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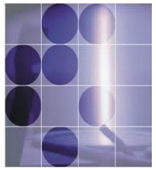


Electron Induced Damage in Silicon

-TRIM and TCAS Simulations-

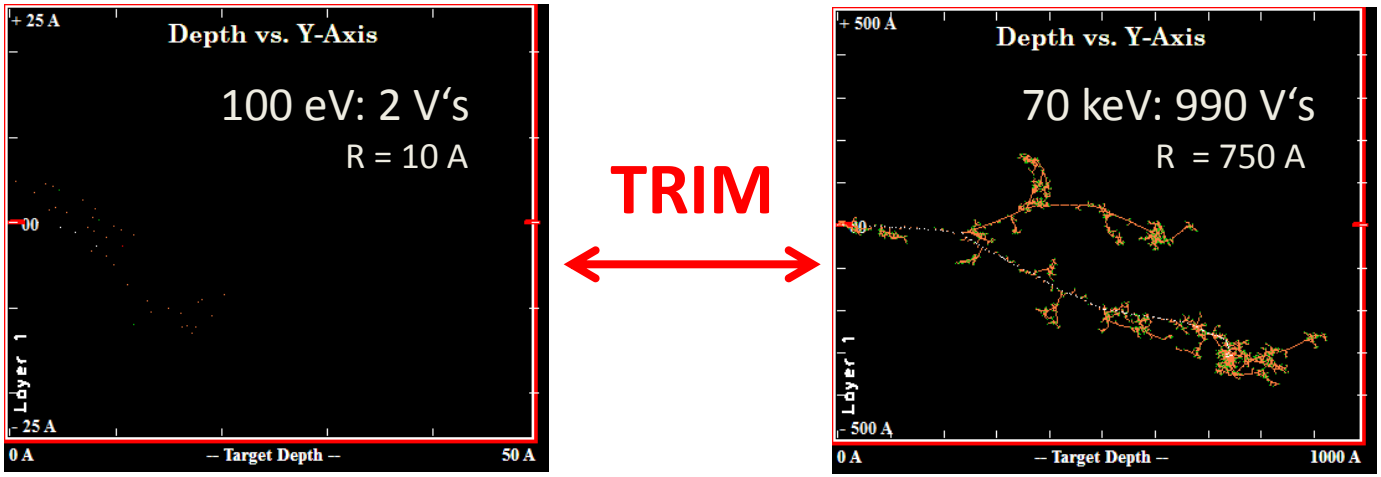
Gunnar Lindström, University of Hamburg
Gregor Kramberger, Jozef Stefan Institute, Ljubljana

Outline:

- **Motivation**
- **Mott-formula and approximations**
- **Recoil-Energy Distributions**
- **Partition Ratio and Damage Function**
- **TRIM and TCAS results**
- **Simulations, Random Walk**
- **Conclusions and Outlook**

Motivation:

- Damage caused by heavy particles (n, p, π)
  result from a mixture of (a) point and (b) „cluster“ defects
- Electron Irradiation in e.g. an energy range 1-30 MeV
  could offer an opportunity to correlate exp. results to (a) and (b)
- Maximum Si-recoil energy for **1 MeV** is only **100 eV**,
  for **30 MeV** it is **70 keV**, very similar to MeV neutrons!



Mott scattering

Scattering of relativistic electrons on Coulomb potential of point like charges (later on expanded by including screening):

Dirac theory: **Mott, Proc. Royal Soc. A124 (1929) and A135 (1932)**

$(d\sigma/d\Omega)_{Mott} = (d\sigma/d\Omega)_{Ruth} \cdot R_{Mott}$; $(d\sigma/d\Omega)_{Ruth}$ relativistic Rutherford-scattering

$R_{Mott} = A(E.\Theta) \cdot |F|^2 + B(Z,E,\Theta) \cdot |G|^2$

F, G complex functions, expansion with $D_k(\alpha Z,\beta)$ and Legendre Polynoms $P_k(\cos\Theta)$

Expansion only conditionally convergent, **exact numerical solution difficult!**

Numerical approximation by **T. Lijian et al: Rad. Phys. Chem. 45, 235 (1995):**

$R_{Lijian}(Z,E_k,\Theta) = \sum_{j=0}^{4} a_j(E_k) \cdot (1-\cos\theta)^{j/2}$ und $a_j(E_k) = \sum_{k=1}^{6} d(j,k) \cdot (\beta - \beta^*)^{k-1}$

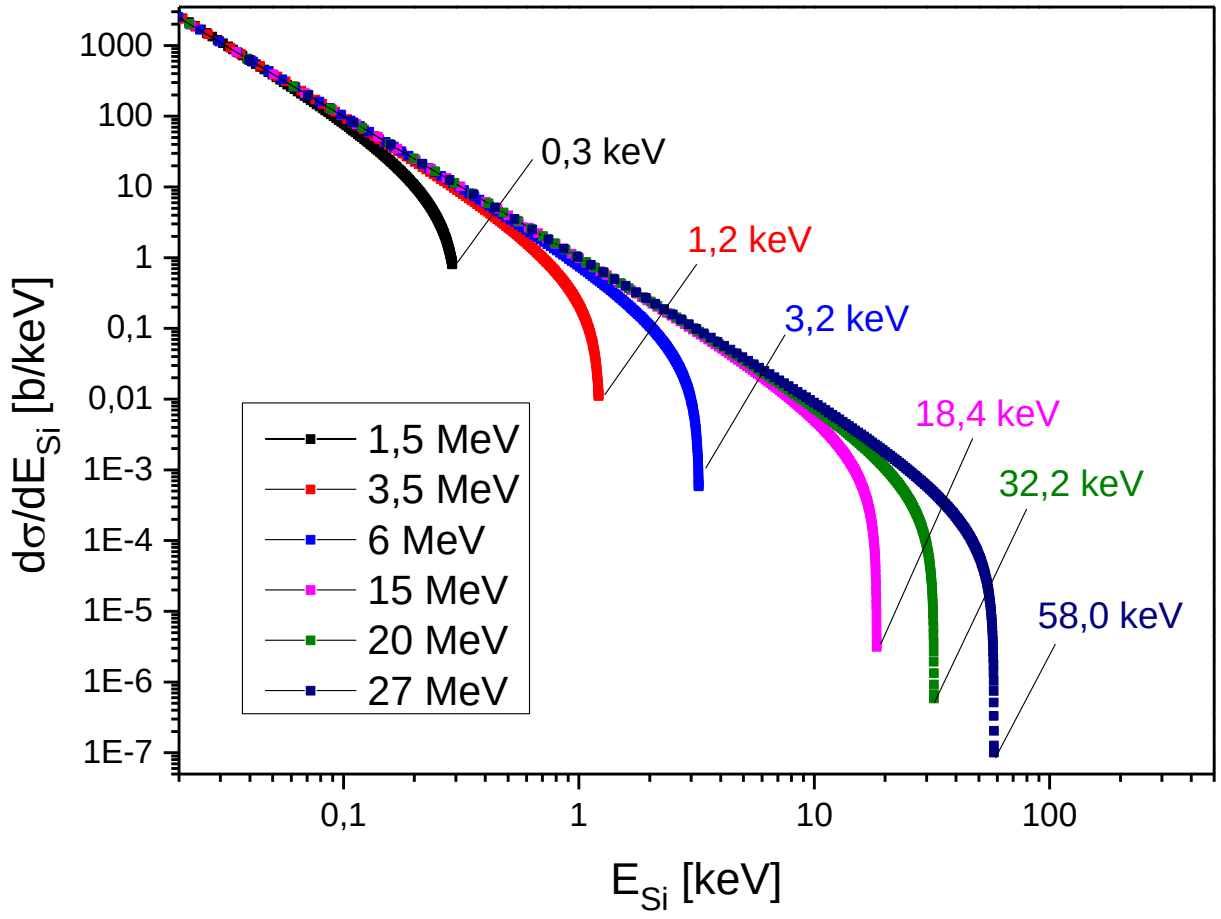
Deviations from exact Mott: < 1% for 30 keV-900 MeV; Z = 1-89

Be aware of simple formula, often found in textbooks: $d\sigma/d\Omega = (d\sigma/d\Omega)_R \cdot (1-\beta^2\sin^2\Theta/2)$

Recent good approach also by: **M.J. Broschini et al, Rad. Phys. Chem. , preprint April 2013**

Recoil Energy Distributions

Mott scattering, Lijians approach



Partition Function Q

describes that part of the energy loss which is responsible for NIEL
J. Lindhard et al., Mat. Fys. Medd. Dan. Vid. Selsk., vol 33, pp. 1-42, 1963.

Practical applications: use analytical approximation
M.T. Robinson, J. Nucl. Materials, vol.216, pp 1-28, 1994
J. Akkermann and J. Barak, IEEE Trans. Nucl. Sci. 53, 6 (2006)
I. Jun et al.; IEEE Trans Nucl. Sci 56, 6 (2009)

For Si ions in Si:

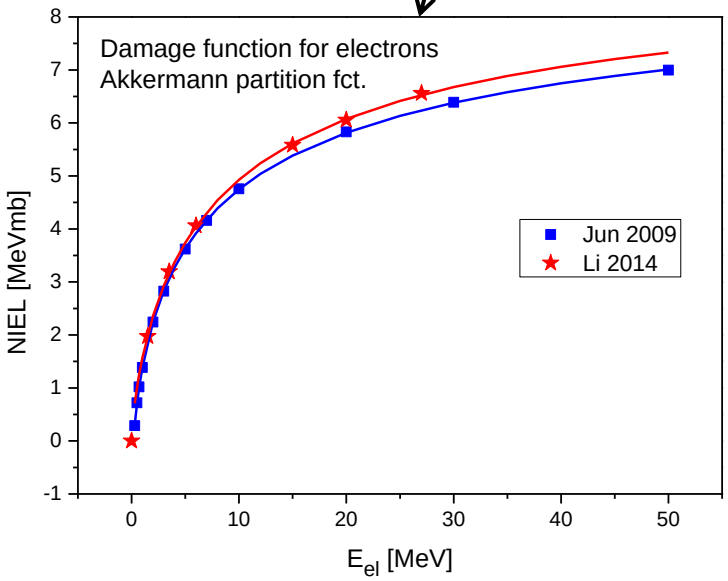
$Z_1 = Z_2 = 14$; $M_1 = M_2 = 28$

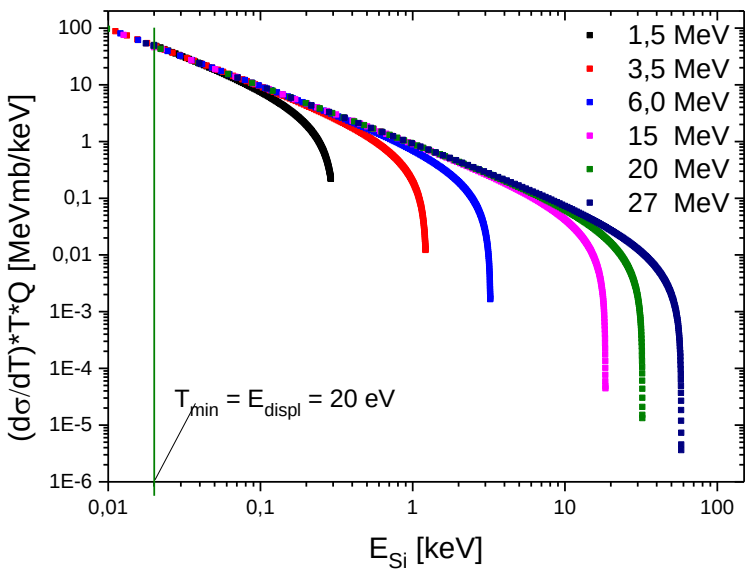
Q(T) = $[1+k \cdot g(\varepsilon)]^{-1}$; k=0,1463; $\varepsilon = T/E_L$, T = recoil energy, E_L = 41,05 keV

$g(\varepsilon) = 0{,}74422\varepsilon + 1.6812\varepsilon^{3/4} + 0{,}90565\varepsilon^{1/6}$ (Jun from Akkermann)

Damage function-1

$$\text{NIEL} = \int_{Tmin}^{Tmax} \left(\frac{d\sigma}{dT}\right) Q(T) T dT$$





5% difference between present results and Jun,
Jun: with atomic screening in relativ. Rutherford scattering

Monte Carlo Codes for Damage Cascades

TRIM:

James F. Ziegler, IBM
Last update: 2013

- **amorphous material**
- Full damage cascades
- Broad choice of inputs
- graphic design

- Direct 2D graphic output
- No of vacancies
- Output tables: V(ok), **I: ??**

TCAS*

Matthias Posselt, HZDR
Last update: April 2014

- **Single crystal Si <100>**
- Full damage cascades
- Broad choice of inputs
- LINUX by command

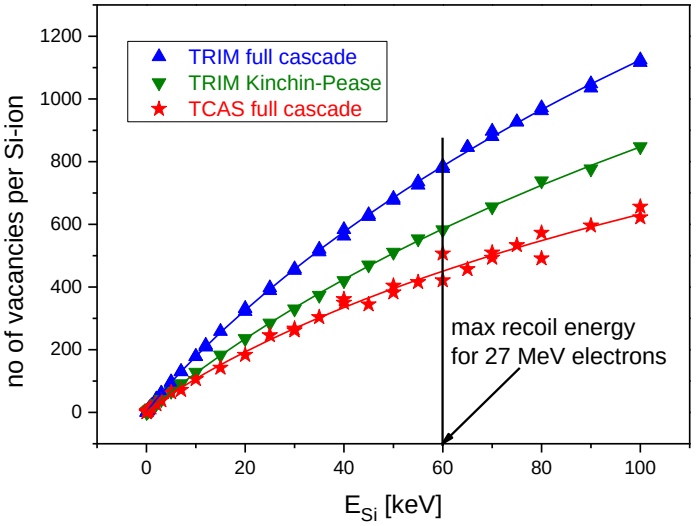
- graphic output included
- **V and I tables**
- **+ Intracasc. recombin.**

!! BCA-code (binary collision approximation), Zero K only !!

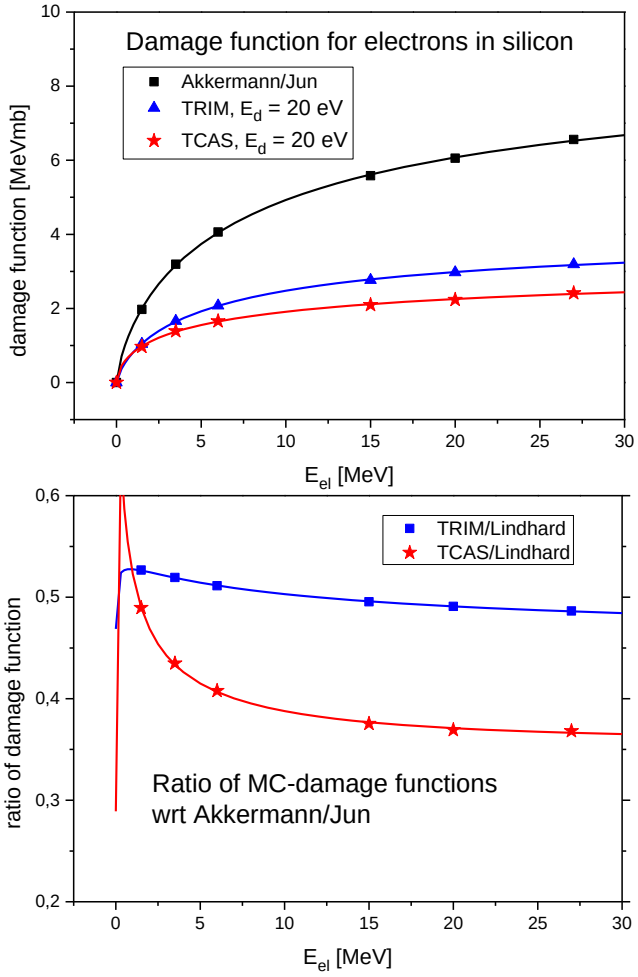
*** Many thanks to Matthias Posselt for continuous help**

TRIM and TCAS results – Damage function-2

No of V‘s (TRIM) resp. V/I‘s (TCAS) per ion

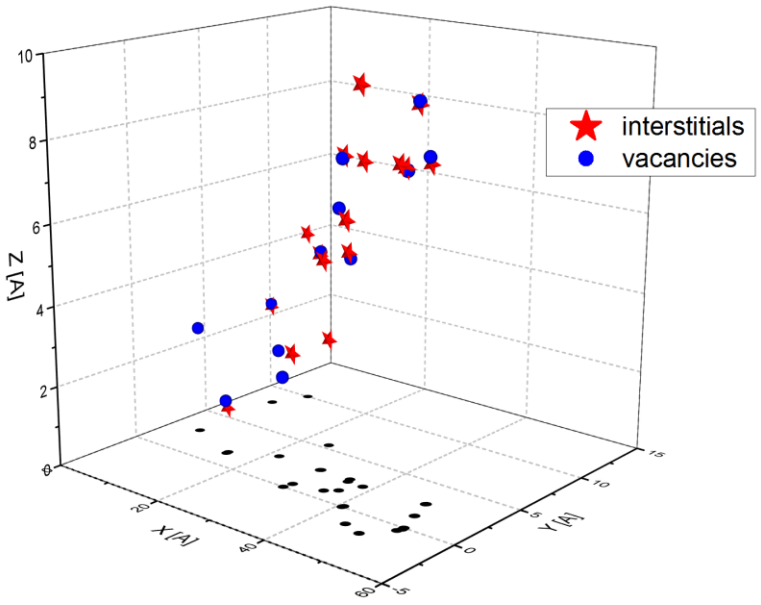


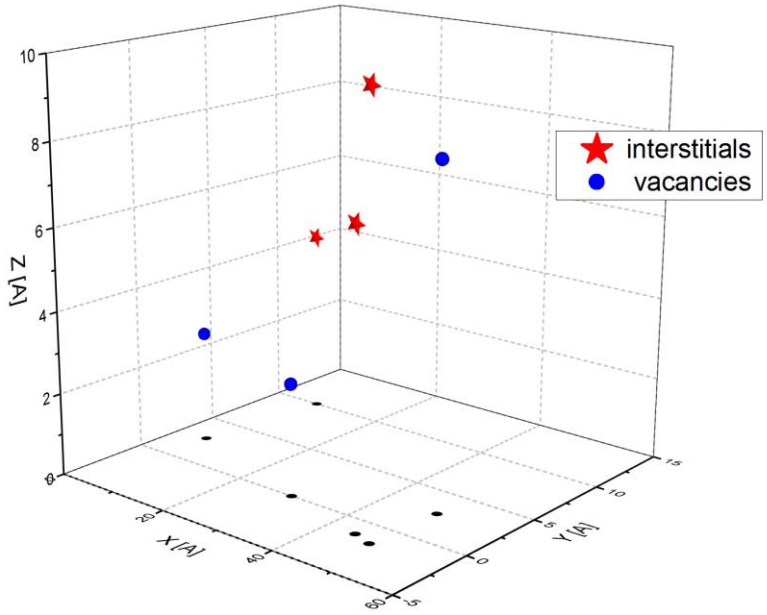
TRIM: E_d= 20 eV, average per 100 ions
TCAS: E_d= 20 eV, average per 10 ions
TRIM/TCAS = 1,8
Kinchin-Pease: approximation
TCAS believed to be more reliable



TCAS simulations 3D distributions

Example 1: E_{Si} = 1 keV (max. recoil for E_{el} = 3,5 MeV)





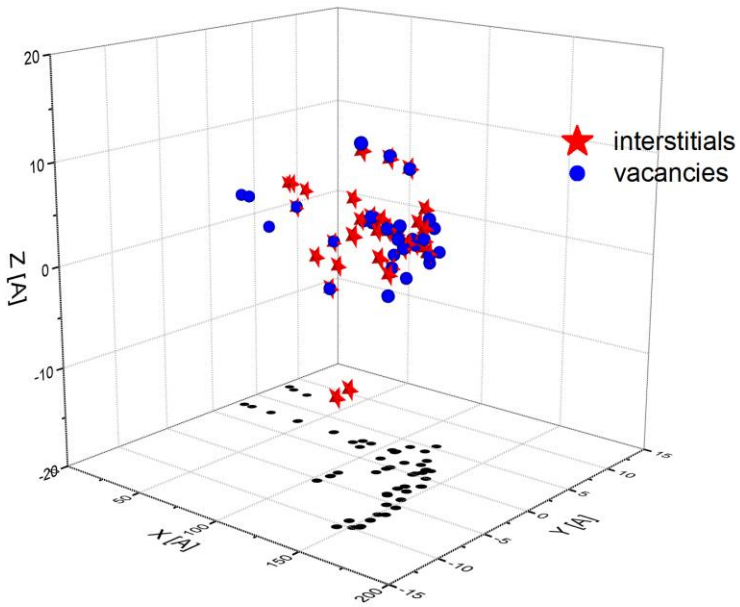
16 V/I produced in cascade
Scale: x, y, z: 60, 20, 10 Å

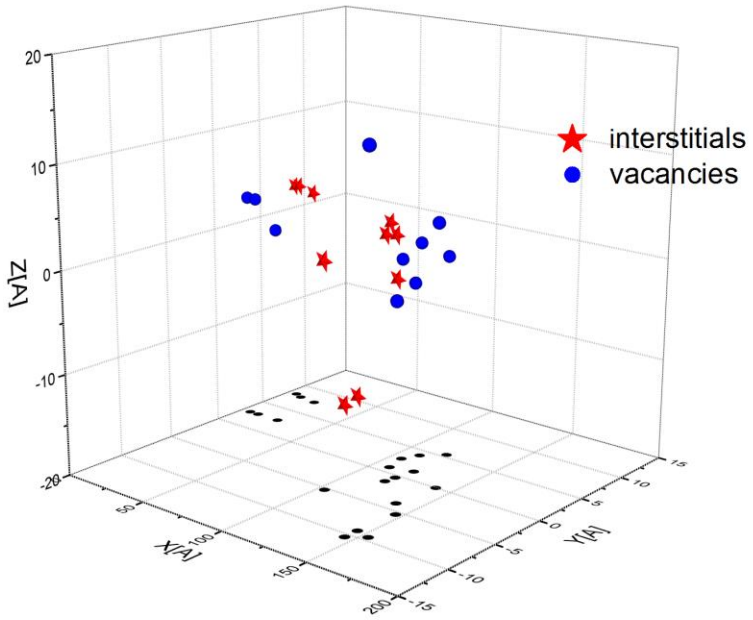
3 V/I after recombination (20%)

R_{rec}= 4 Angstrom (lattice constant: 5,43 A)

TCAS simulations 3D distributions

Example 2: E_{Si} = 3 keV (max. recoil for E_{el} = 6 MeV)



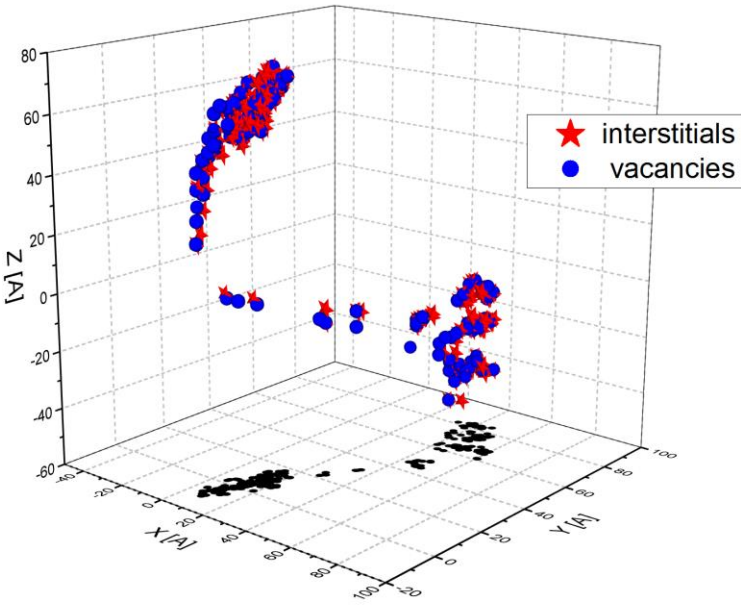


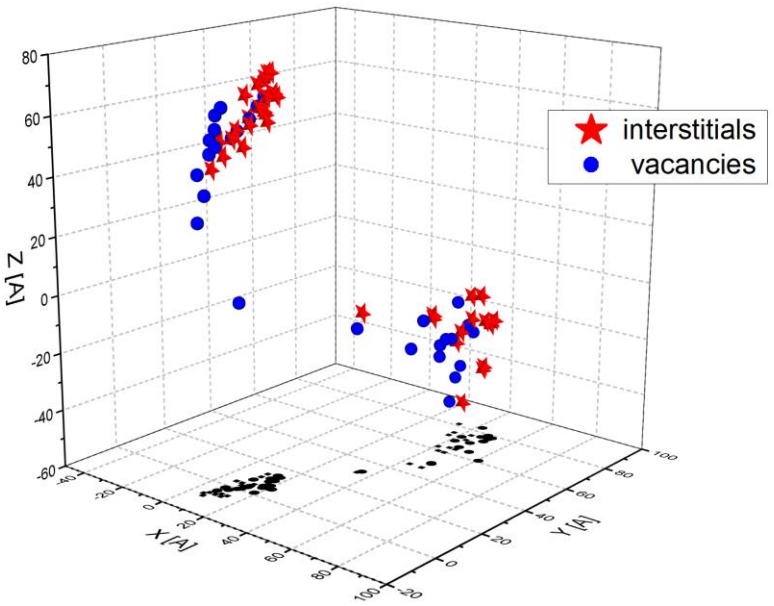
36 V/I produced in cascade
Scale: x, y, z: 200, 30, 40 Å

10 V/I after recombination (20%)

TCAS simulations 3D distributions

Example 3: E_{si} = 20 keV (max. recoil for E_{el} = 15 MeV)



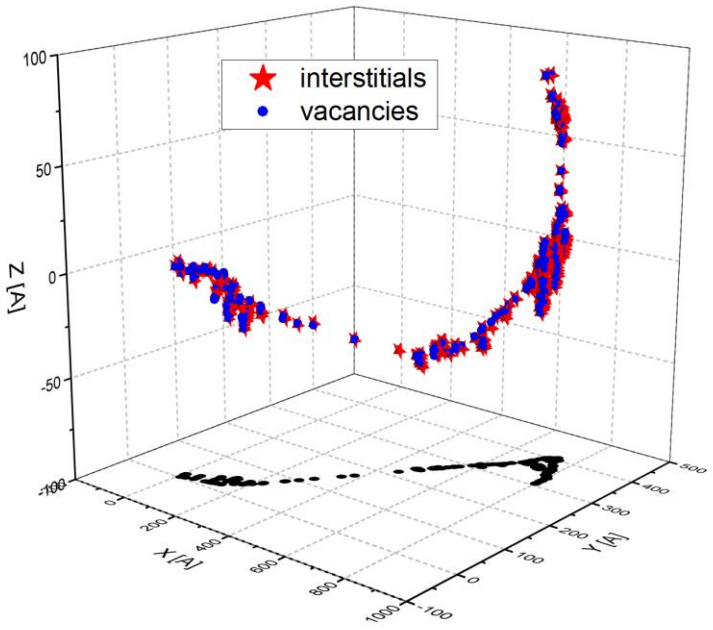


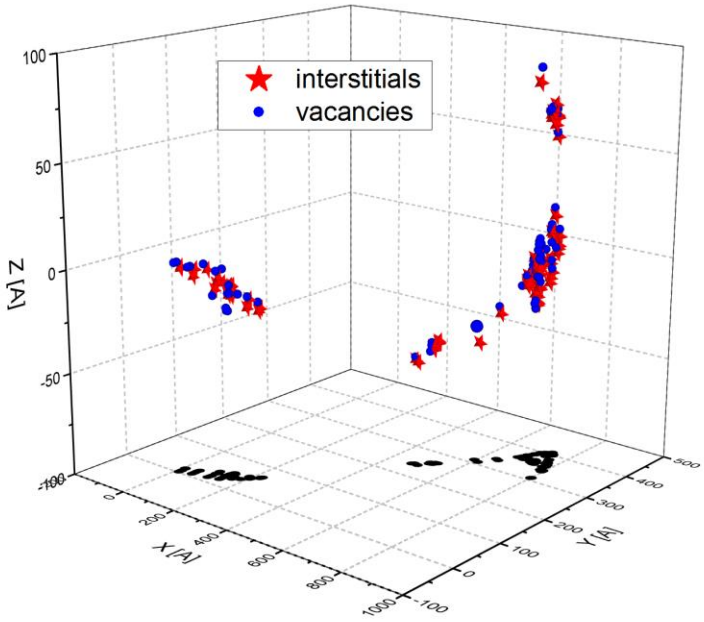
210 V/I produced in cascade
Scale: x, y, z: 150, 120, 140 Å

36 V/I after recombination (20%)

TCAS simulations 3D distributions

Example 3: E_{si} = 60 keV (max. recoil for E_{el} = 27 MeV)





474 V/I produced in cascade

86 V/I's after recombination (20%!)

X,y,z: 1200, 600, 200 Å

Attn: these are only examples for one ion each!
simulations done for 10 ions at each recoil energy

Random Walk of Defects

Contributed by Gregor

Procedure:

Input from TCAS (original cascade without intra-cascade recombination)

1. Correct for „doubles“, if so move V or I by one lattice distance
2. Do initial recombination of V-I, after that: V+V->V_2 and I+I->I_2
3. Start with the random walk:
   a. Find minimum distance *d* between any two I or V.
   b. Set “adaptive time step” according $t_{step}=\frac{d^2}{2 \cdot D_{V,I}}$
   c. Move all defects with steps in *x,y,z* distributed randomly according to Gaussian with width given by $\sigma = \sqrt{2 \cdot D \cdot t_{step}}$
   d. Loop over all defects and look for interactions. If two defects interact, create (or annihilate) a new defect with given properties and include it in the next step (parents -> child hierarchy)
   e. Repeat from step a-e as many times as required

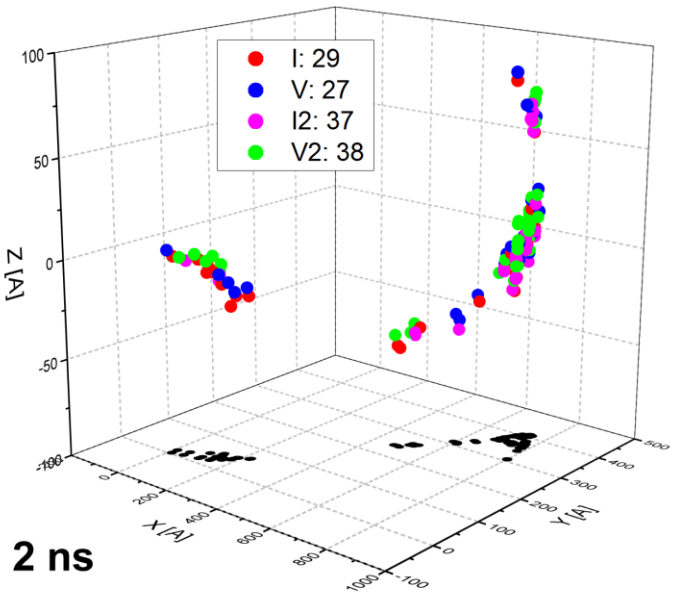
Assumptions

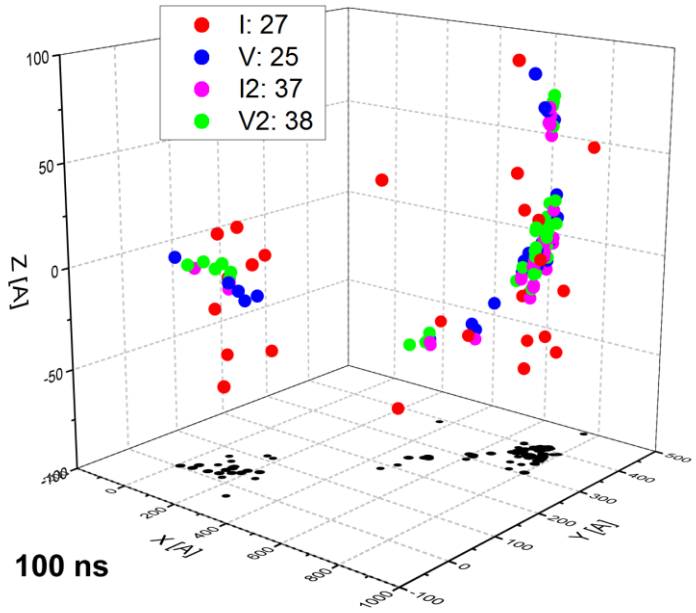
- Diffusion constants: S.M. Myers et al. JAP 104 (2008). dependece on charge states neglected
- D assumed independent on lattice orientation
- Reaction occurs if two defects are within given radius at given time step - (ON/OFF) decision, will be improved to calculate probability based on distance. This is one of the most important improvements needed.

Software

- TCAS for generation of V,I
- Random Walk is a c++ ROOT based library.
  - Inputs:
    - Table with interaction radii, R_{VI} = 4 A, R_{VV} = 7.7 A, R_{II} = 7.9 A
    - Table with possible reactions, so far only: V+I, V+V, I+I
    - Diffusion constants, only for I and V, V_2 and I_2 assumed immobile
  - Visualization based on ROOT

Example: Si-recoil energy of 60 keV

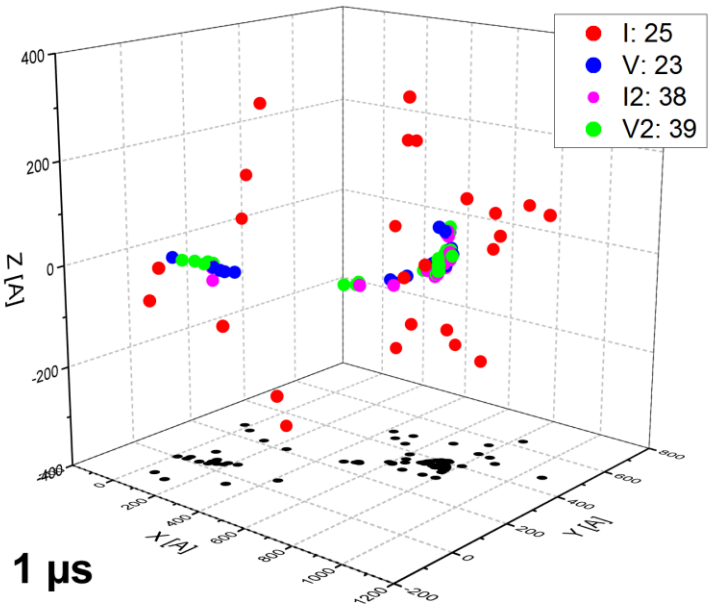


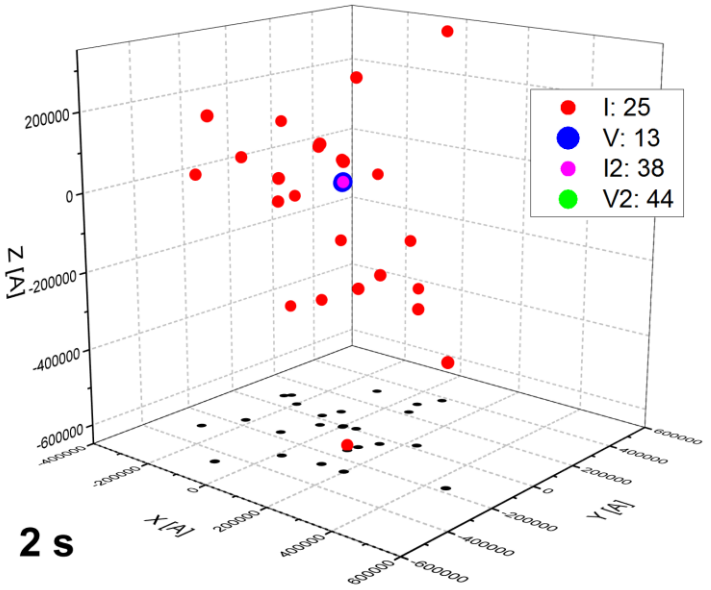


t=2 ns: not much migrations yet,
a lot of I2 and V2 formed
in or close to initial cascade
Scale: x, y, z: 1200, 600, 200 Å

t= 100 ns: I2 and V2 not much changed
I's migrate out of the initial
cascade
Scale: x, y, z: 1200, 600, 200 Å

Example: Si-recoil energy of 60 keV





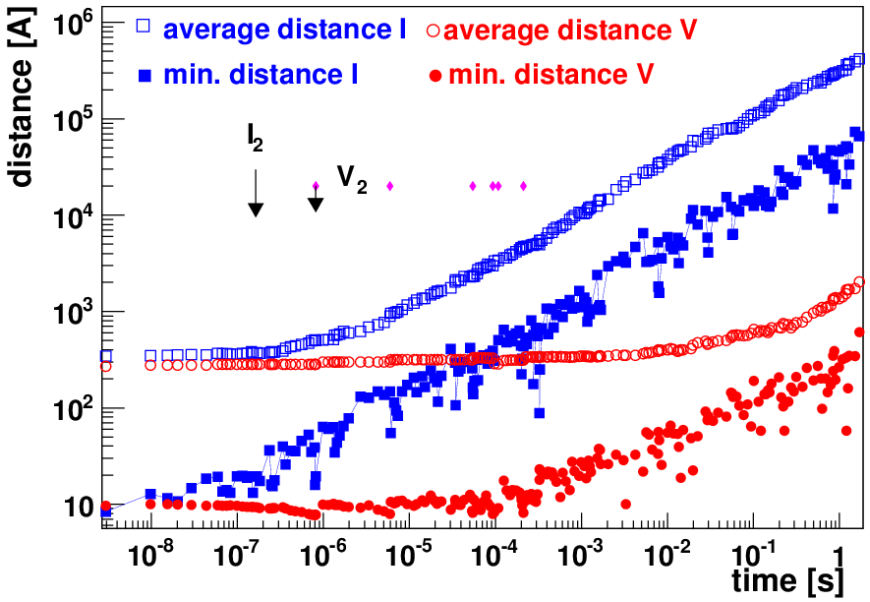
t = 1 µs, original cascade still in place (I2, V2 assumed to be immobile), ongoing fast migration of I‘s

Scale: x, y, z: 1400, 1000, 1000 Å

t = 2s, 25 of the initial 103 I‘s have moved throughout the detector volume! Finally: more V2 than I2 formed!

Scale: x, y, z: 100, 120, 100 µm!

Example: Si-recoil energy of 60 keV



At 1 s: average distance I: 32 µm! **At 1 s: average distance V: 0,14 µm!**

Interstitials migrate much faster than vacancies,
hence they evade disordered regions more likely,
More V_2 than I_2 formed as seen for t > 1µs

Conclusions and Outlook

- Mott scattering implemented from Lijians parameterization, be aware of simple textbook equations, especially for heavier atoms
- Partition function used from Akkermann and Jun, small deviations in displacement function due to atomic screening in Rutherford equation (Jun)
- Displacement function derived from TRIM and TCAS deviate from traditional approach, TCAS believed to be more reliable than TRIM
- TCAS offers simulation for single crystals (Si: <100>) and a direct output for both vacancies and interstitials plus recombination within initial cascade, leaving 20% surviving for migration
- Random walk studies reproduce TCAS recombinations and show development of I, V, V-V and I-I as fct. of time. Interstitials move faster and hence evade damage sites especially seen after longer times (µs)
- TRIM and TCAS are binary code collision approximations, describing damage production as sequence of 2 body interactions (cascades)
- More realistic (?): MD model, based on many body interactions, local heating, melting, amorphization, recrystallisation taken into account, see C. Inguimbert et al., IEEE NS 57, 4 (2010) and literature cited there
- Future approach: start with MD, followed by random walk as in this report

Kinchin-Pease approximation

Kinchin and R.S. Pease, The displacement of atoms in solids by radiation, Rep. Prog. Phys., vol. 18, p. 1, 1955

Describes number N_{FP} of produced Frenkel pairs for an energy E_{PKA} of a primary knock on atom by a simple analytic equation:

$$N_{FP} = 0.8 \cdot (E_{PKA} / 2T_{d,av}) \text{ for } E_{PKA} > 2T_{d,av} / 0.8$$

$T_{d,av}$ *: average displacement energy*

This simple equation should be taken with great care, see one of the figures (slide 8) in this report. It is incuded in SRIM/TRIM as one of the options, does not describe TRIM nor TCAS results.

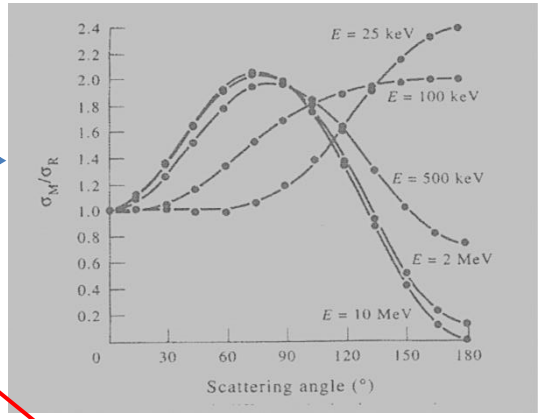
Molecular Dynamics Simulation

Based on many body interactions in contrast to BCA, binary code 2 body collisions, as in TRIM, TCAS.

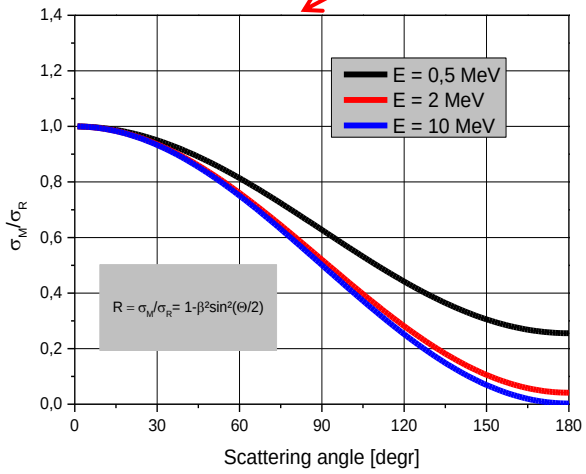
- *In contrast to Kinchin-Pease non-linear effects primarily at low E_{PKA}*
- *Displacements can be generated even for $E_{PKA} < E_d$!*
- *Initially huge no of FP produced, cooling down to RT within few ps*
- *After stable condition reached (< 10 ps) no of FP roughly as in BCA*
- *Isolated point defects are predominantly interstitials (see Gregor)*
- *Amorphous clusters may be produced in cascade core*

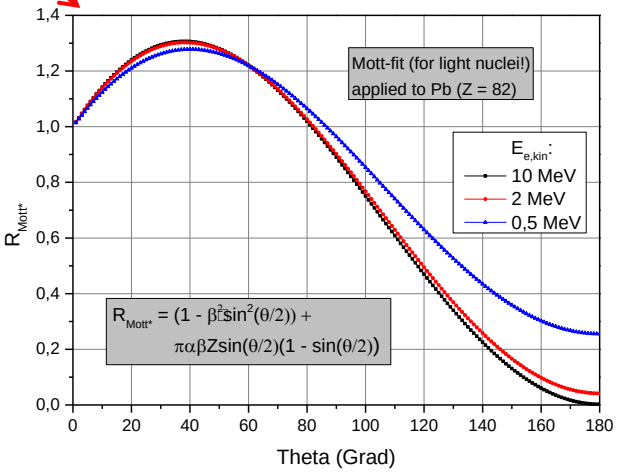
For further reading start with citations given in:
C. Inguimbert et al: „Effective NIEL“ in Silicon: Calculation Using MolecularDynamics Simulation Results, IEEE NS Vol 57, No 4, 2010

$\sigma_{Mott}/\sigma_{Ruthf}$ für Pb nach Lijian
Punkte: exakte Mott-Formel
Linien: Fit nach Lijian



Simple approaches don‘t work





Simple textbook equation
παZ«1; SI: **παZ=0,3 !**

Better approach for light nuclei