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SMR/1758-4

"Workshop on Ion Beam Studies of Nanomaterials:
Synthesis, Modification and Characterization"

26 June - 1 July 2006

Fully atomistic approach for ion-channeling analysis of defects in Si

Giorgio Lulli
CNR-IMM Institute
Bologna, Italy

Consiglio Nazionale delle Ricerche
Istituto per la Microelettronica e i Microsistemi

Fully atomistic approach for ion-channeling analysis of defects in Si

Giorgio Lulli
CNR-IMM Institute Bologna (Italy)

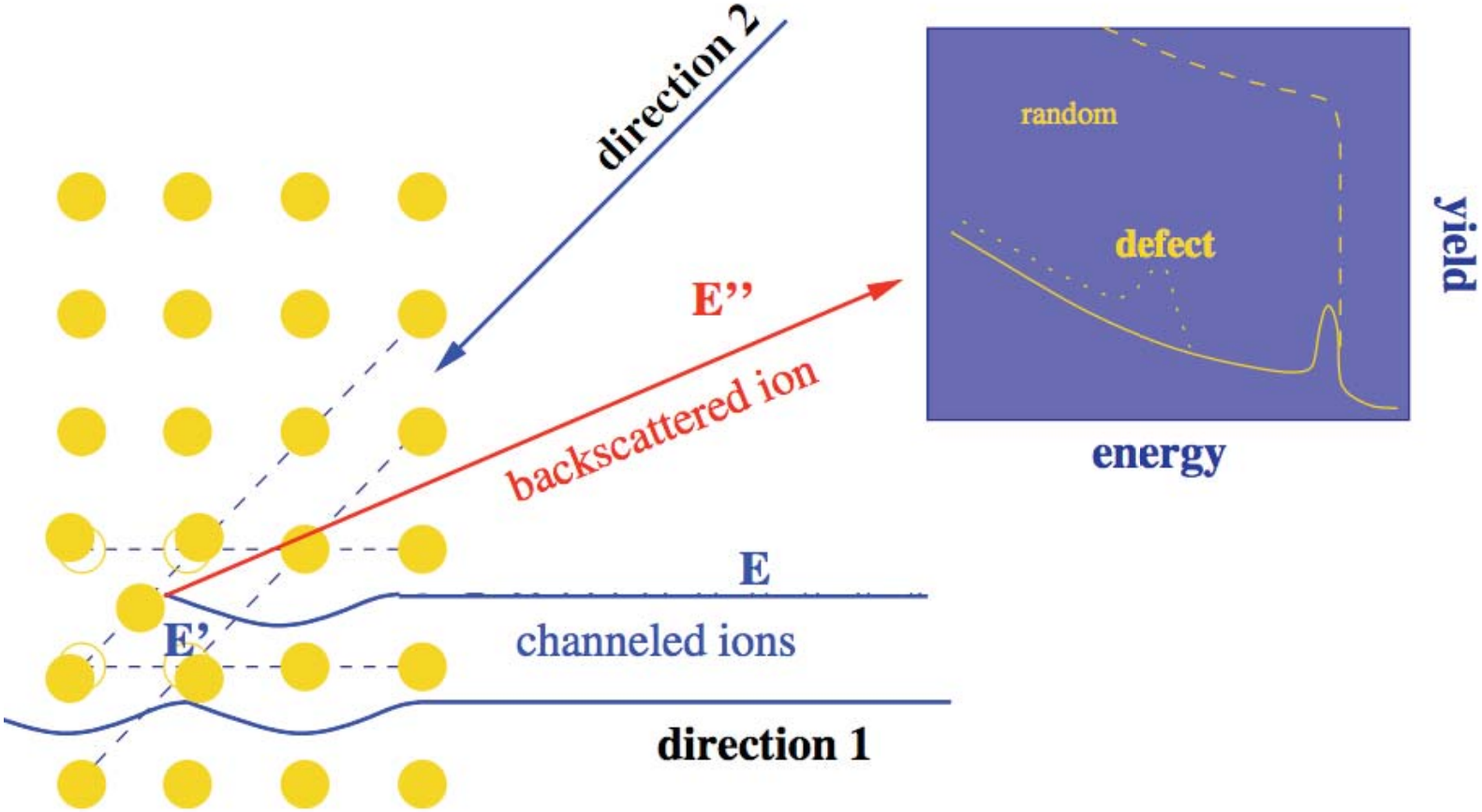
Motivation

- ion-implantation doping of Silicon
- developing predictive MC-BCA model of ion implantation (ion and defect profiles)
- comparison simulation - experiment (RBS-C)

Objective

Interpreting the macroscopic RBS-C response of ion irradiated Si with models of lattice defects obtained from atomistic calculations

RBS channeling and defects



MATERIALS ANALYSIS BY ION CHANNELING

Submicron Crystallography

LEONARD C. FELDMAN
Bell Laboratories
Murray Hill, New Jersey

JAMES W. MAYER
Cornell University
Ithaca, New York

S. THOMAS PICRAUX
Sandia National Laboratories
Albuquerque, New Mexico

1982

ACADEMIC PRESS

A Subsidiary of Harcourt Brace Jovanovich, Publishers

New York London
Paris San Diego San Francisco São Paulo Sydney Tokyo Toronto

CHAPTER 4

DECHANNELING BY DEFECTS

4.1 Introduction

Many properties of materials are dominated by defects. Thus the processing of materials requires the control of defects during different treatments, such as diffusion of dopant impurities in semiconductors, work hardening of metals, and surface-alloy formation by ion implantation. Channeling effect measurements can be used to investigate or to monitor the controlled introduction and removal of structural defects during material processing. In this chapter we demonstrate how the channeling effect is sensitive to structural defects.

The previous chapters treated the crystal as perfect in that particles once channeled remained in channeling trajectories. An imperfect crystal contains defects that introduce distortions in the crystal structure; defects provide a mechanism for the scattering of channeled particles into nonchanneling trajectories. This scattering process is referred to as dechanneling and is the primary concern of this chapter. Each type of defect has a particular influence on the trajectory of a passing particle and can be associated with a corresponding dechanneling factor σ_D. The partition of the particle trajectories into channeled and dechanneled components by means of a dechanneling factor is used in Chapter 5 to determine the number of defects and their depth distribution in the crystal.

… the “Bible” of RBS-C

RBS-C characterization ⟷ **physics of defects (silicon)**

- mature technique
- already well developed in the 80's

- major achievements: last 15 years (computation)
- still in progress

Radiation Effects, 1979, Vol. 41, pp. 195–202
0033-7579/79/4104-0195$04.50/0

LOCATION OF SELF-INTERSTITIAL ATOMS IN BORON-IMPLANTED SILICON BY MEANS OF RUTHERFORD BACKSCATTERING OF CHANNELLED IONS

GERHARD GÖTZ and GERALD SOMMER†

Sektion Physik der Friedrich-Schiller-Universität Jena, DDR 69 Jena, Max-Wien-Platz 1

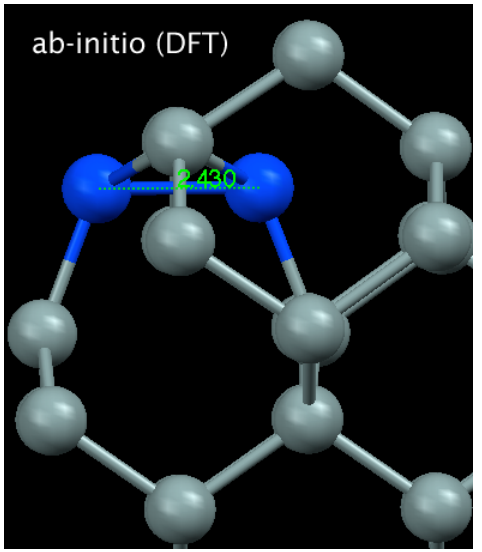
(*Received January 9, 1979*)

For locating self-interstitial atoms in silicon by means of Rutherford backscattering of channelled ions, boron has been implanted at room temperature and at the temperature of liquid nitrogen. The employed implantation doses were $2 \cdot 10^{14}$ cm^{-2} and $7 \cdot 10^{15}$ cm^{-2}, respectively. The experiments have been performed at 300 K and at 120 K to reduce ionization-stimulated annealing. The beam of 1.4 MeV He^+-ions was highly collimated.

To obtain the configuration of implantation-induced self-interstitial atoms symmetry considerations have been performed.

The location experiments presented indicate the existence of isolated self-interstitial atoms in silicon. Under the conditions of these experiments the interstitial atoms assume a ⟨110⟩ split configuration of orthorhombic symmetry.

interatomic distance = 2.88 Å



Radiation Effects, 1982, Vol. 59, pp. 117–124
0033-7579/82/5904-0117$06.50/0

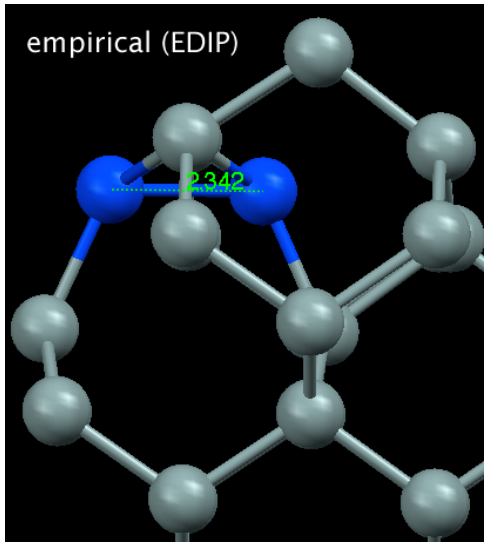
A STUDY ON THE SELF-INTERSTITIAL STRUCTURE OF RADIATION DAMAGED SILICON BY MEANS OF THE DOUBLE ALIGNMENT CHANNELING TECHNIQUE

K. MORITA† and H. D. CARSTANJEN

Department of Physics, University of Munich, Munich, W. Germany

(*Received March 24, 1981*)

The angular distribution of 2.8 MeV helium ions backscattered from silicon crystals containing self-interstitials has been calculated by channeling computer simulations for a double alignment channeling configuration. The structures of the self-interstitial defects are assumed to be the split ⟨110⟩ interstitial and the split ⟨100⟩ di-interstitial with various inter-atomic distances. The obtained profiles of the backscattering yield are found to show shapes characteristic for each structure which can be used for differentiating between these structures. When comparing these profiles with experimental profiles obtained with the same double alignment channeling configuration in a previous study one finds reasonable agreement for the split ⟨110⟩ interstitial defect with an inter-atomic distance of 1.76 Å.



What's (almost) new

- interpretation of RBS-C measurement in ion-implanted Si (low defect concentration) based on a physical model of the disordered lattice

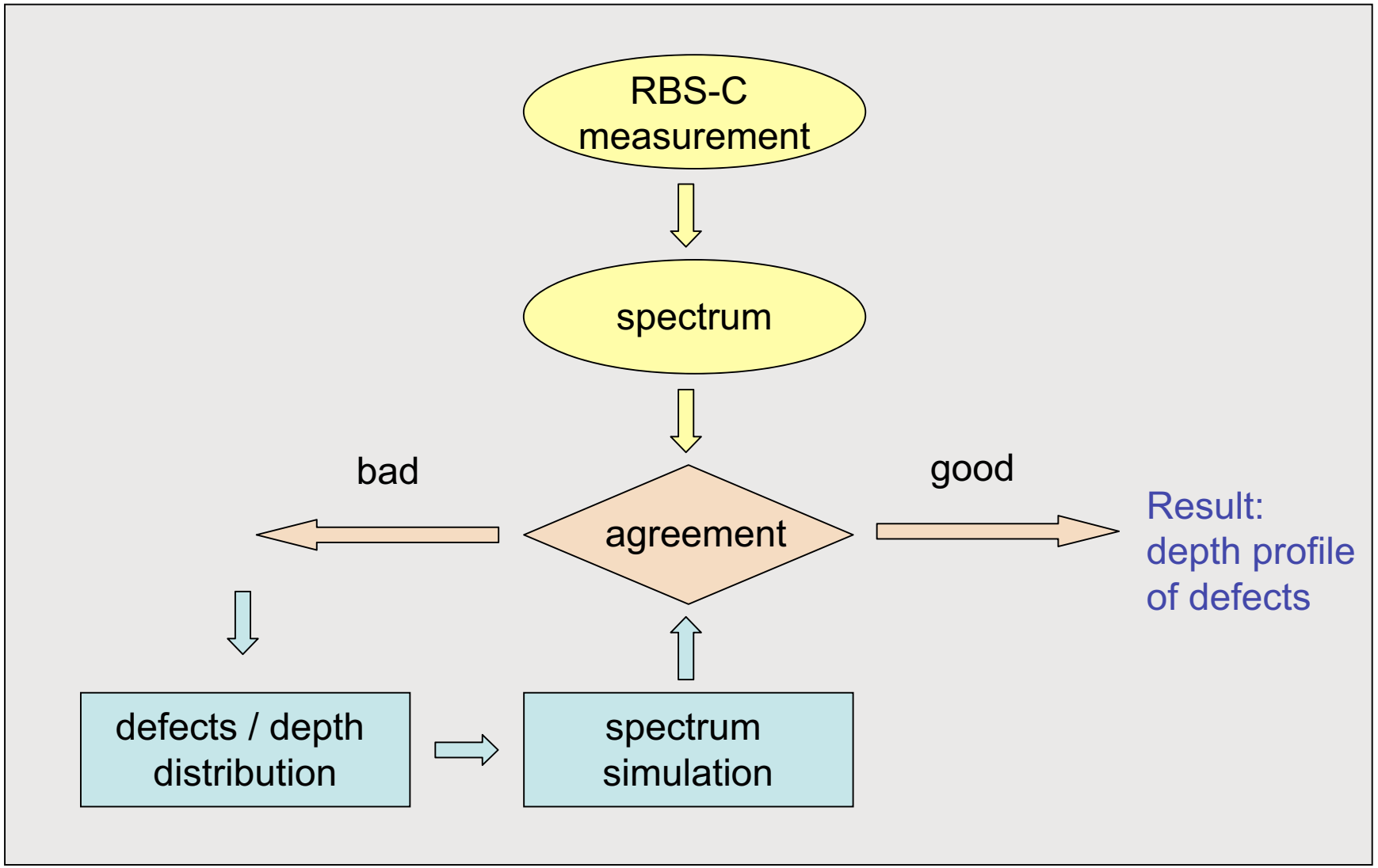
- the simulation of spectra takes its input from theoretical models obtained by atomistic calculations

Experiment

- **substrate**: (100) Si FZ 500Ω•cm *n*-type
- **implantation**: Si^+ 180 keV 10^{14} cm^{-2} RT
  (as-implanted, low defect concentration ~ few %)
- **characterization**: multiaxial RBS-C He^+ 2MeV
  orientations: <100>, <111>, <112>, <113>, {110}, {100}, <130>, <120>, <110>

What is needed

- experimental (multi-axial) RBS-C analysis
- physical model for computation of defects
- procedure to build up a large (~10^6 atoms) model sample of disordered lattice
- MC-BCA simulation of RBS-C spectra from the model sample (code BISIC)

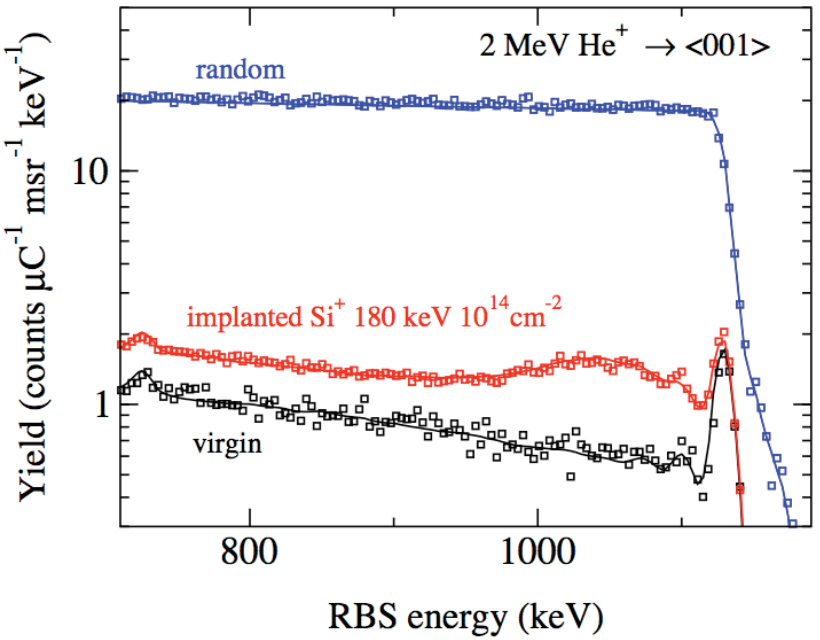

RBS-C measurement
spectrum
bad
good
agreement
Result: depth profile of defects
defects / depth distribution
spectrum simulation

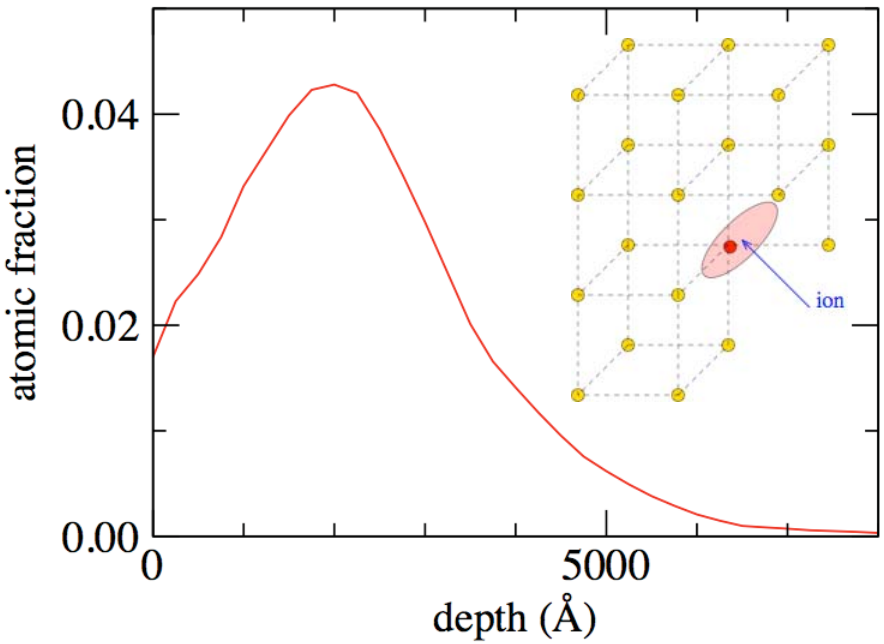
Point defects: what does the Bible say ?

In the spirit of Chapter 5 a complete treatment would consider the flux distribution of the channeled particles and the position of the isolated atoms in the channel. In real crystals the position of isolated host atoms, the self-interstitial, is not well known at the high defect concentrations ($\gtrsim 1\%$) typically required for channeling effect studies of defects. In practice a random distribution of atom positions within the channel is assumed. With this assumption a detailed knowledge of the flux distribution of the channeled particles is not required, and only the fraction of the particles that remain channeled is utilized. This follows because the dechanneling probability for a given channeled particle is independent of the trajectory when all atom positions in the channel have the same occupational probability. Consequently, one obtains a unique dechanneling factor for point defects in this *random position* approximation.

The preceding analysis was based on a single scattering approximation where the dechanneling is solely caused by single collisions to angles

Random position approximation

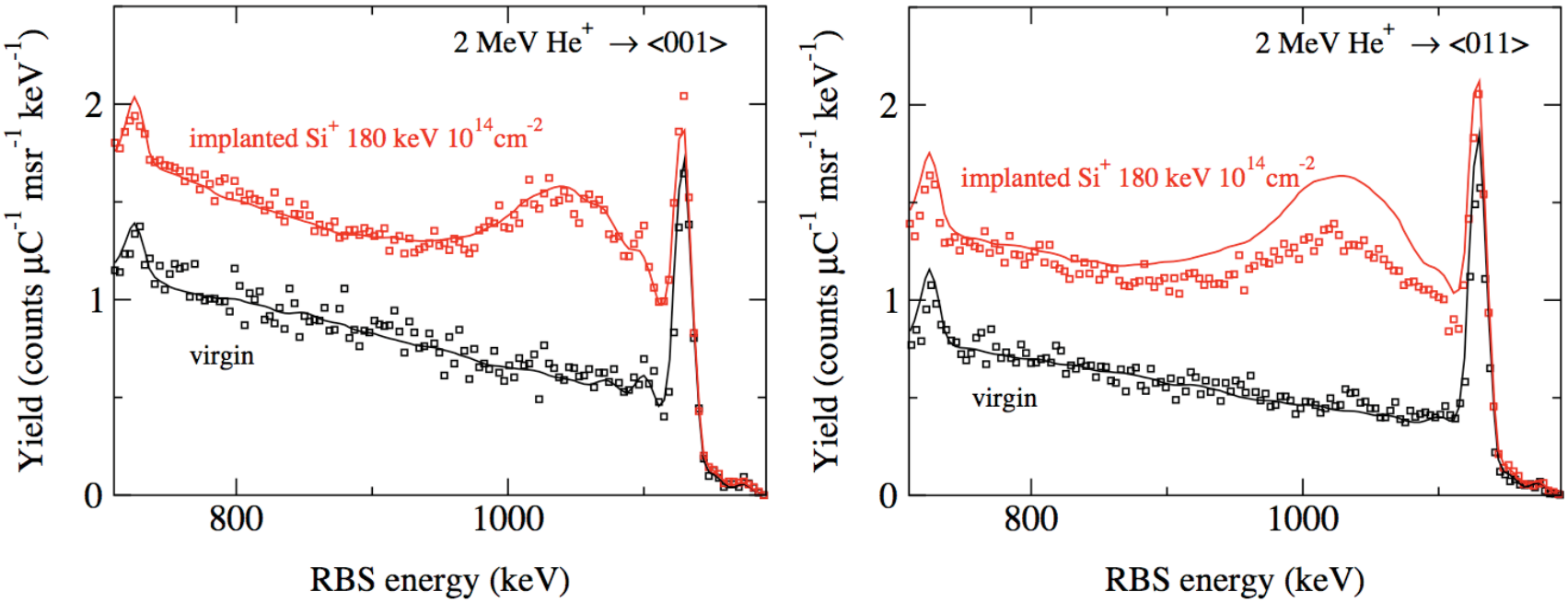




- treatment of defects as in the “two-beams” approximation[1]
- isotropic model

[1]E. Bøgh, Can. J. Phys. 46 (1968) 653

Random position approximation



random model is isotropic, experimental damage is not

Physical model of defects

accommodating extra-atoms or vacancies according to energy minimization criteria

interatomic forces for energy minimization:

1) first-principle or *ab-initio* (e.g. DFT)

2) semi-empirical (e.g. Tight-Binding)

3) empirical: Stillinger-Weber, Tersoff, EDIP ….

Example of empirical model: the EDIP potential

The energy of a configuration $\mathbf{R_i}$ is expressed as a sum over single atom energies, $E = \sum_i E_i$, each containing two– and three–body terms :

$$\boldsymbol{E}_i = \sum_j V_2(R_{ij}, Z_i) + \sum_{j,k} V_3(R_{ij}, R_{ik}, Z_i) \text{ where:}$$

$$V_2(r, Z) = A[(\tfrac{B}{r})^{\rho} - \exp(-\beta Z^2)] \exp(\tfrac{\sigma}{r-a})$$

$$Z_i = \sum_{m \neq i} f(R_{im})$$

$$f(r) = \begin{cases} 1 & \text{if } r < c \\ \exp(\frac{\alpha}{1-(\frac{r-c}{b-c})^{-3}}) & \text{if } c < r < b \\ 0 & \text{if } r > b \end{cases}$$

$$V_3(R_{ij}, R_{ik}, Z_i) = g(R_{ij}) g(R_{ik}) h(\cos\theta_{ijk}, Z_i)$$

$$g(r) = e^{\frac{\gamma}{r-b}}$$

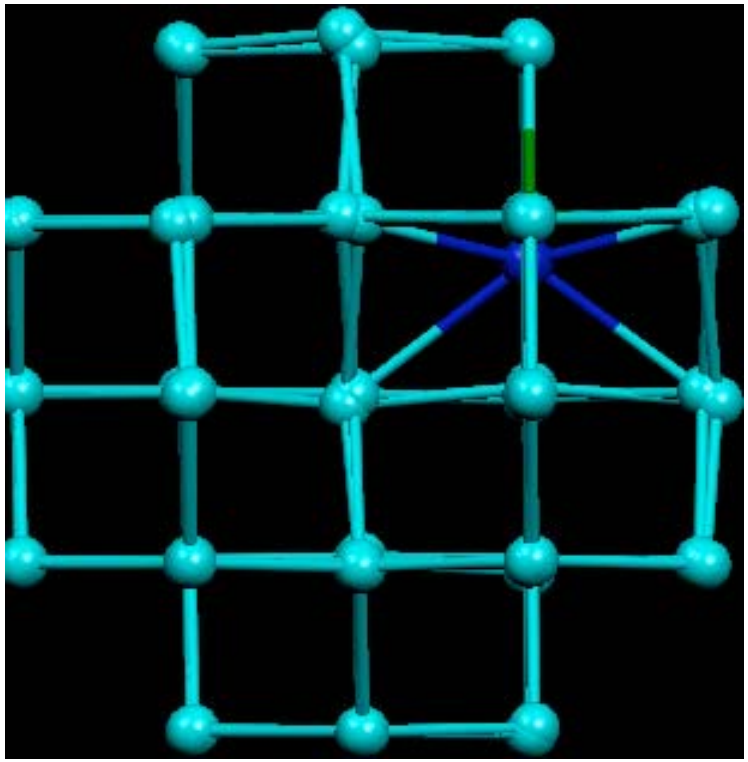
$$h(l, Z) = \lambda[(1 - e^{-Q(Z)(l+\tau(Z))^2}) + \eta Q(Z)(l + \tau(Z))^2]$$

$$\tau(Z) = u_1 + u_2(u_3 e^{-u_4 Z} - e^{-2u_4 Z})$$

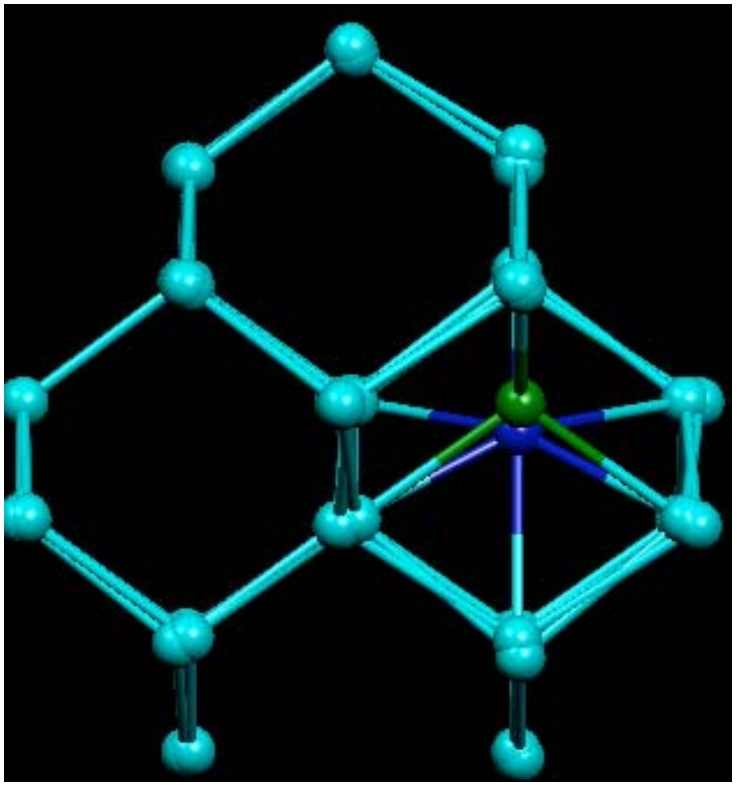
$$Q(Z) = Q_0 e^{-\mu Z}$$

Here i, j and k label the atoms of the system, $V_2(R_{ij}, Z_i)$ is an interaction between atoms i and j representing pairwise bonds, and $V_3(R_{ij}, R_{ik}, Z_i)$ is the interaction between atoms i, j and k centered at atom i representing angular forces. A(eV), B(Å), ρ, a(Å), c (Å), σ (Å), λ (eV), γ (Å), η, Q_0, μ, β, α are empirical parameters.

Tetrahedral and hexagonal interstitial

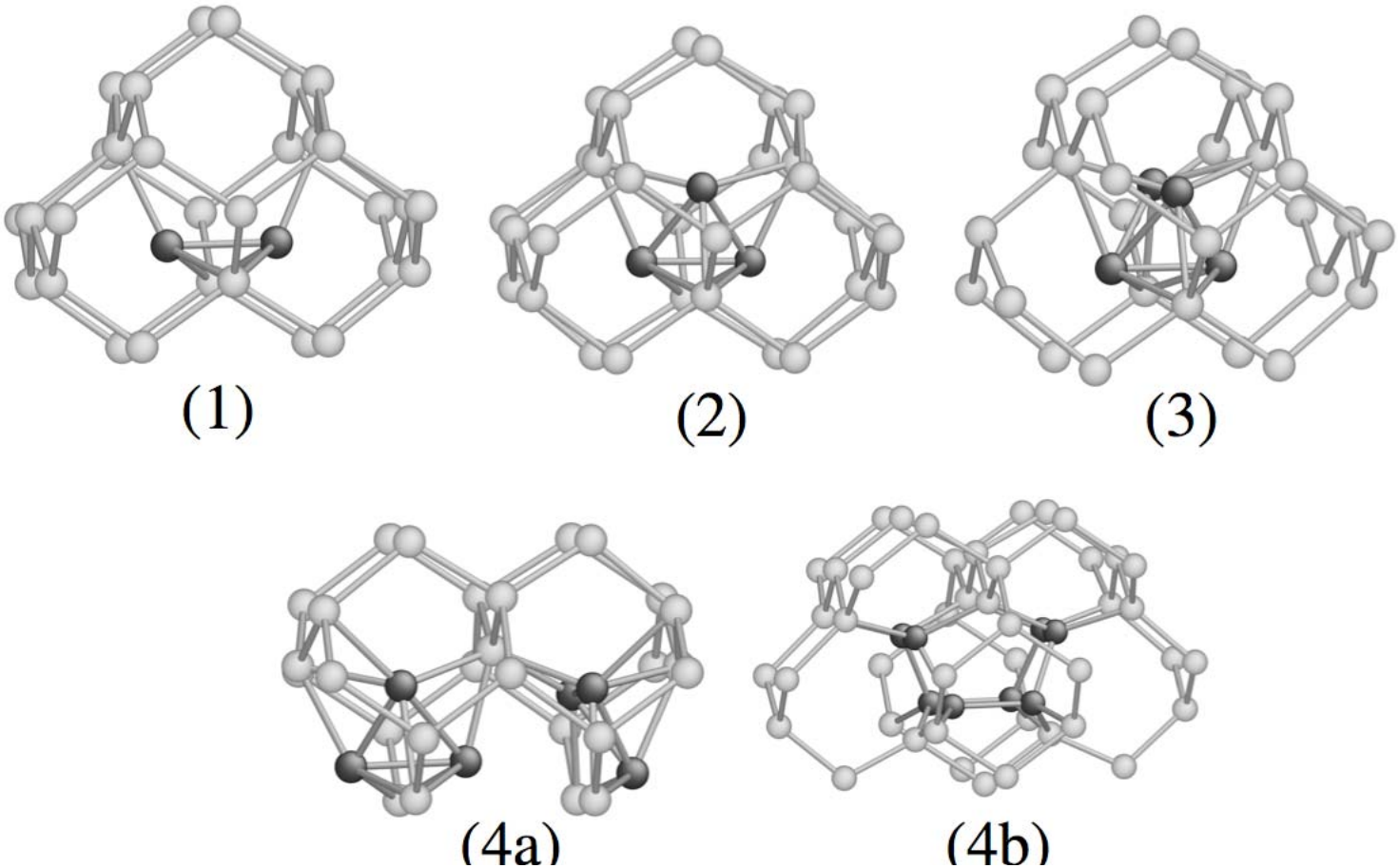


<100> view

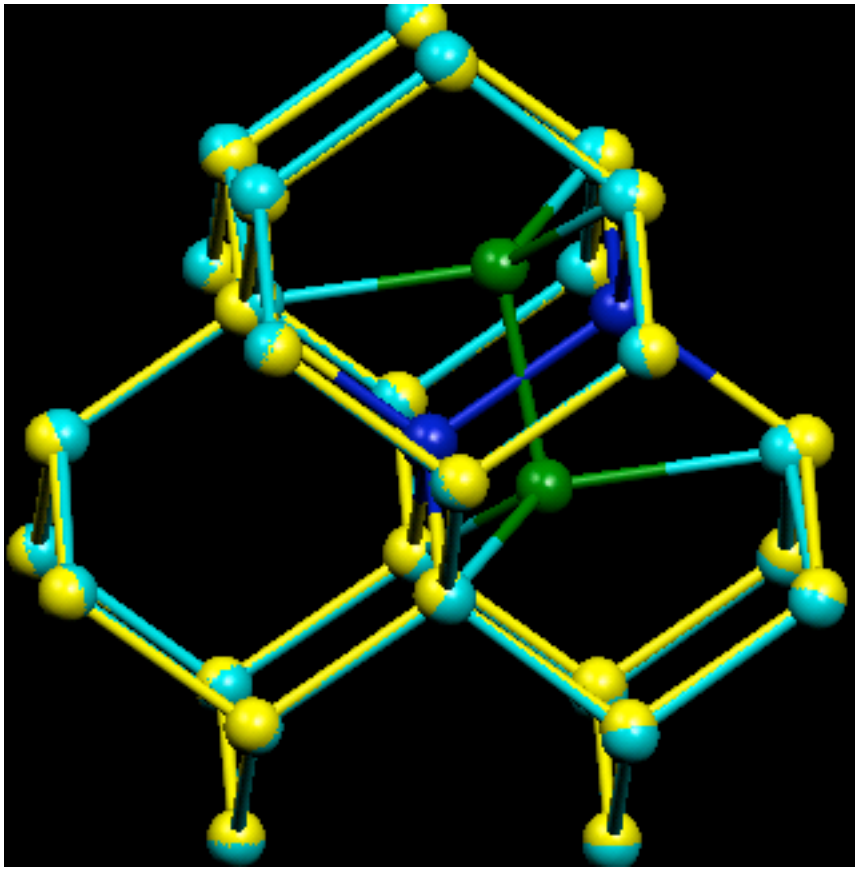


<110> view

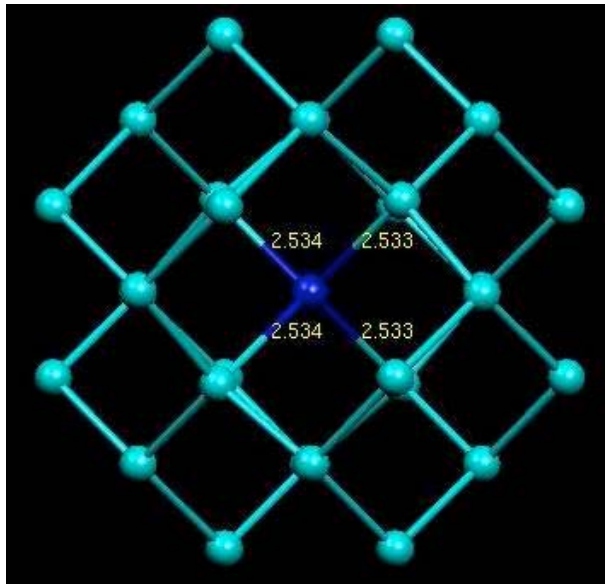
Split-like interstitial defects



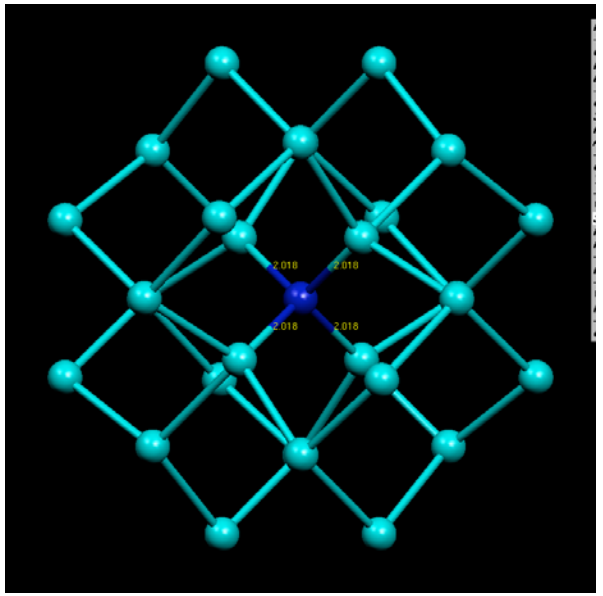
Bond-defect



Limitation of empirical potentials: the Si-vacancy



EDIP vacancy



DFT vacancy

amount and sign of the deformation differ
but both give an isotropic RBS-C response

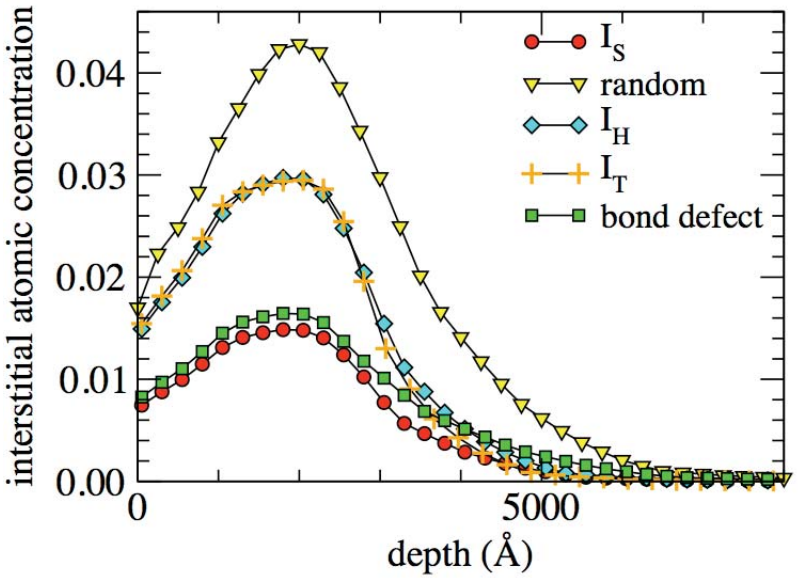
Strain

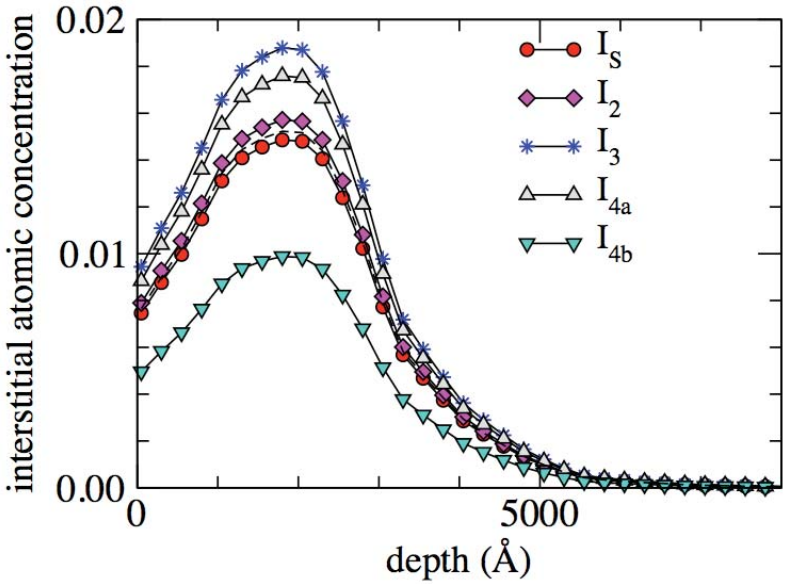
- Energy minimization (relaxation) induces strain in the lattice, which increases disorder, as detected by RBS-C

- Strain, which depends on the model (defect, interaction potential) has implication both on the quantification of defects and on their multi-axial response

I_s	1.45
I_2	0.95
I_3	1.03
I_{4b}	1.35

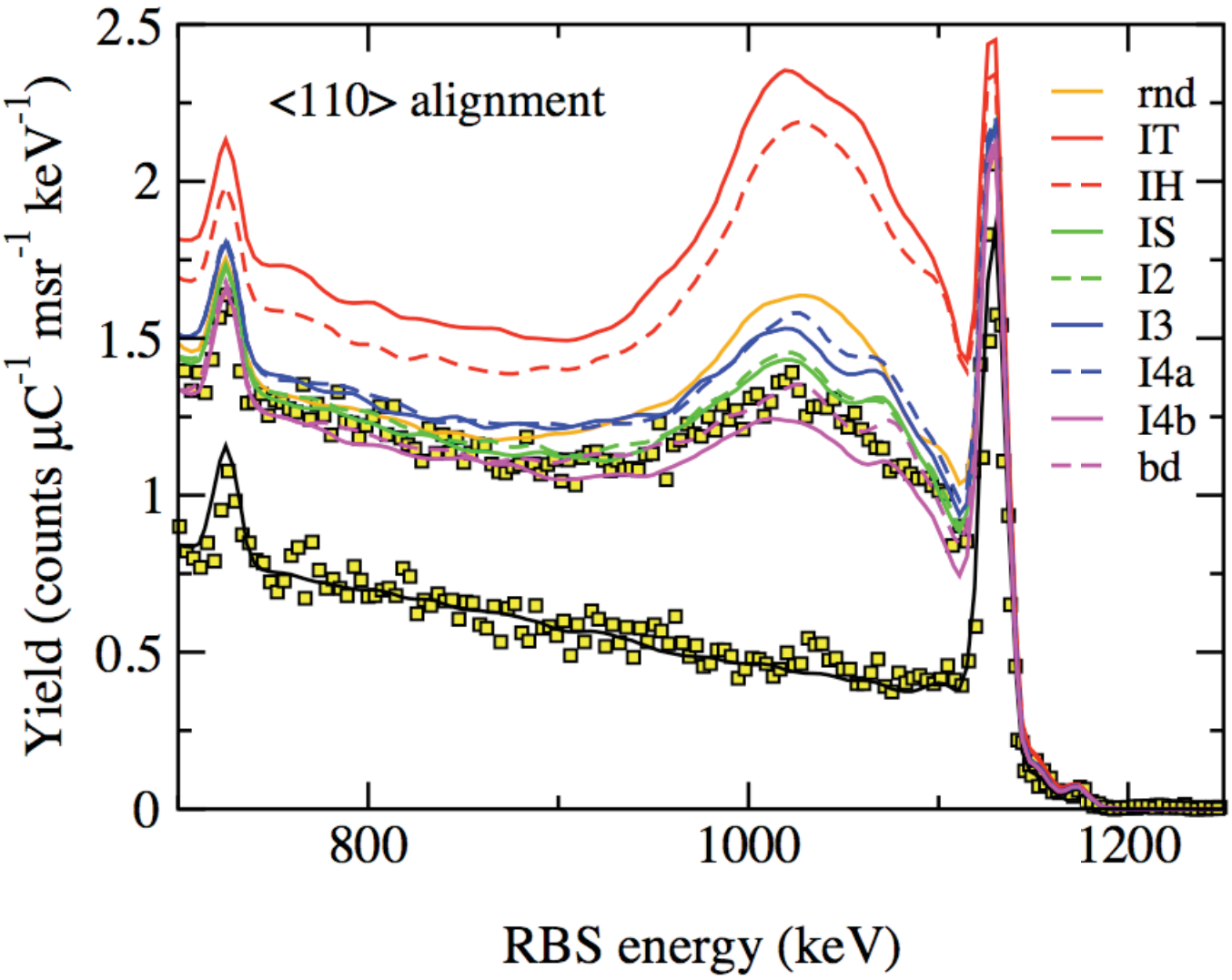
Volume expansion (in atomic volume units Ω) introduced per extra-atom by various split-like interstitial defects

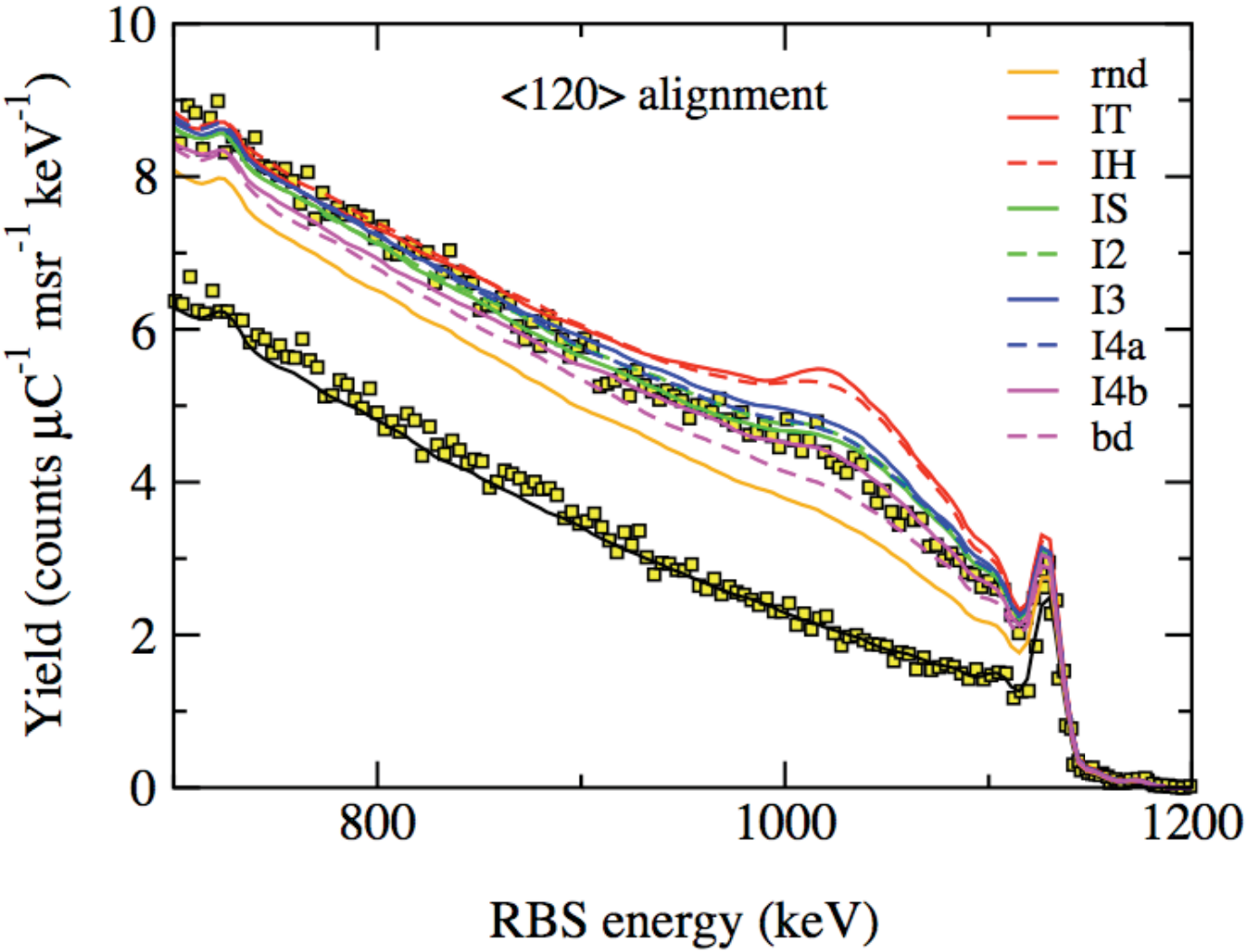




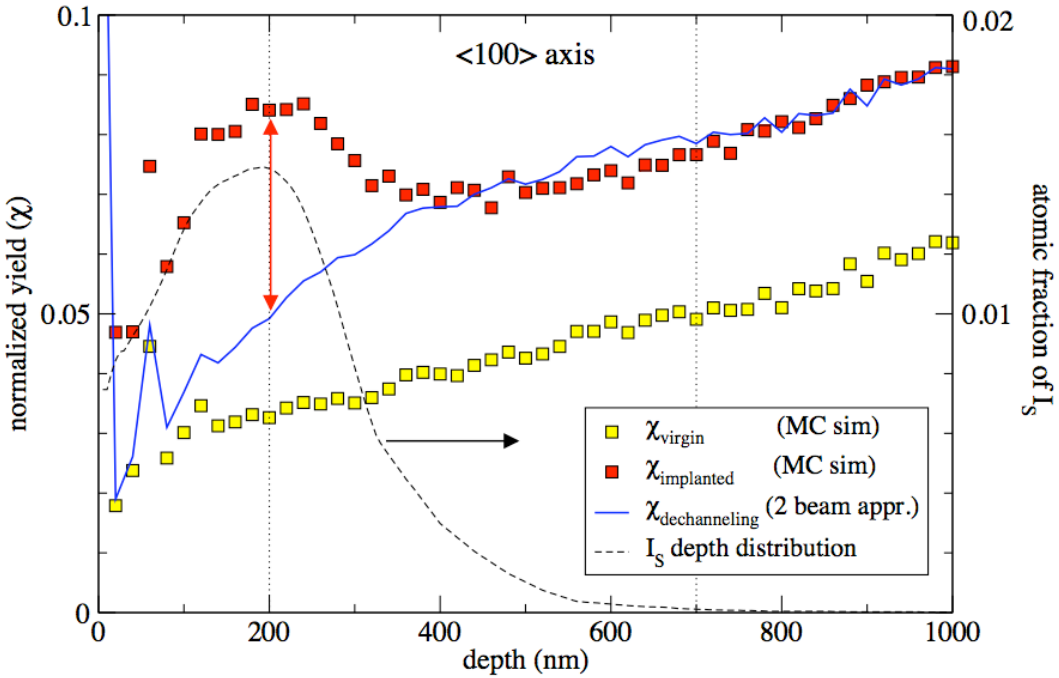
different defects ⇒ different profiles to fit <100> RBS-C

different scattering factor, different lattice strain


<110> alignment
rnd
IT
IH
IS
I2
I3
I4a
I4b
bd
Yield (counts μC-1 msr-1 keV-1)
RBS energy (keV)
0
0.5
1
1.5
2
2.5
800
1000
1200


<120> alignment
rnd
IT
IH
IS
I2
I3
I4a
I4b
bd
Yield (counts μC-1 msr-1 keV-1)
RBS energy (keV)
0
2
4
6
8
10
800
1000
1200

RBS-C signature (two-beams approximation)



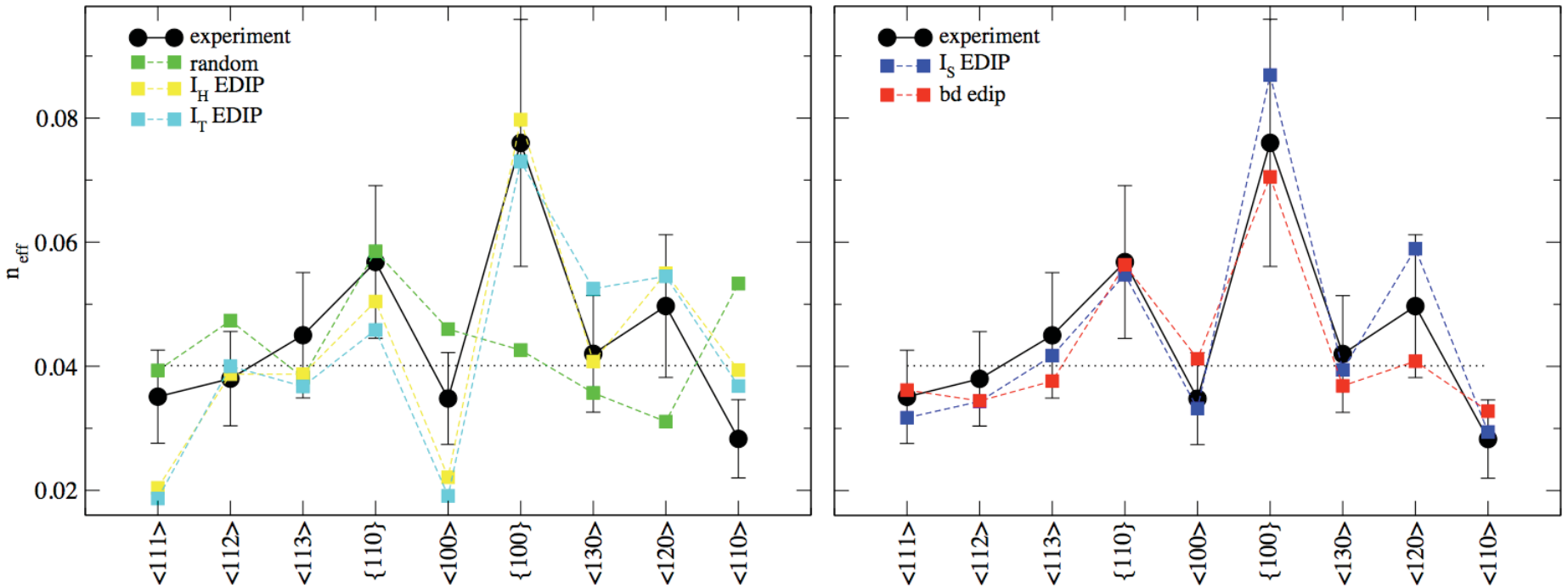
$$\chi_{implanted}(z) = \chi_{dechanneling}(z) + [1 - \chi_{dechanneling}(z)]\frac{n_d(z)}{N} f$$

$$\chi_{dechanneling}(z) \simeq \chi_{virgin}(z) + [1 - \chi_{virgin}(z)]\sigma I(z)$$

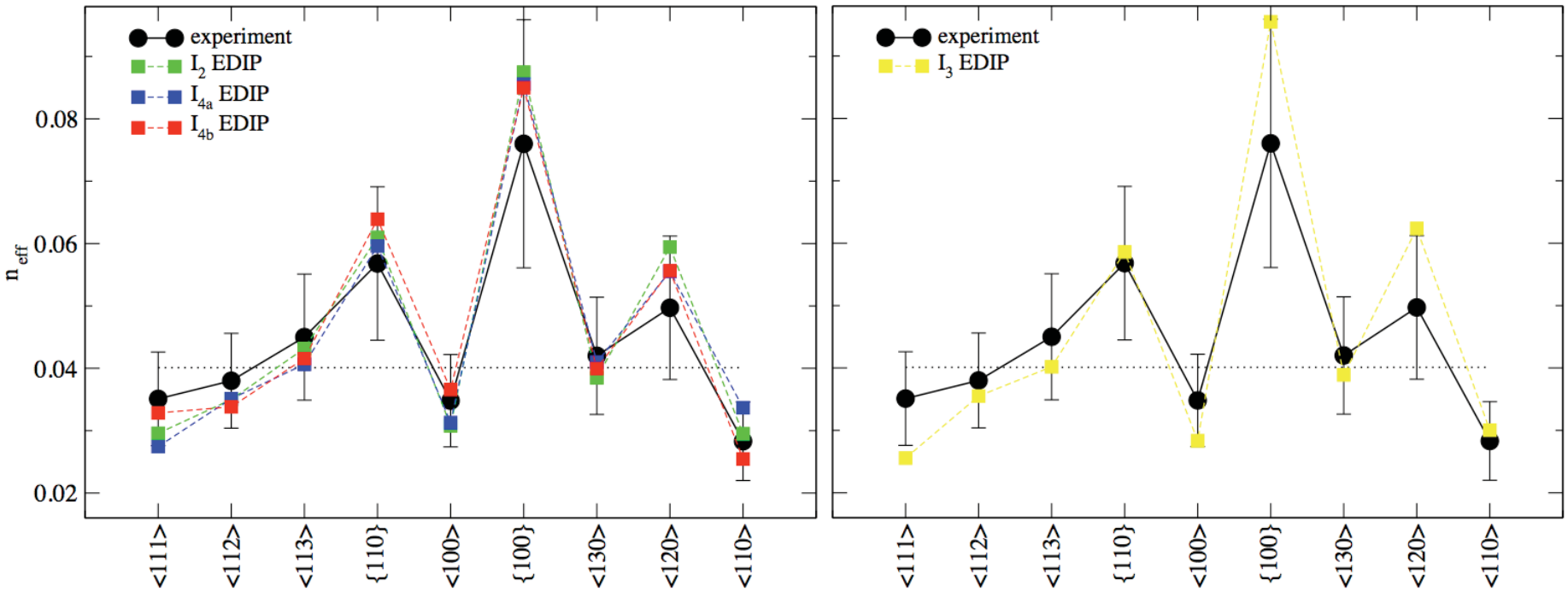
$$\sigma = \frac{\chi_{dechanneling}(z_0) - \chi_{virgin}(z_0)}{[1 - \chi_{virgin}(z_0)]\, I} \qquad (z_0 = 700nm)$$

$$n_{eff}(z) = \frac{n_d(z)}{N} f = \left[\frac{\chi_{implanted}(z) - \chi_{dechanneling}(z)}{1 - \chi_{dechanneling}(z)}\right] \qquad (z = 200nm)$$

Elementary interstitials

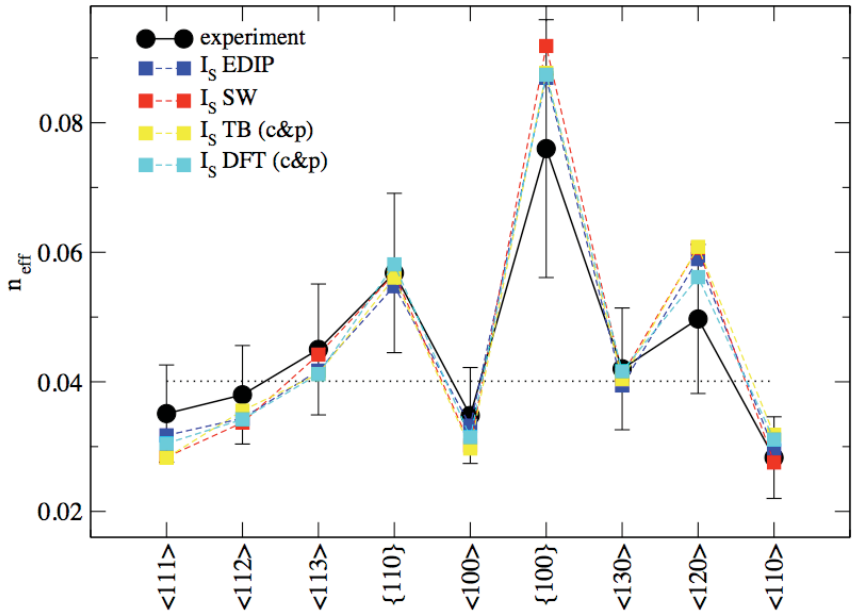


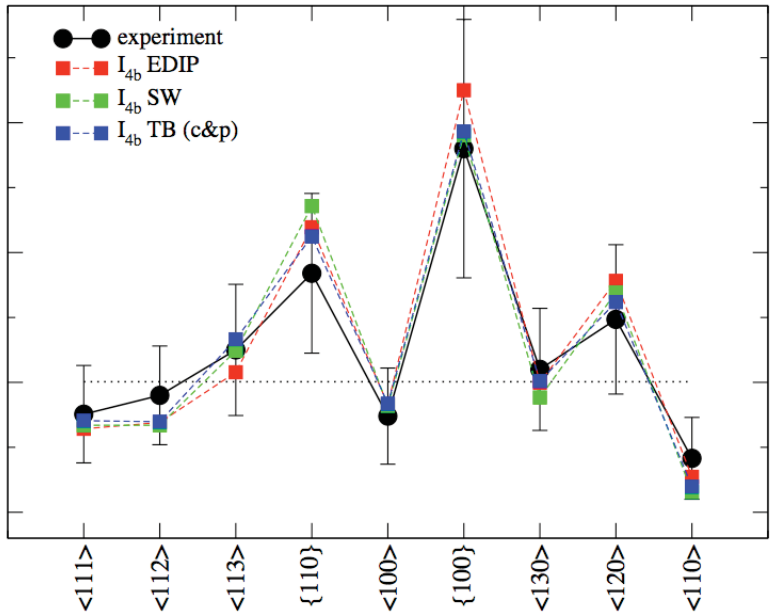
Clustered interstitials

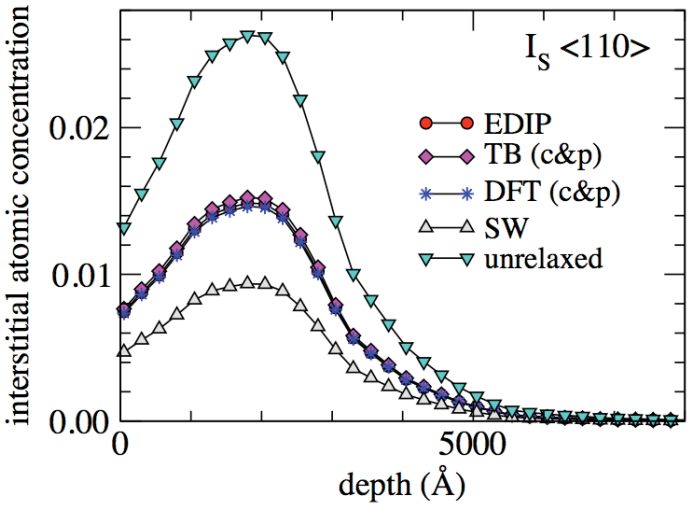


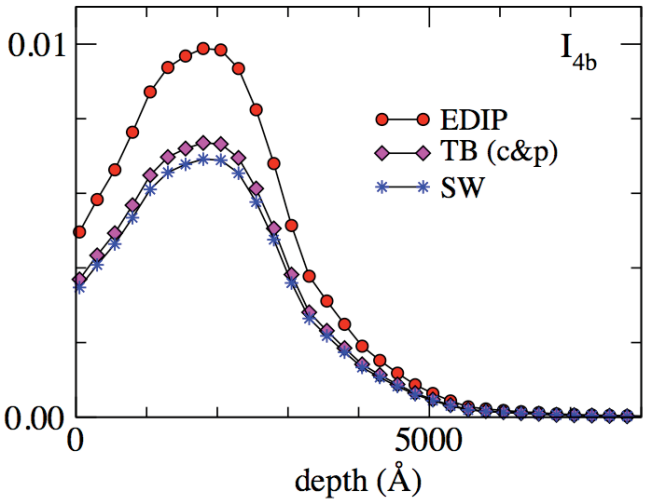
fine, … but

do results depend on the model of atomic interaction?


experiment
I_S EDIP
I_S SW
I_S TB (c&p)
I_S DFT (c&p)
n_{eff}
0.08
0.06
0.04
0.02
<111>
<112>
<113>
{110}
<100>
{100}
<130>
<120>
<110>

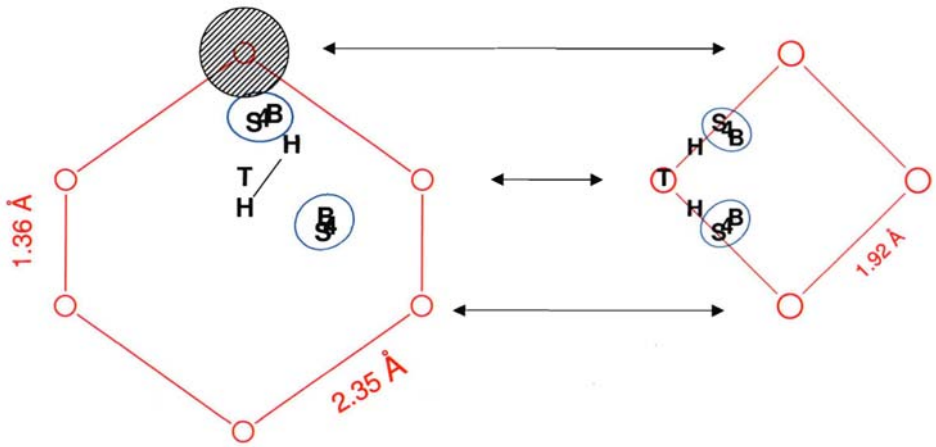

experiment
I_{4b} EDIP
I_{4b} SW
I_{4b} TB (c&p)
<111>
<112>
<113>
{110}
<100>
{100}
<130>
<120>
<110>


I_S <110>
EDIP
TB (c&p)
DFT (c&p)
SW
unrelaxed
interstitial atomic concentration
0.02
0.01
0.00
0
5000
depth (Å)


I_{4b}
EDIP
TB (c&p)
SW
0.01
0.00
0
5000
depth (Å)

Comparing fitting with different defects/models

model	*deviation*
I_{4K} *TB*	3.21e-3
I_{4K} *EDIP*	3.73e-3
I_s *EDIP*	3.78e-3
I_s *DFT*	4.01e-3
I_2 *EDIP*	4.52e-3
I_{4K} *SW*	4.35e-3
I_{4C} *EDIP*	4.98e-3
bd_EDIP	5.08e-3
I_s *SW*	5.15e-3
I_s *TB*	5.25e-3
I_2 *TB*	6.25e-3
I_s *unrel.*	6.33e-3
I_3 *EDIP*	6.62e-3
I_{4C} *TB*	6.85e-3
I_3 *TB*	7.34e-3
IH EDIP	9.63e-3
IT EDIP	1.10e-2
random	1.735e-2



<110> and <100> projections of the average interstitial positions in silicon. Tetrahedal (T), Hexagonal (H), Split-<110> (S), Bond defect (B) and Tetra-Interstitial (4). The shaded sphere has a radius R_L. The atoms have a radius ρ.

Final remarks

- atomistic simulation of RBS-C measurements based on physical models of defects has been investigated
- some of the interstitial defect models considered (the split family, plus bond defect) reproduce multi-axial measurements within the estimated uncertainty, whereas others (random, hexagonal and tetrahedral) do not

Final remarks

- qualitative conclusions do not depend on the model of atomic interaction
- quantitative of defects do depend both on the interatomic potential and on defect type
- the uncertainty on the amount of defects may vary more than ~ 2, due to the differences in scattering factors and lattice strain associated with different defects and different atomic interaction models

Papers on the subject

- S. Balboni, E. Albertazzi, M. Bianconi, and G. Lulli *Atomistic modeling of ion channeling in Si with point defects: the role of lattice relaxation* Phys. Rev. B **66** 045202 (2002).
- G. Lulli, E. Albertazzi, M. Bianconi and S. Balboni *Computer simulation of ion channeling in Si containing structurally relaxed point defects* Nucl. Instrum. Methods B **211** 50 (2003).
- M. Bianconi E. Albertazzi, S. Balboni and G. Lulli *Analysis of ion implanted silicon by RBS--channeling: influence of the damage model* Nucl. Instrum. Methods B **219/220** 232 (2004).
- G. Lulli, E. Albertazzi, M. Bianconi, A. Satta, S. Balboni and L. Colombo *Interpretation of ion channeling spectra in ion implanted Si with models of structurally relaxed point defects and clusters* Phys. Rev. B **69** 165216 (2004).
- M. Bianconi, E. Albertazzi, S. Balboni, L. Colombo, G. Lulli and A. Satta *Channeling characterization of defects in silicon: an atomistic approach* Nucl. Instrum. Methods B **230**, 185 (2005).
- G. Lulli, E. Albertazzi, M. Bianconi, A. Satta, S. Balboni, L. Colombo, and A. Uguzzoni *Investigation of heavily damaged ion implanted Si by atomistic simulation of Rutherford Backscattering channeling spectra* Nucl. Instrum. Methods B **230** 613 (2005).