Simulation of defect formation in different hadron irradiation environments

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For details see ROSE/TN/2001-02, submitted to NIM

Motivation

Reasons for this simulation study

No really microscopic NIEL simulation exists

● ● ●

NIEL scaling seems to be often misinterpreted.

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Modern simulation codes allow to attempt a truly microscopic NIEL calculation.

Experimental data from the ROSE (CERN RD48) collaboration shows NIEL violation in some cases.

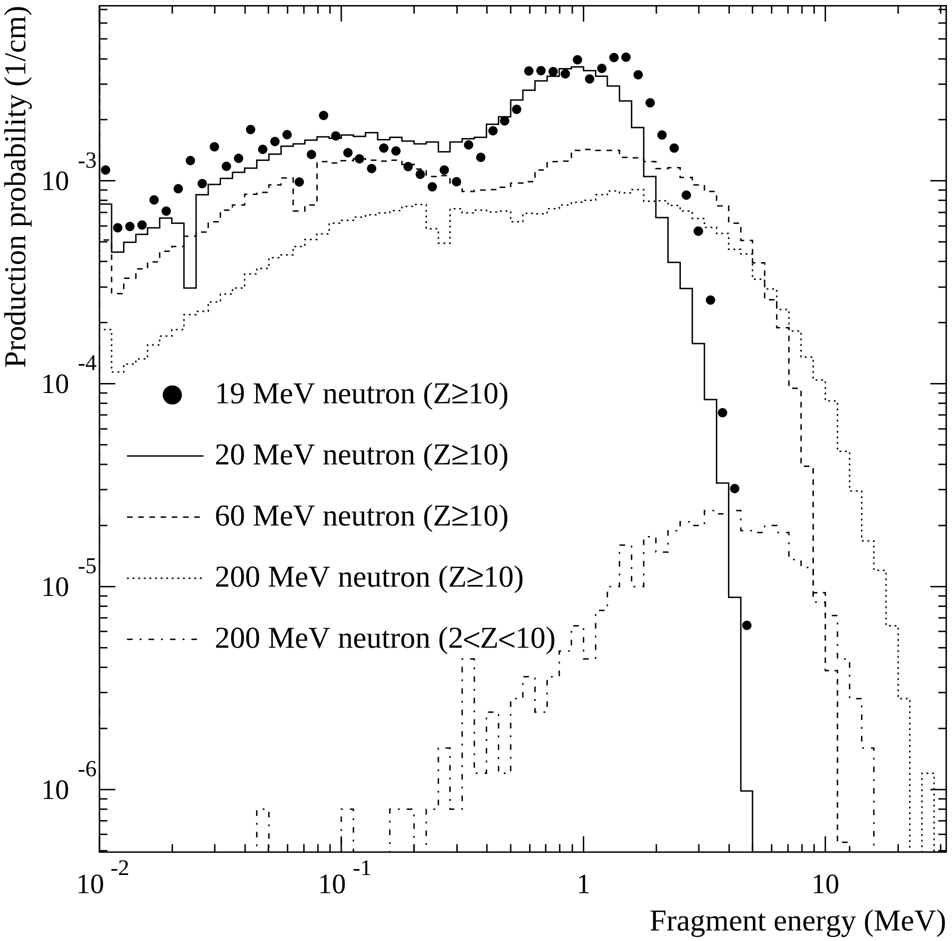
Especially,

Oxygen enriched silicon behaves differently under neutron and proton irradiation when compared to standard Si.

Understanding of possible NIEL violation and effects of oxygen can be significant for LHC and other forthcoming experiments.

High Energy hadronic Interactions

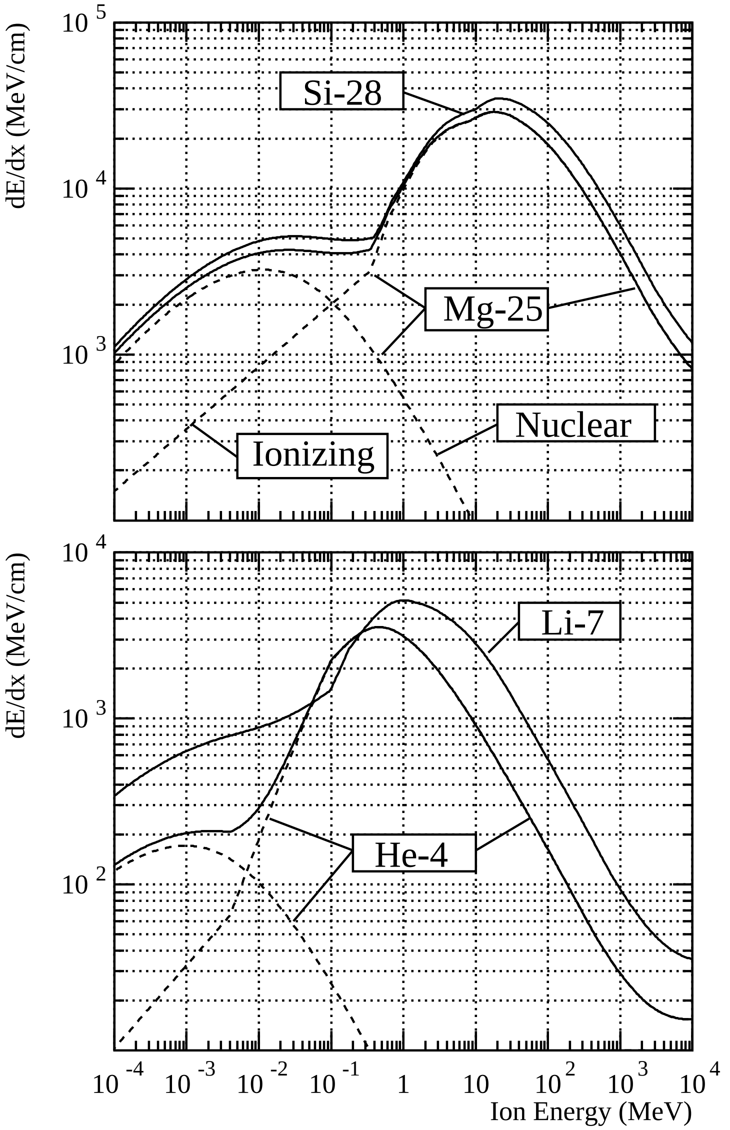
Recoil spectra of $>$20 MeV hadrons on Si



Typical recoil energies up to few tens of MeV

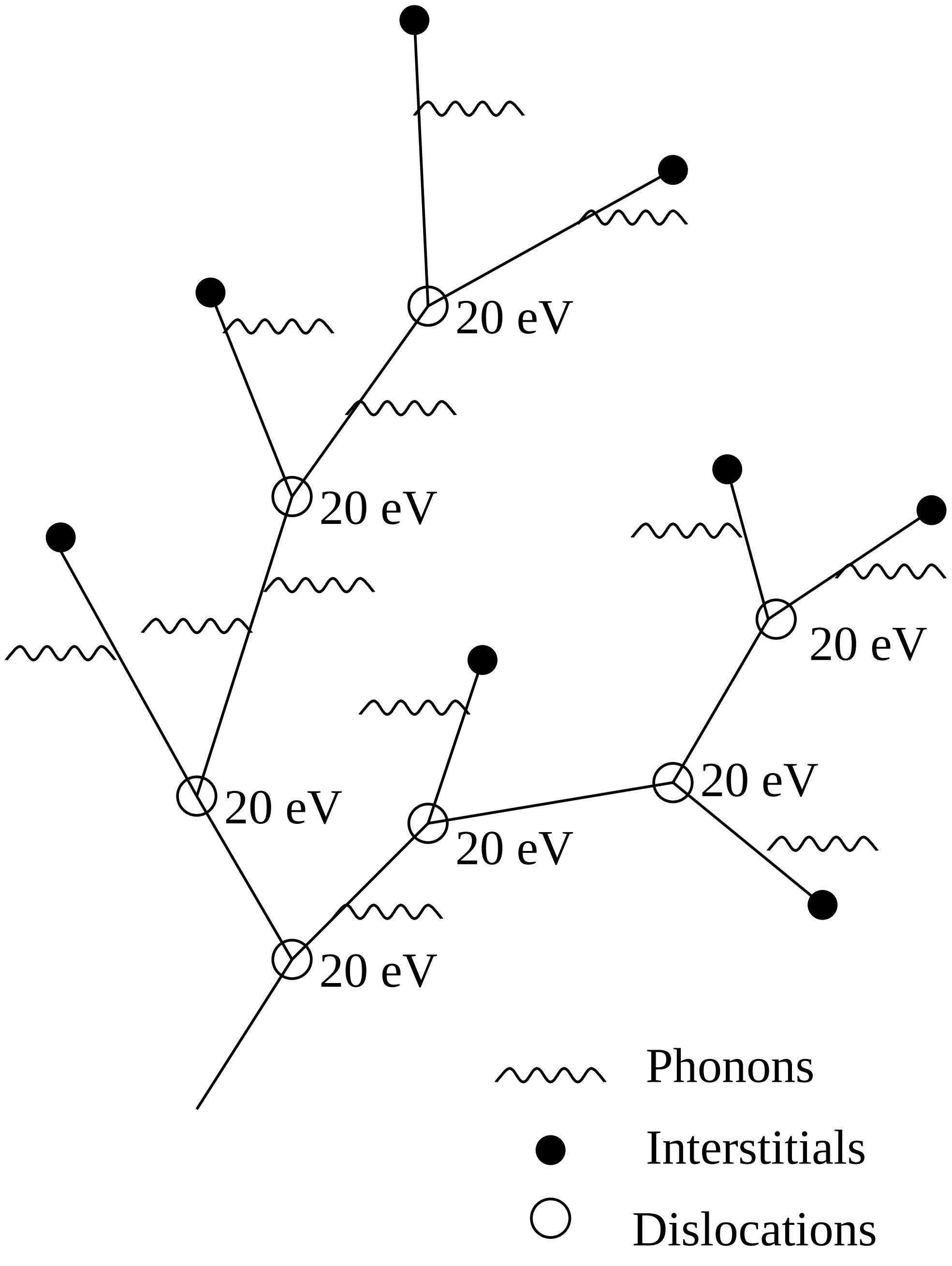
Stopping of nuclear fragments in Si

Calculated dE/dx for various ions in Si



NIEL is important only at low ion energies → saturation

Schematic of Atomic Cascade



TRIM simulation of full atomic cascade

Generate explicitly all recoils above dislocation threshold E_D=20 eV

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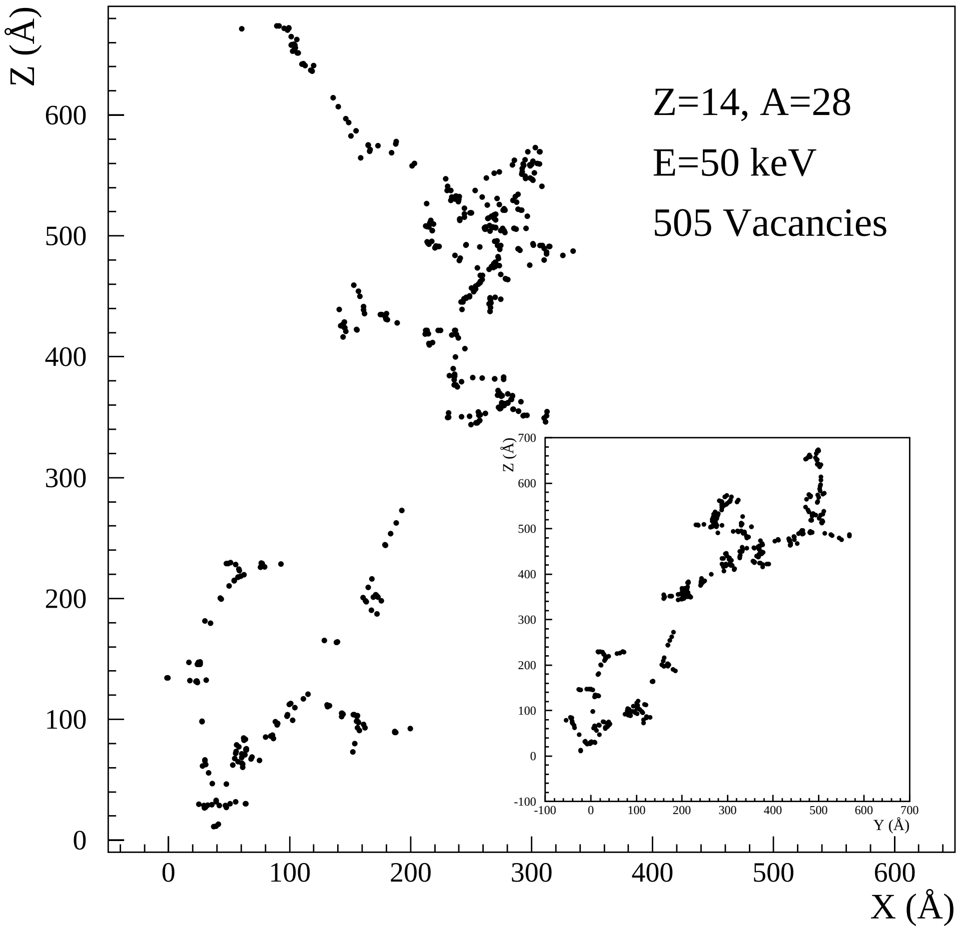
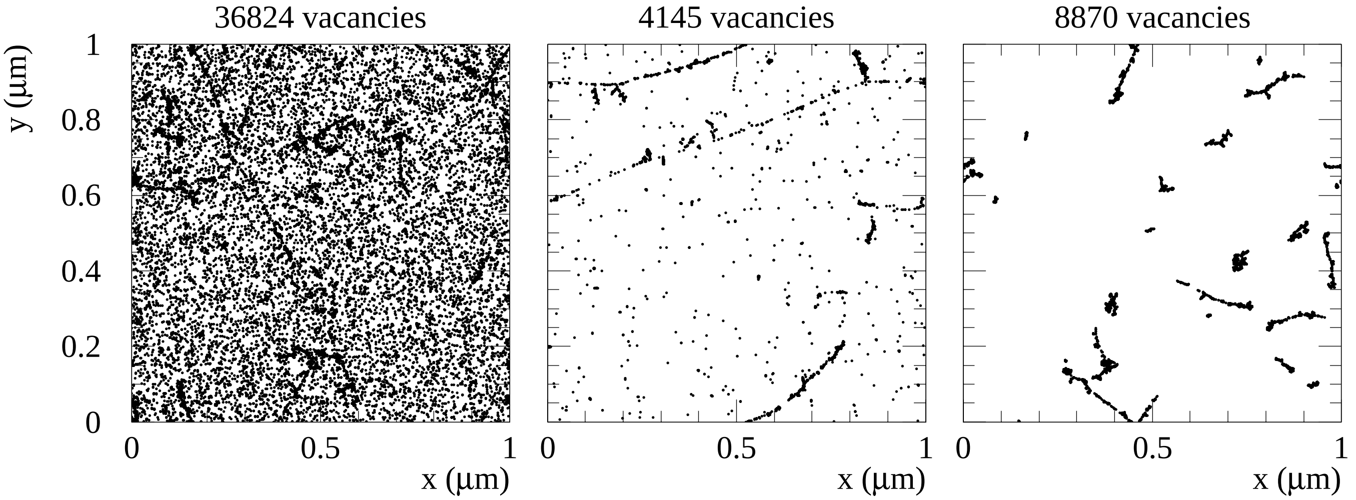
Exact knowledge of all vacancy and interstitial positions (except lattice structure) created by the h-Si interaction



Vacancy densities at high fluences

Projections of vacancy positions

Project through 1 μm of depth after fluence 10^{14} cm^{-1}



10 MeV Proton **24 GeV/c Proton** **1 MeV Neutron**

10 MeV protons

Mainly isolated point defects (remember depth dimension)

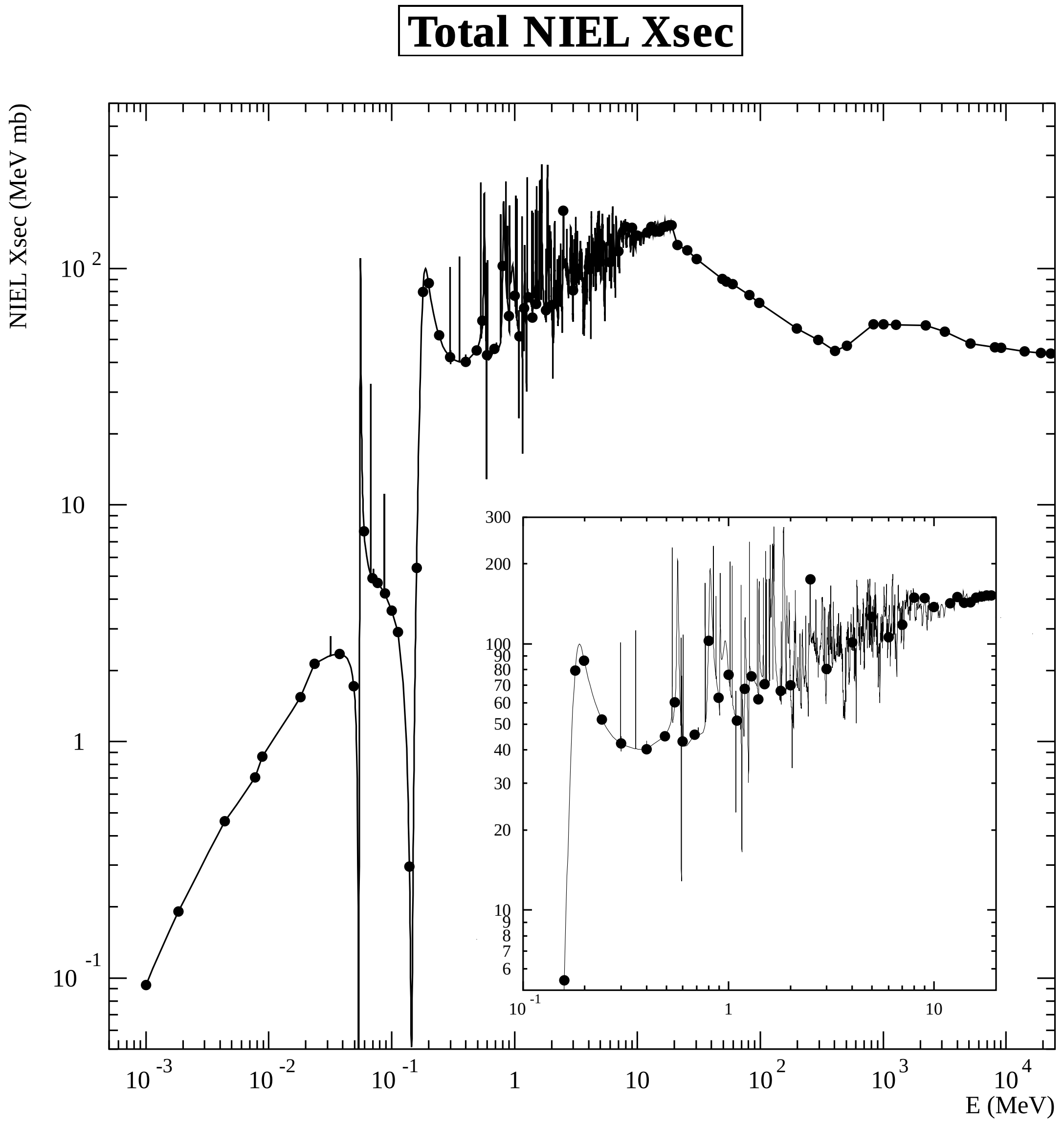
24 GeV/c protons

Isolated point defects and clusters

1 MeV neutrons

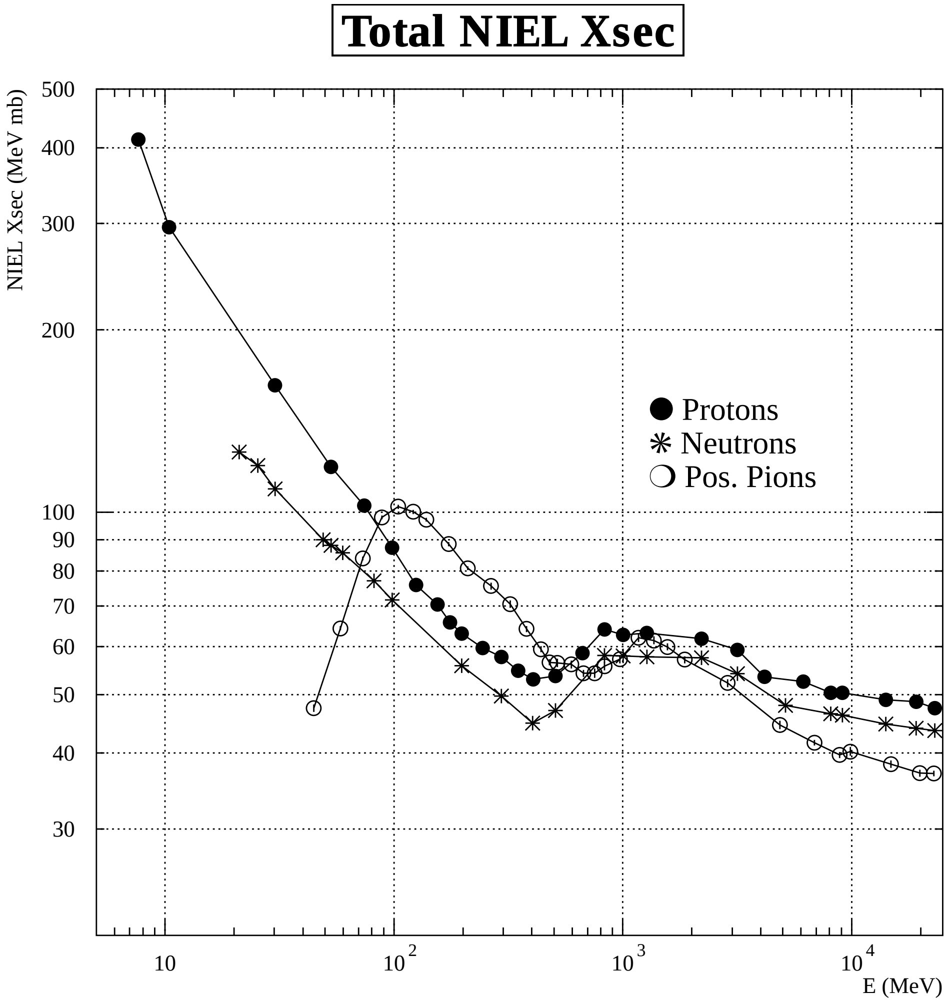
Almost only clusters

NIEL of Neutrons



DEFINED value for 1 MeV neutrons:
NIEL Xsec = 95 MeV mb

NIEL Xsec of High-Energy Hadrons



Agreement with previous work / expt. at high energy
Consistent with pion data at Δ-resonance
Lower than older work for low-energy protons.

Partitioning of NIEL

NIEL itself is further partitioned into

- **dislocations (≈20 eV per case)**
- **phonons (all collisions transferring less than 20 eV)**

Kinchin-Pease:

$$\left\{ \begin{array}{ccc} \nu = 1 & \text{if} & E_D < E_\nu < 2.5 E_D \\ \nu = \frac{E_\nu}{2.5\, E_D} & \text{if} & E_\nu > 2.5 E_D \end{array} \right\}$$

E_ν=NIEL, ν=Number of dislocations.

⇒ 40% of NIEL goes into dislocations (=damage).

These simulations:

	10 MeV proton	24 GeV/c proton	1 MeV neutron
Total NIEL Xsec	292	47.2	76.9
Phonons	147	27.2	44.1
Displacements	145	20.0	32.8
Displace./Total	50 %	42 %	43 %

Possibly slight dependence on type of irradiation

Defect Migration - Davies Model

Vacancies and interstitials migrate and recombine with each other and with impurities

Different recombination probabilities $P(X,Y)$ for all defect (impurity) pairs, i.e. reaction $X+Y \rightarrow XY$

Relative formation rate of defect XY:

$$\frac{P(X,Y)[Y]}{\sum_i P(X,Z_i)[Z_i]}$$

$[Y]$, $[Z_i]$=concentration of Y and Z_i.

Reasonable model if defects uniformly dispersed

Not applicable in clusters with varying density

Random walk + Davies Model I

After hadron irradiation the defects tend to be clustered

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Assumption of uniform dispersion not valid

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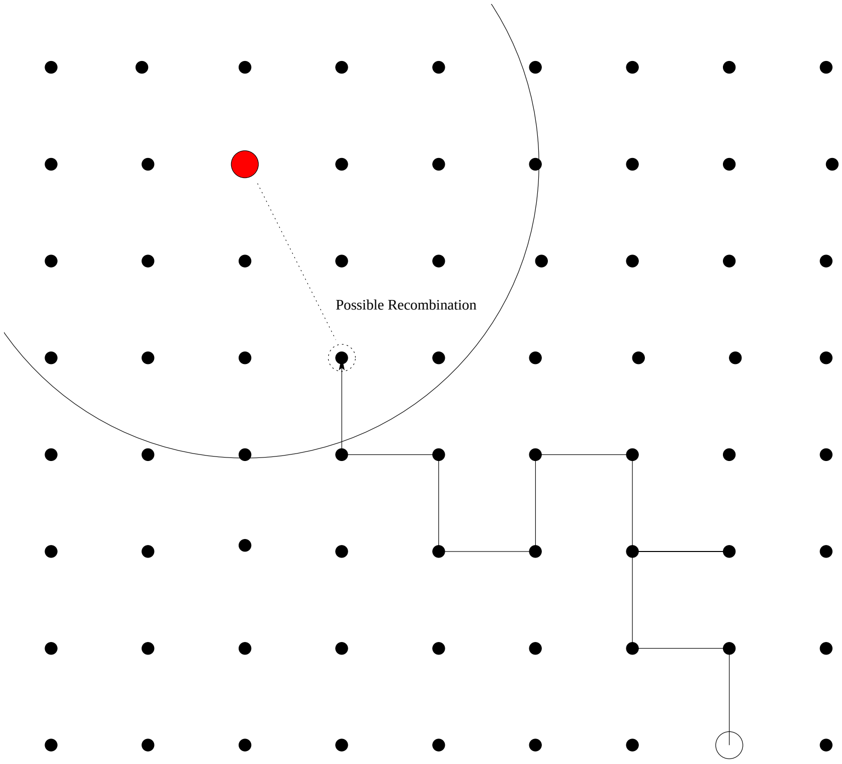
Treat each defect initially as a random walker which jumps from one lattice site to the other.



Random walk + Davies Model II

Some assumptions of the model

- **Interstitial diffuse 1000$\times$ faster than vacancies**
- **The $P(X,Y)$-values implicitly account for interactions between the defects**
- **Values of $P(X,Y)$ are the same within and outside cluster.**
- **$P(X,Y)$ values extracted from fits to DLTS data.**

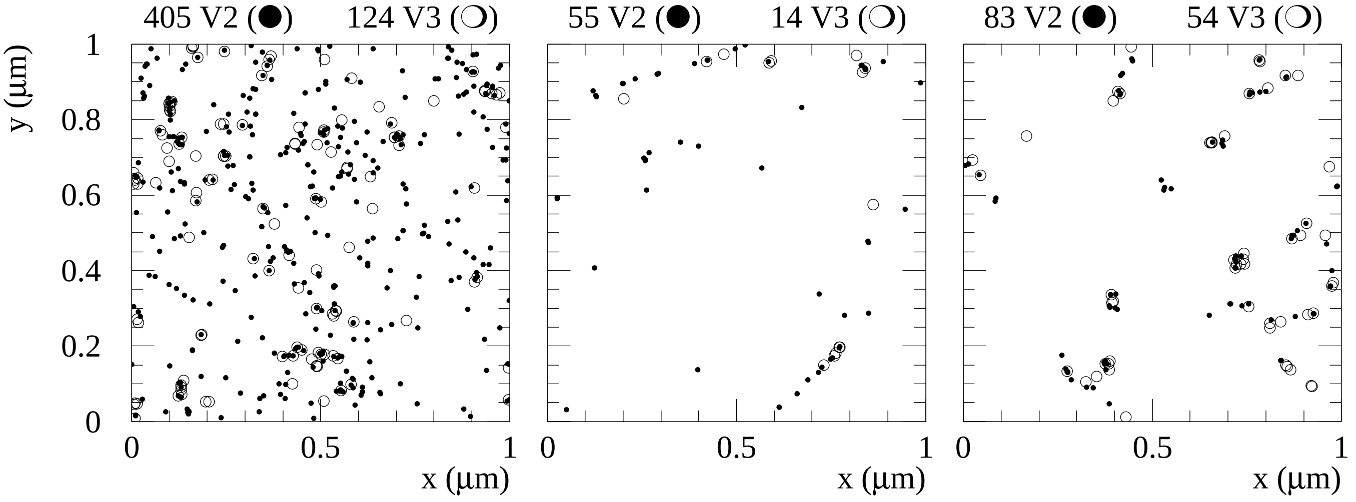
Basic simulation procedure

1. **Take final vacancy/interstitial constellation after TRIM**
2. **Allow for immediate recombinations (randomly in order of inter-defect distance)**
3. **Random walk the defects – after each step check recombination**
4. **Defects which escape cluster undergo Davies' treatment (assuming uniform distribution of previously produced defects)**
5. **Proceed in fluence steps (16 steps from 10^{12} to 10^{15} cm^{-2})**

Defect Densities after Migration

Projections of V2 and V3 positions

Project through 1 μm of depth after fluence 10^{14} cm^{-1}



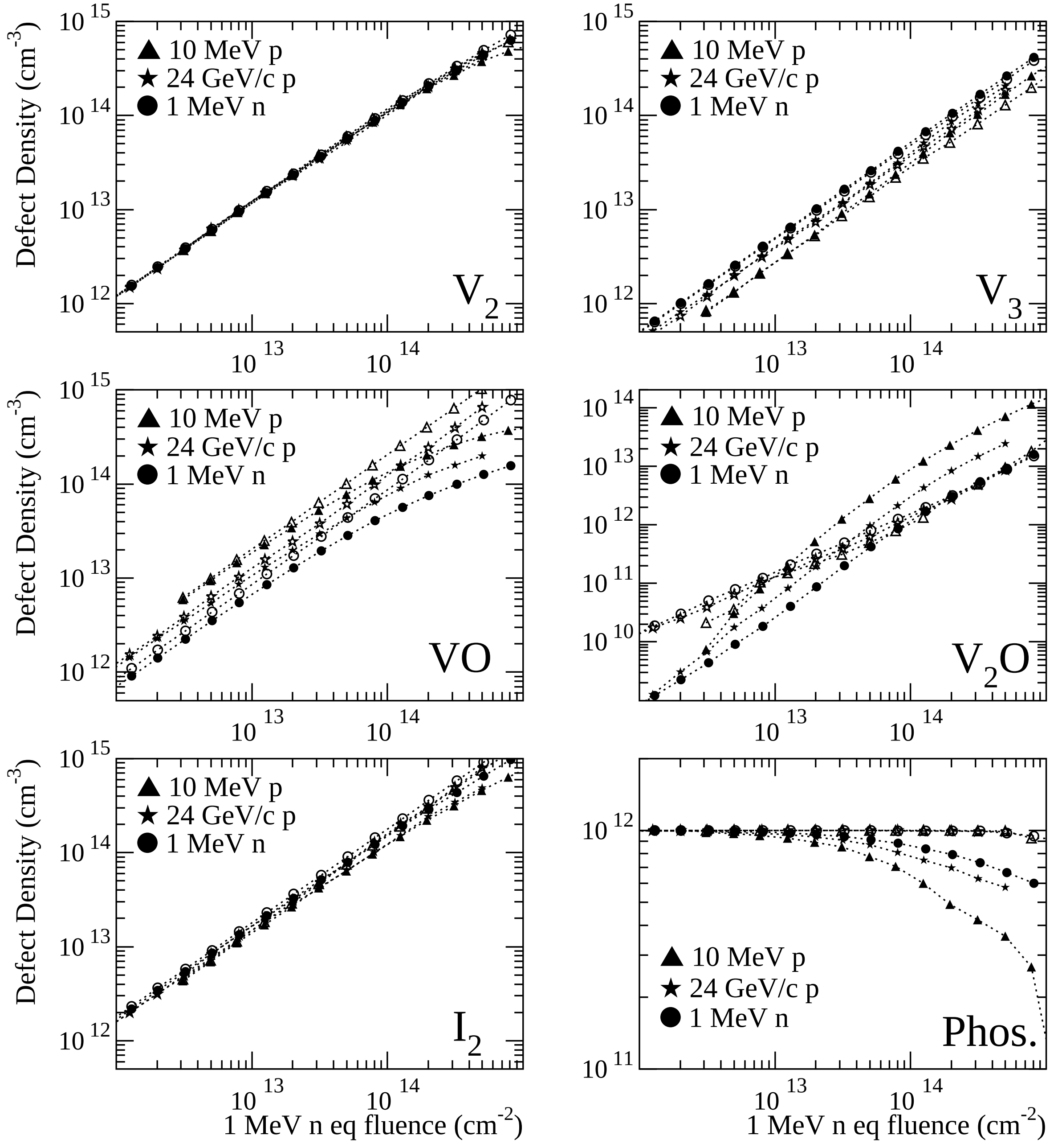
10 MeV Proton **24 GeV/c Proton** **1 MeV Neutron**

Some degree of clustering still remaining

Fraction of vacancies ending up in different composite defects:

Irradiation type	$[VO]/[V]_{ini}$	$2\times[V_2]/[V]_{ini}$	$3\times[V_3]/[V]_{ini}$	$N\times[V_N]/[V]_{ini}$
10 MeV proton	**0.0133**	**0.0191**	**0.0075**	**0.0025**
24 GeV proton	**0.0105**	**0.0231**	**0.0119**	**0.0041**
1 MeV neutron	**0.0064**	**0.0227**	**0.0150**	**0.0056**

Evolution of Defect Densities



Open symbols [O]=5×10^{17} cm^{-3}, Solid symbols [O]=5×10^{15} cm^{-3}

Shockley-Read-Hall predictions

Defect occupancies can be calculated from standard SRH theory

However,

Significant uncertainties in

- **defect energy levels**
- **capture cross sections for e and h**

Reasonable guess $\sigma_p = \sigma_h = 2 \times 10^{-15}$ cm^{-2}

Defect type	**Energy (eV)**	f_i	**I$_{\mathrm{leak}}$ (μA/defect)**
V$_2$	**E$_c$-0.42**	2×10^{-5}	9×10^{-14}
V$_3$	**(E$_c$-0.47)**	7×10^{-4}	6×10^{-13}
V$_2$O	**(E$_c$-0.55)**	**0.3**	1×10^{-11}

$$\boxed{N_{\mathrm{eff}} = |[P] - f_1 \times [V_2O] - f_2 \times [V_2] - f_3 \times [V_3]|}$$

With above SRH values and simulated defect concentrations N_{eff} and I_{leak} are orders of magnitude too low

Effect of clustering

V2 and probably V3 have 3 charge states in the band-gap

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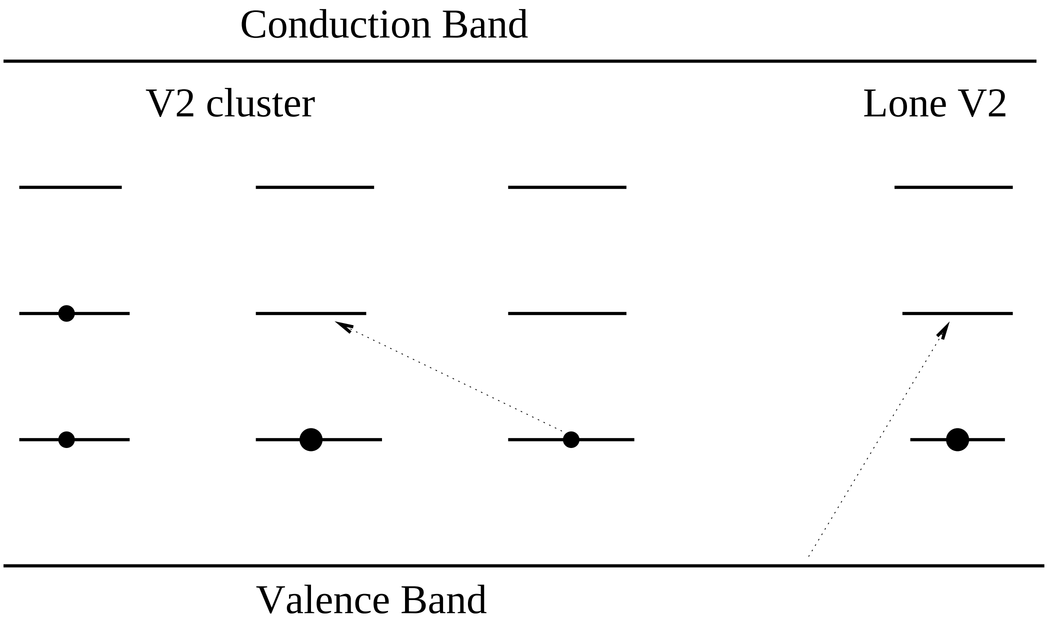
If defects are clustered, transitions between defect levels can amplify the occupancies predicted by simple SRH theory



Effect predicted to be seen at local densities of $10^{16} - 10^{18}$ cm^{-3}

Cluster Enhancement over SRH

Use local density within radius R around each defect

Defect type	R (Å)	1 MeV neutron f_c^i	1 MeV neutron E_i	24 GeV/c proton f_c^i	24 GeV/c proton E_i
V_2	100	0.70	288	0.51	277
V_3	100	0.65	281	0.57	274
V_2	200	0.87	64	0.64	58
V_3	200	0.85	62	0.74	58

Defect type	R (Å)	10 MeV proton f_c^i	10 MeV proton E_i	200 MeV π^+ f_c^i	200 MeV π^+ E_i
V_2	100	0.35	269	0.56	279
V_3	100	0.51	271	0.59	276
V_2	200	0.41	55	0.70	59
V_3	200	0.64	56	0.77	59

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Split V2 and V3 in clustered and non-clustered components

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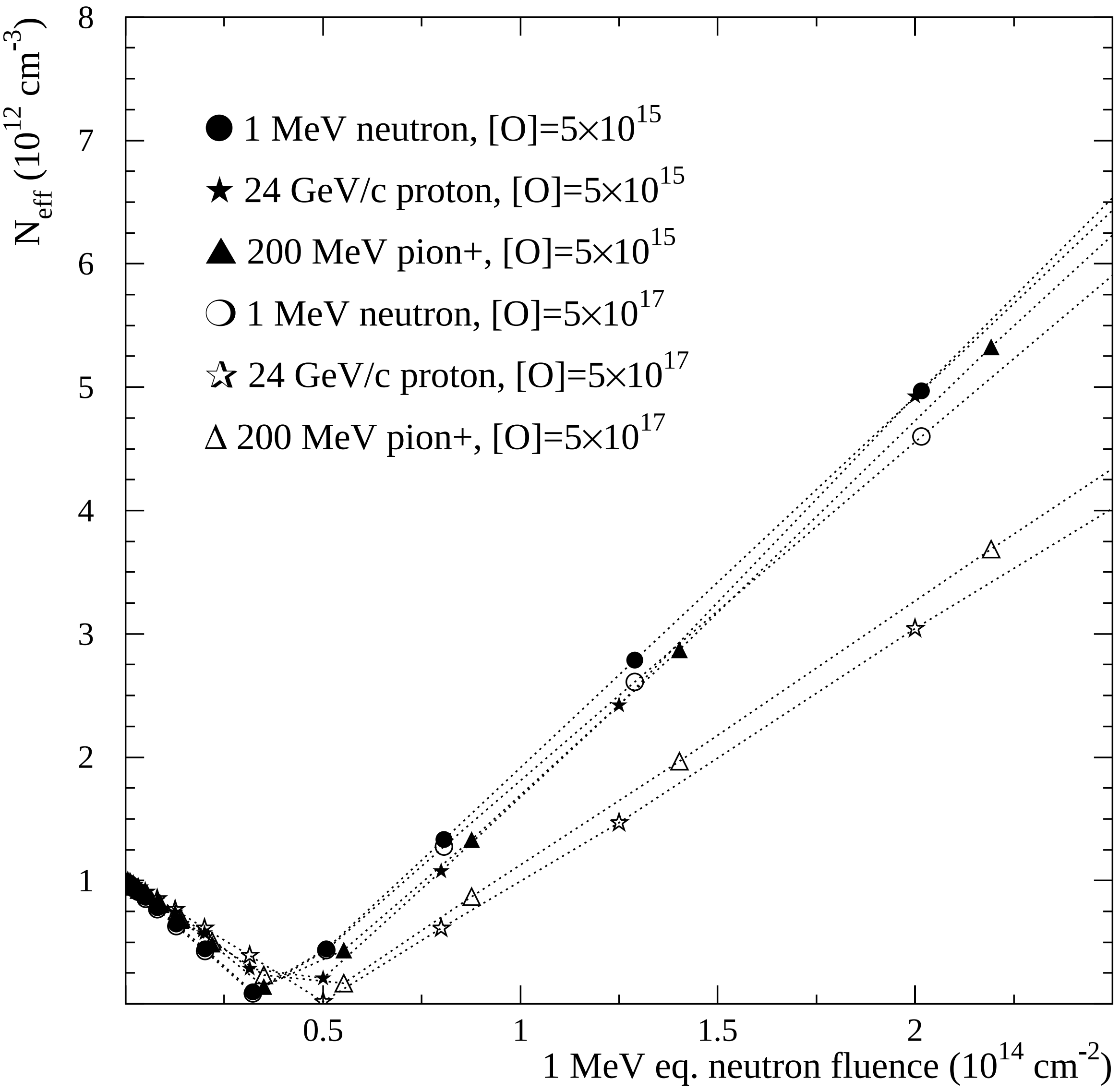
$$N_{\text{eff}} = \left|[P] \; - f_1[V_2O] - f_2\{E_2 f_c^2 + (1 - f_c^2)\}[V_2] \right.$$
$$\left. - f_3\{E_3 f_c^3 + (1 - f_c^3)\}[V_3]\right|$$

Best fit to data with R=100 Å values.

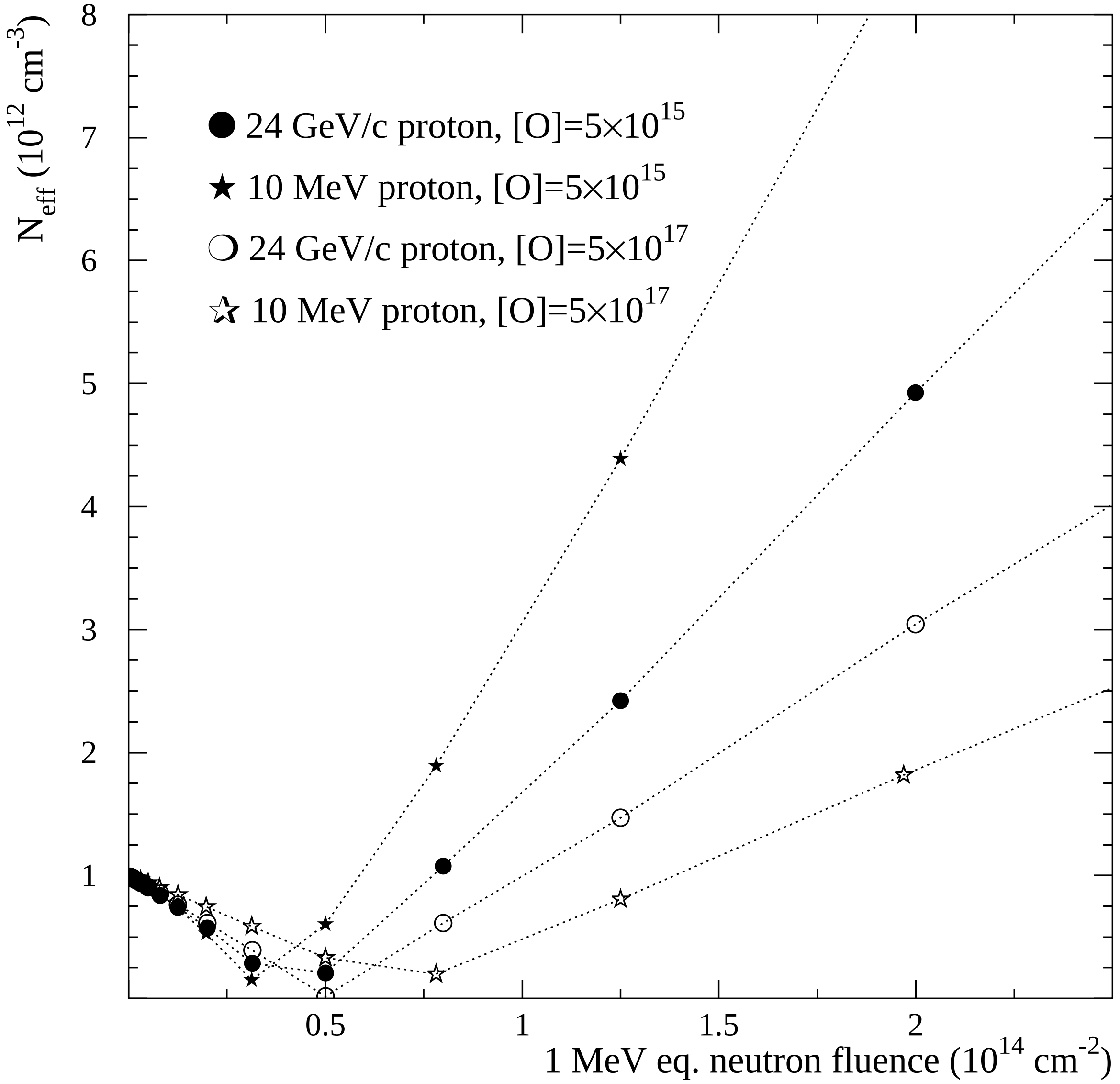
Changes of N_{eff}



Experimentally observed effect of oxygen reproduced (although not quite as pronounced as in experiments)

N_{eff} for 10 MeV protons

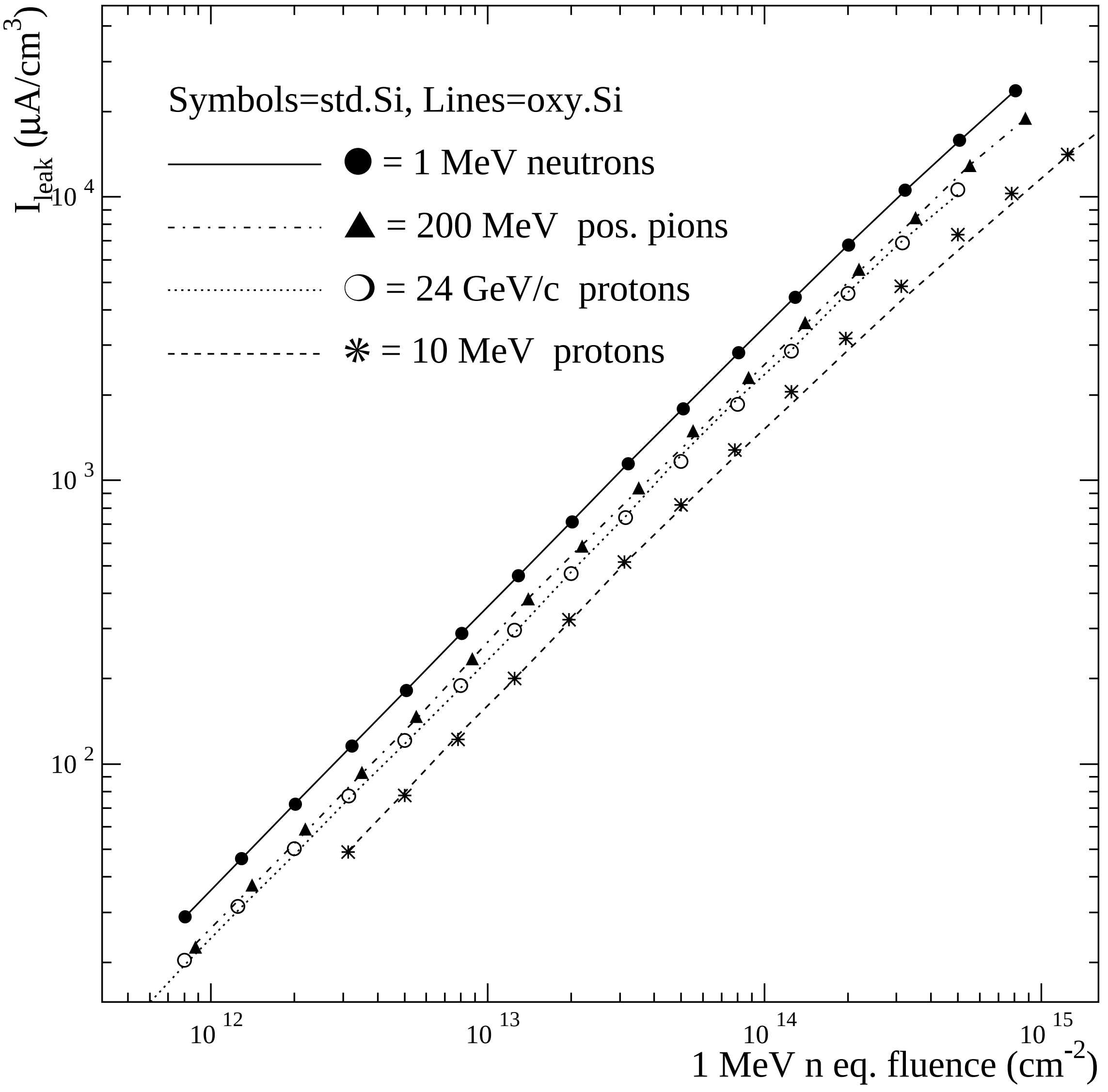
Assume simulated hardness factors
H(10 MeV p)/H(24 GeV/c p)=6.2



Large oxygen effect for 10 MeV protons, scaling violation

Changes of $\boldsymbol{I}_{\text{leak}}$

Assume simulated hardness factors
H(10 MeV p)/H(24 GeV/c p)=6.2



Apparent NIEL violation – but maybe correct !

NIEL scaling violation ?

NIEL cannot be directly measured
&
Neutron damage at 1 MeV varies a rapidly

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Experimental uncertainty for 1 MeV neutrons

Recent experiments (Bechevet et al) for relative damage (α and β) show NIEL violation in standard Si.

	α	β
9 MeV p	**13.3**	**4.3**
10 MeV p	**9.9**	**3.4**
24 GeV/c p	**2.54**	**0.56**
Ratio	**3.9–5.2**	**6.1–7.7**

These are fairly consistent with the simulations

Is NIEL violation reasonable ?

The prediction that NIEL is violated arises from a few almost model-independent facts

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Concentrations of defects (V2, V3, ...) are fixed by experimental DLTS data and ’cannot’ be wrong by orders of magnitude

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Need a mechanism to amplify level occupancies above SRH theory

Intercenter charge transfer seems a natural candidate

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The presumably dominant defect V2 scales with NIEL

&

Different degree of V2 (and V3) clustering for various irradiation types

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NIEL scaling violation

Conclusions I

NIEL scaling usually OK within factor of ~ 2

but do not trust it blindly because

It can fail badly for oxygenated silicon

It does not seem to be exact for standard silicon either

Discrepancies seem to be largest for low-energy protons

especially

Measured 1 MeV neutron damage values should be treated with care

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Would be better to use 24 GeV/c protons as reference

Conclusions II

Model predictions are consistent with experiments on standard and oxygenated silicon

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The V2O defect and SRH enhancement due to clustering of V2 are both needed for this

However, there are several assumptions, which can be considered as almost free parameters.

The present assumptions seem reasonable, but one can easily think of others which would not provide the same consistency

Can check model and assumption with

- **10 MeV proton data for std and oxy silicon**
- N_{eff} **data immediately after (cold) irradiation**