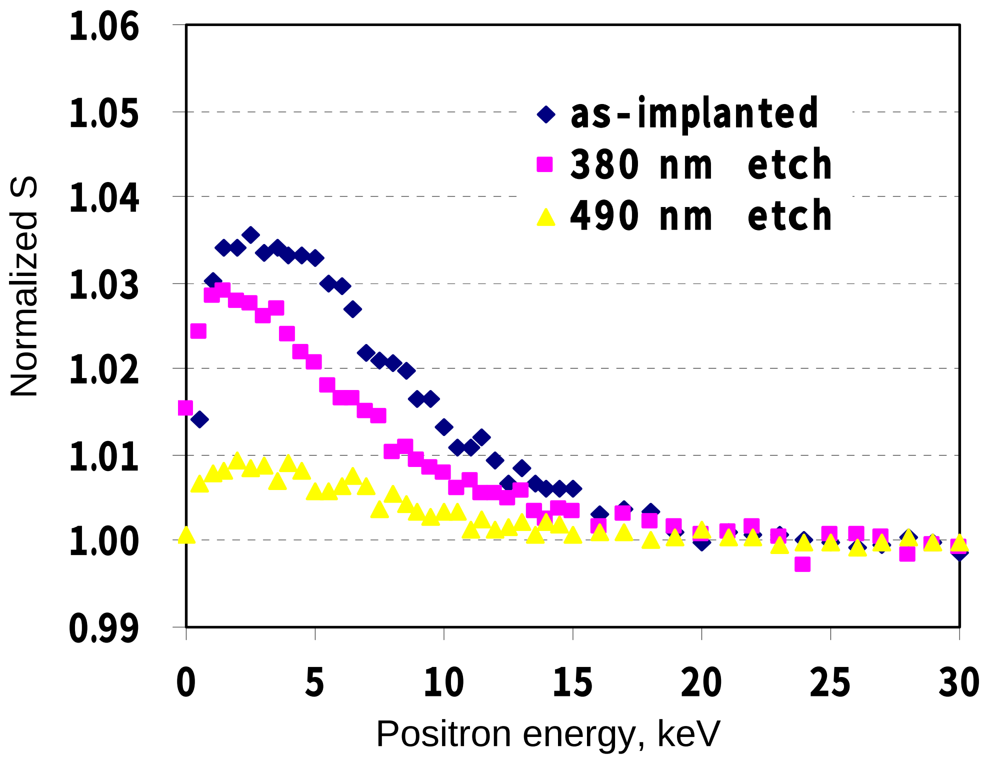


Vacancy-argon complexes in Si

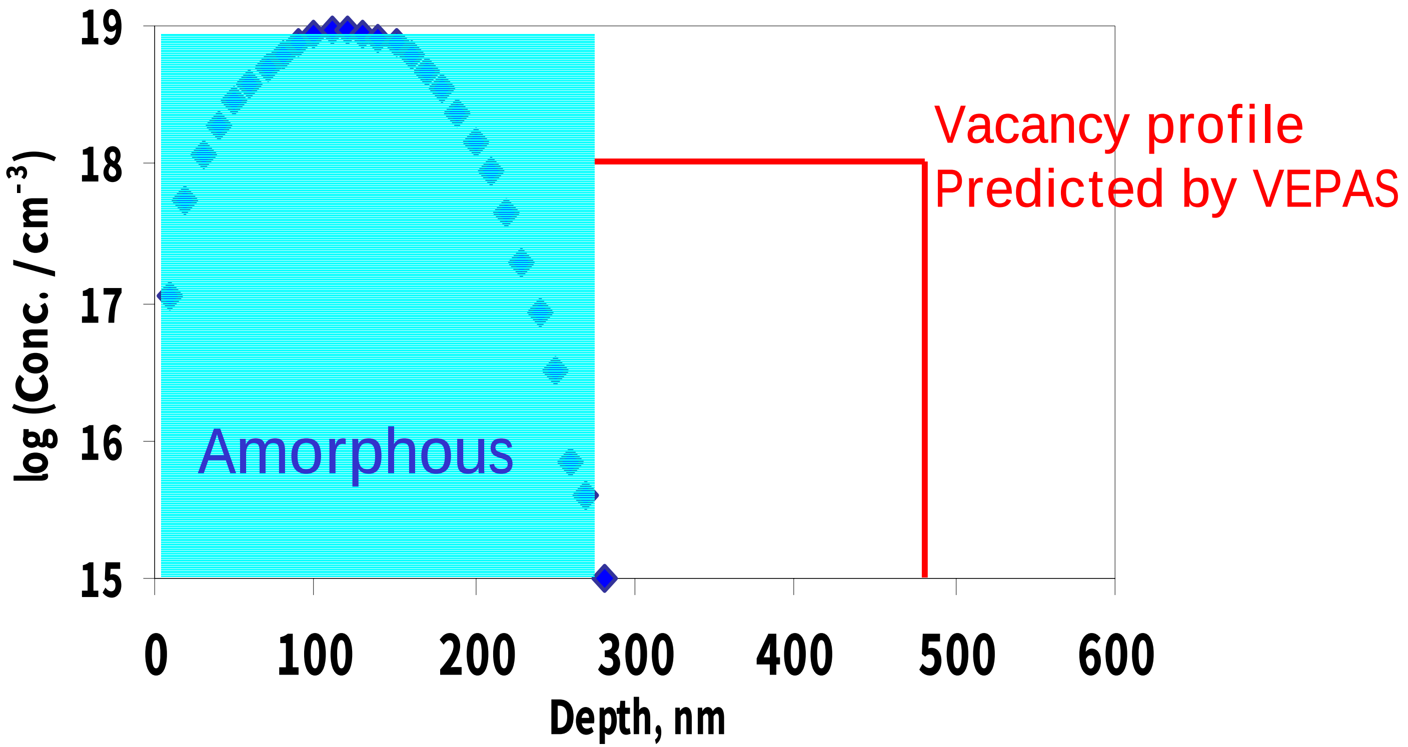
$1x10^{15}$ Ar^{+}/cm^{2}, 100 keV

> The critical dose for amorphization
Mean projected range: 114 nm
Straggling range: 41 nm

S-E curves for the as-implanted sample



Vacancy profile in Ar ion-implanted Si



Defects are induced beyond the implantation profile.

Lifetime & CEB measurements

Lifetime & CDB ratio curves in Ar ion-implanted Si

Positron lifetime @ 3 keV

Ar ion implanted region:

Top surface – 200 nm: 302 ps (98%)

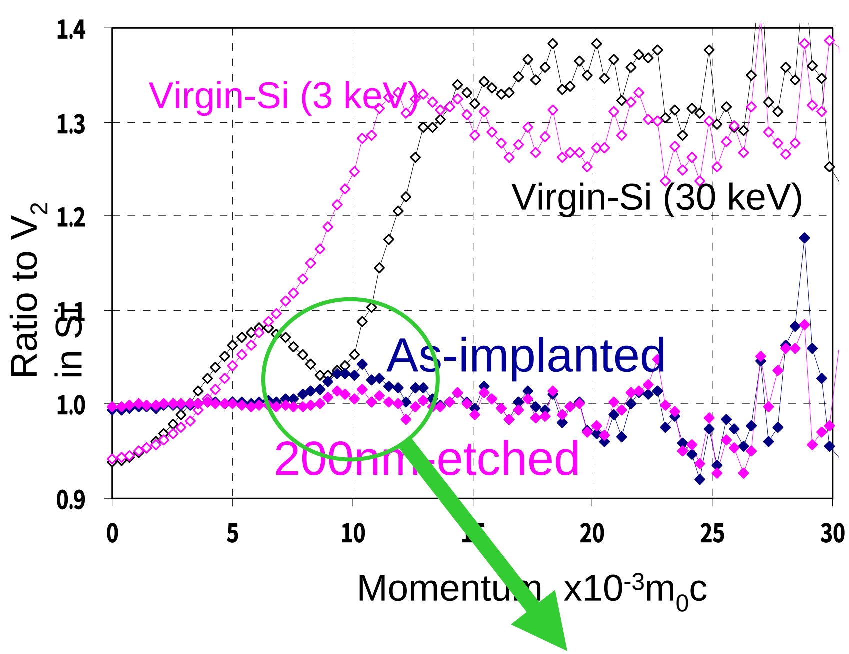
Size: Divacancies

Beyond the implanted region:

200 nm – 400 nm depths: 301 ps (92%)

Size: Divacancies

CDB ratio spectra @ 3 keV



Due to Ar atoms ?

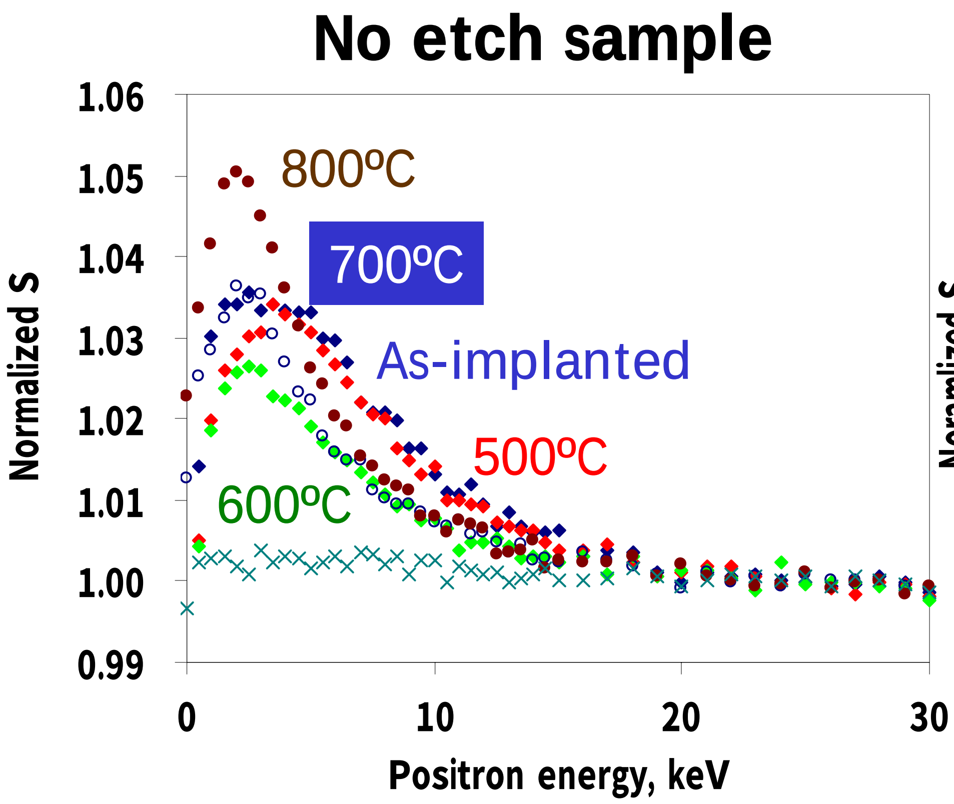
In the implanted region: Amorphous

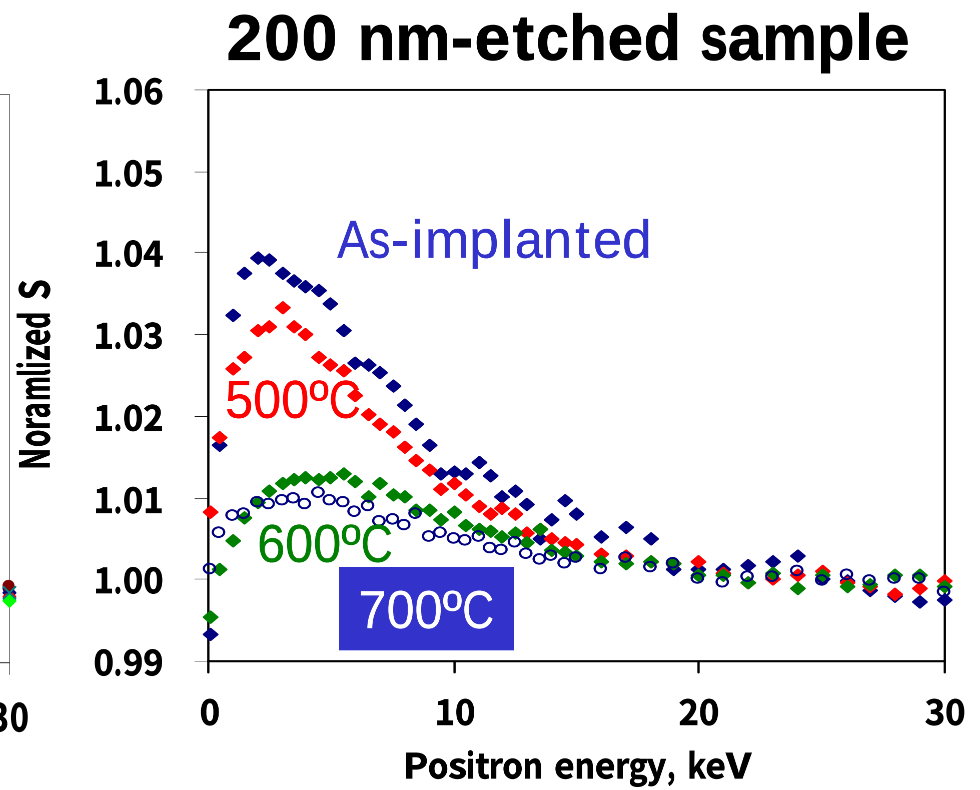
Passivation by Ar atoms?

Beyond the implanted range: Divacancies

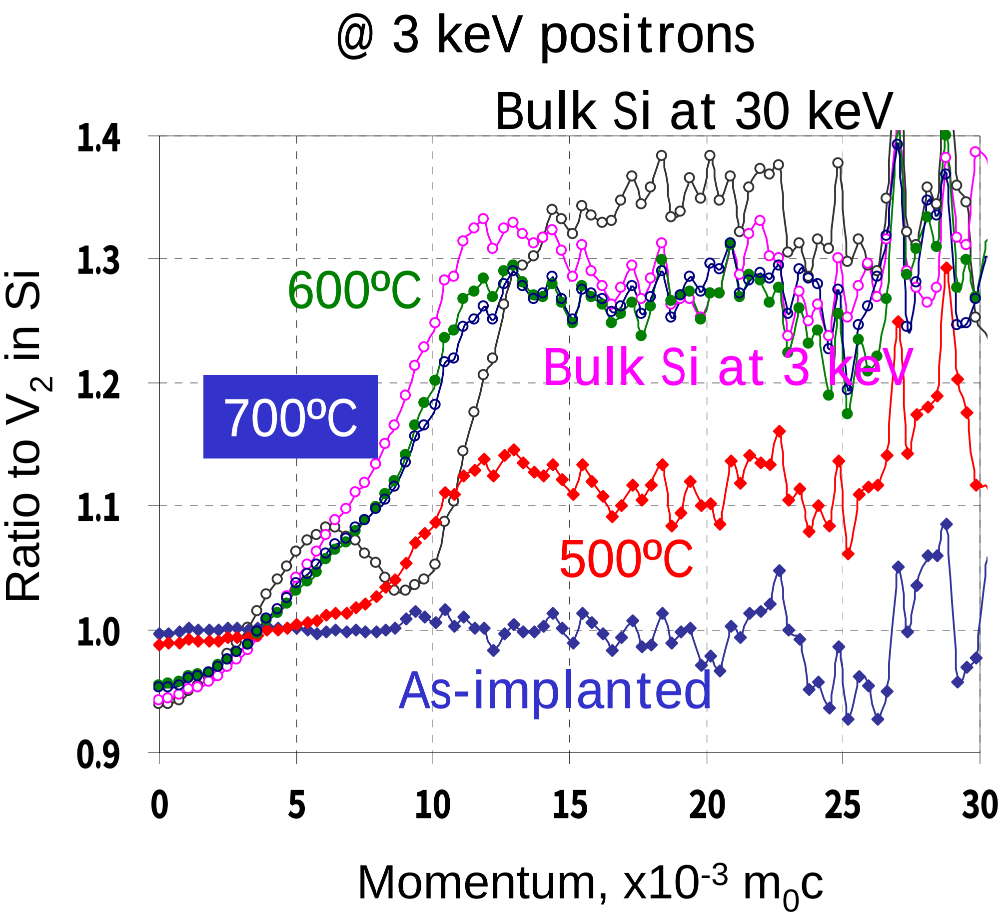
S-E curves for the Ar ion implanted Si after annealing

$1x10^{15}$ Ar^{+}/cm^{2}, 100 keV





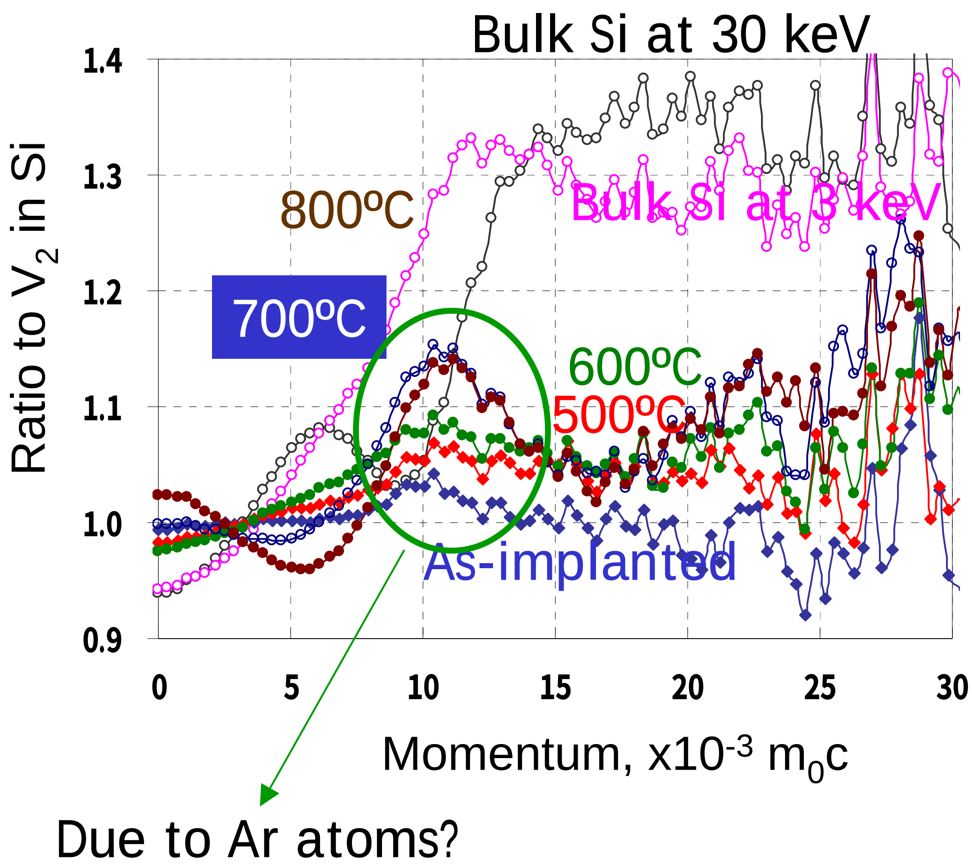
CDB and lifetime for Ar ion-implanted Si
200 nm - 400 nm



500ºC	Lifetime(Size)	330 ps, 72%
	S parameter	High S
	Peak intensity at $10\times10^{-3}\ m_0c$	None
600ºC	Lifetime(Size)	338 ps, 53%
	S parameter	Low S
	Peak intensity at $10\times10^{-3}\ m_0c$	None
700ºC	Lifetime(Size)	318 ps, 52%
	S parameter	Low S
	Peak intensity at $10\times10^{-3}\ m_0c$	None
800ºC	Lifetime(Size)	291 ps, 65%
	S parameter	Low S
	Peak intensity at $10\times10^{-3}\ m_0c$	None

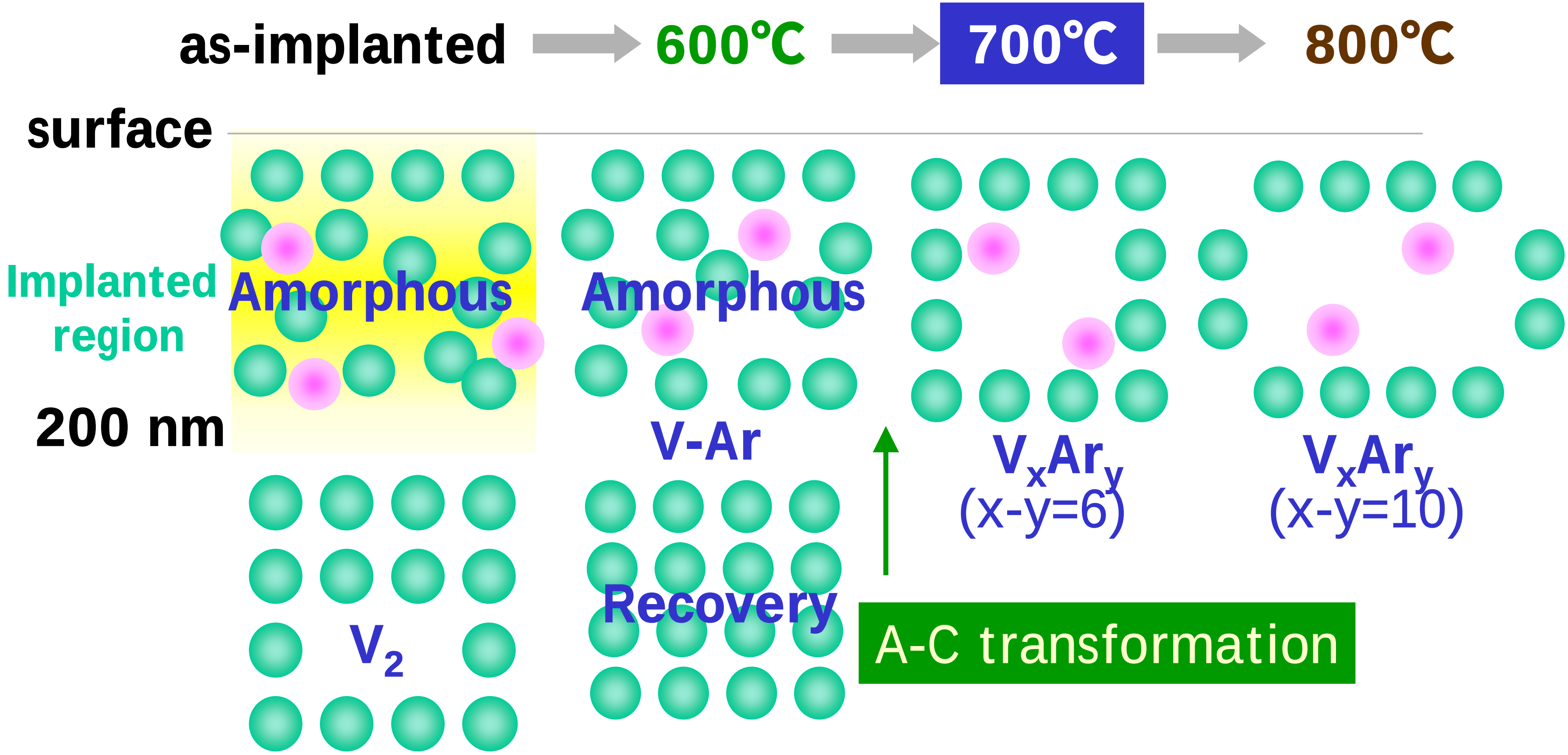
Beyond the implantation range: anneal out at 600ºC

CDB and lifetime for Ar ion-implanted Si
Top surface - 200 nm



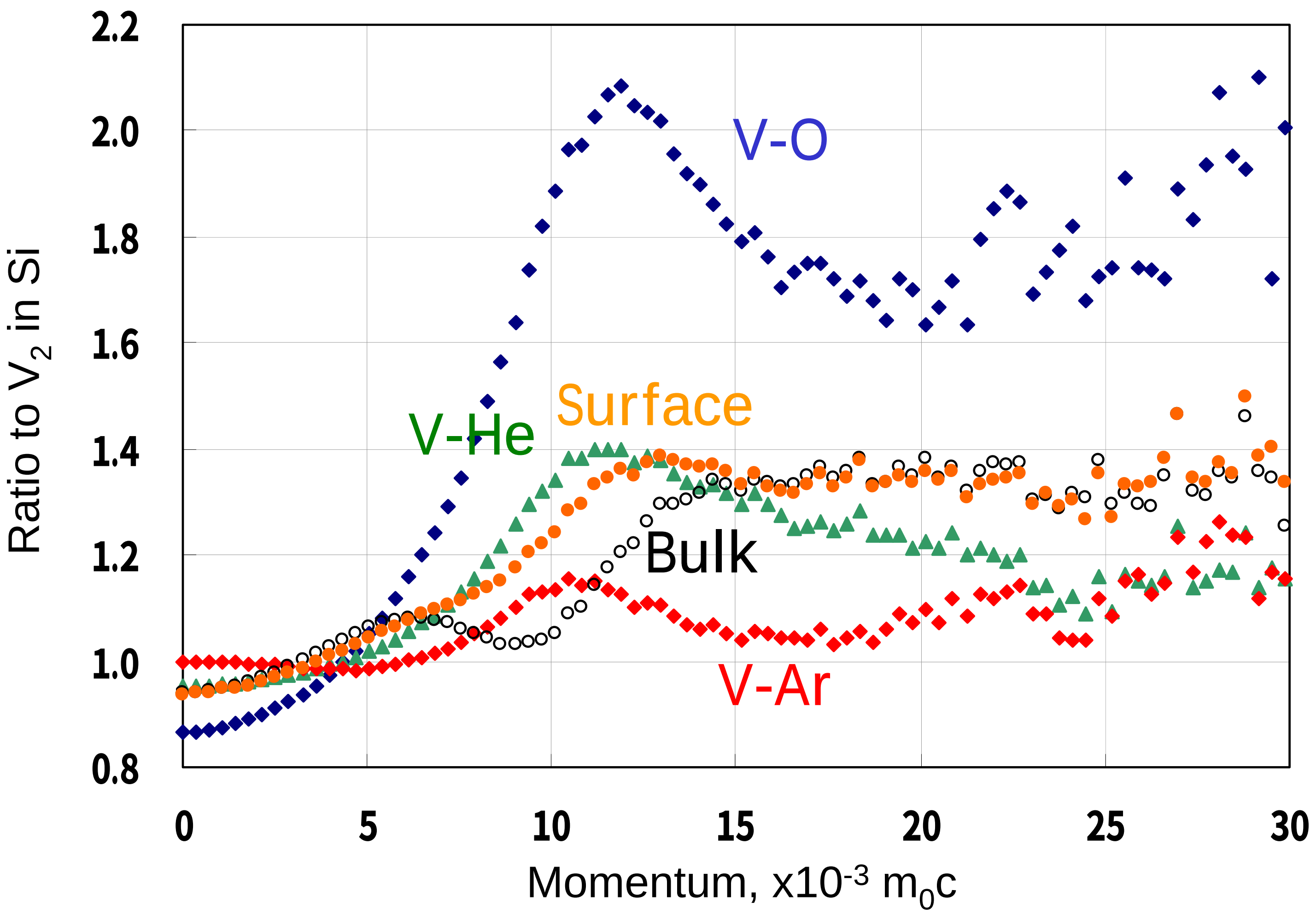
500ºC	Lifetime(Size)	298 ps, 98%
	S parameter	High S
	Peak intensity at 10×10^{-3} m_0c	Medium
600ºC	Lifetime(Size)	297 ps, 98%
	S parameter	High S
	Peak intensity at 10×10^{-3} m_0c	Medium
700ºC	Lifetime(Size)	370 ps, 79%
	S parameter	Higher S
	Peak intensity at 10×10^{-3} m_0c	Strong
800ºC	Lifetime(Size)	408 ps, 83%
	S parameter	Higher S
	Peak intensity at 10×10^{-3} m_0c	Strong

V-Ar complexes behavior in Si



1. A-C trans. temp. is higher. (Usual around 600ºC)
2. Ar atoms are not released from the sample.

CEB ratio curves for V-impurity complexes in Si
- Reference V_2 in Si -



4. Summary

Various V-impurity complexes in Si have been investigated by S-E, CDB, and lifetime measurements using a positron beam.

1. These techniques are useful to identify V-I complexes in Si.
2. Depth resolution-enhanced VEPAS enables us to carry out the layer-by-layer analysis.
3. Much attention should be paid in the analysis of CDB data using a positron beam.
4. The theoretical approach is needed to identify the structure of V-I complexes in Si.