Hadronic Interactions in Si

Neutrons

- **Below 3 MeV mostly elastic (or (n,γ))**
- **Between 3-20 MeV elastic, (n,p), (n,α) etc**
- **Above 20 MeV increasing number of inelastic channels**

Protons

- **Below $\sim$5 MeV only elastic**
- **Up to few tens of MeV elastic and few-nucleon stripping**
- **At high energies elastic and deep inelastic reactions**

Pions

Like protons, but deposit their rest mass (140 MeV) in addition.

Simulation of interactions

Neutrons

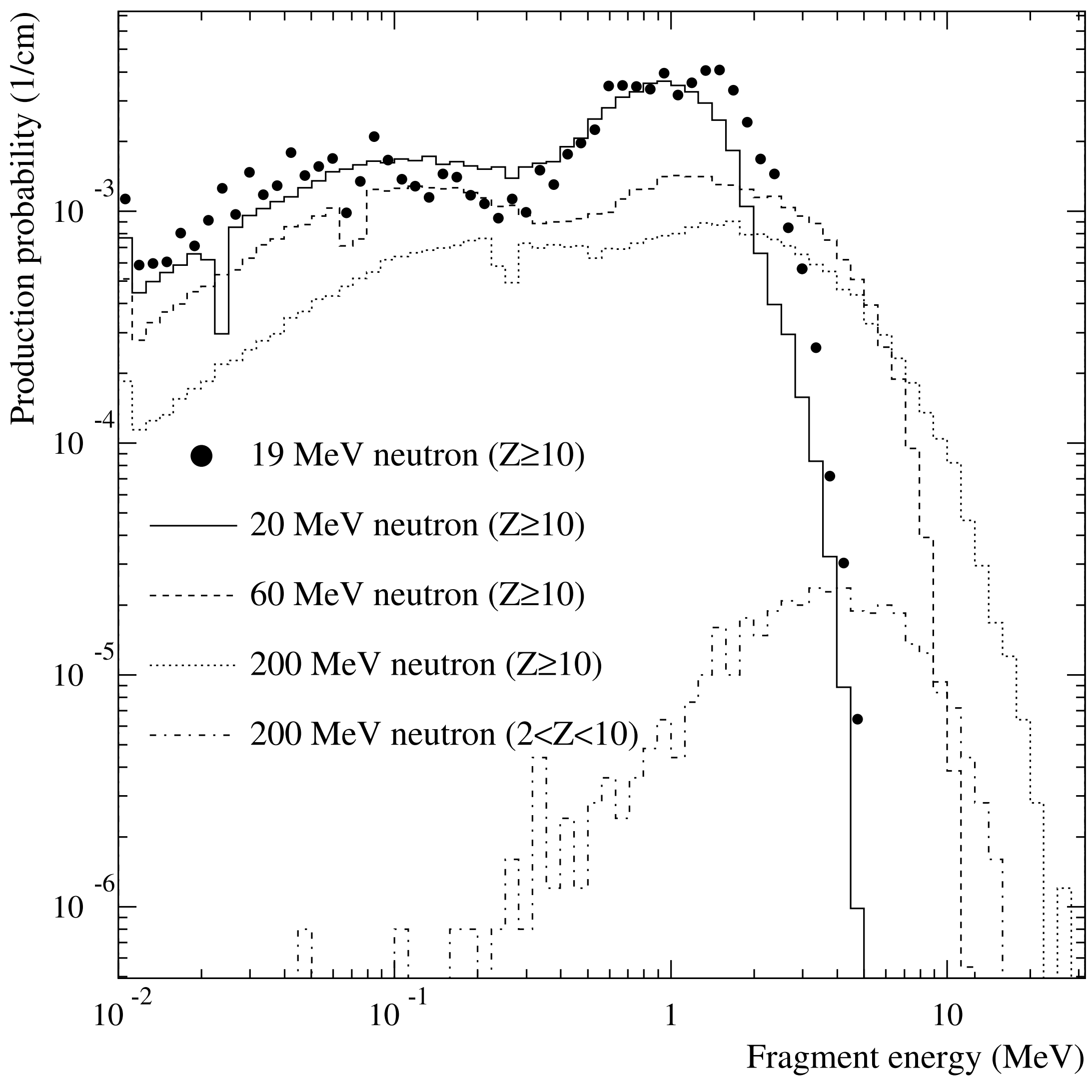
Below 20 MeV direct sampling from ENDFB-VI data.

Above 20 MeV FLUKA event generators

Protons and Pions

Elastic scattering: optical Glauber formalism

Inelastic scattering: FLUKA event generators



Transport of recoils

Use modified version of TRIM85 code

Features:

- **Generate all atomic recoils explicitly down to the threshold of 20 eV**
- **Transport all atomic recoils until their energy is below 20 eV**

Results:

Full final state of each collision with explicit knowledge of all interstitial (I) and vacancy (V) positions.

50 keV recoils - initial vacancies

Lindhard NIEL at 50 keV: $\longrightarrow$ NIEL=$\frac{50\,\mathrm{keV}}{1+k_d g(\epsilon_d)}$ = 29 keV

Kinchin-Pease: N=$\frac{0.8\times\mathrm{NIEL}}{2E_D}$ $\longrightarrow$ N=580

NIEL from simulation =

Dislocation energy (20 eV per IV-pair)
+
Energy transfers of less than 20 eV
+
Energy of ions falling below 20 eV

Simulation:

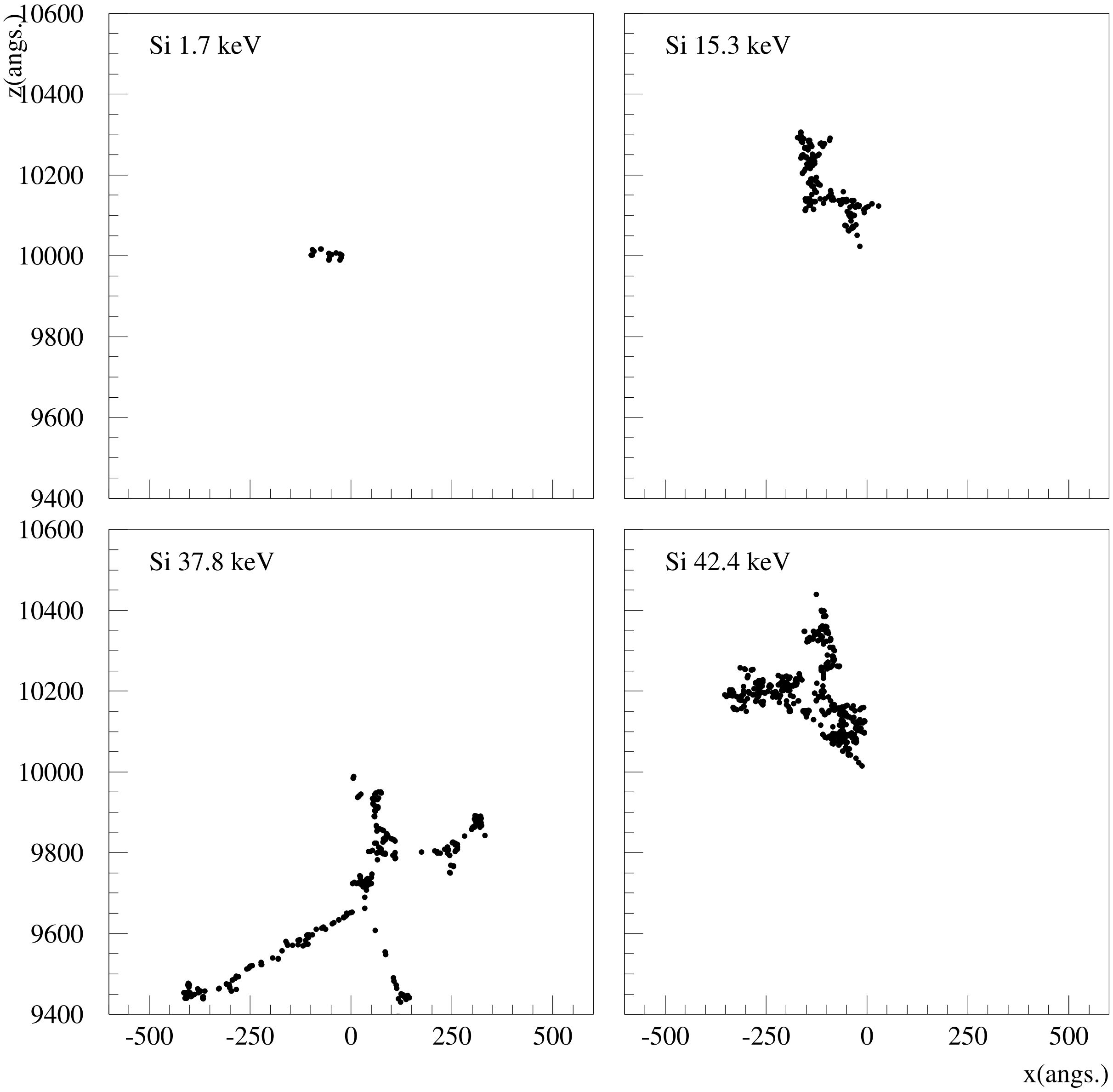
NIEL = 25.1 keV
N = 553

1 MeV neutron interactions

Calculated NIEL Xsec (at 981 keV) : 102 MeV mb

(NIEL varies rapidly with energy for 1 MeV neutrons)

XZ-projection of initial Interstitial positions for 4 neutron events

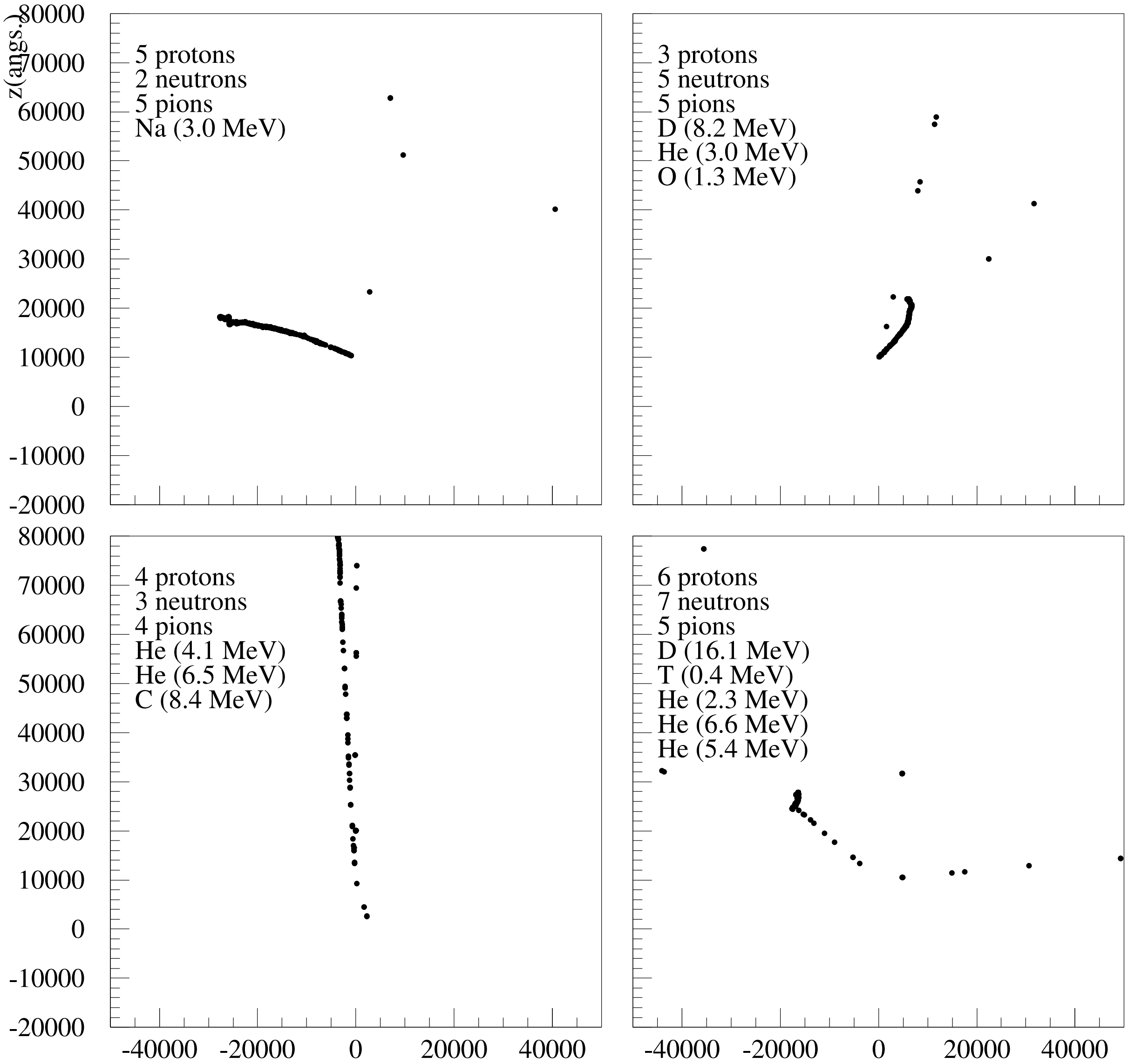


19 GeV proton interactions

Calculated NIEL Xsec : 66 MeV mb

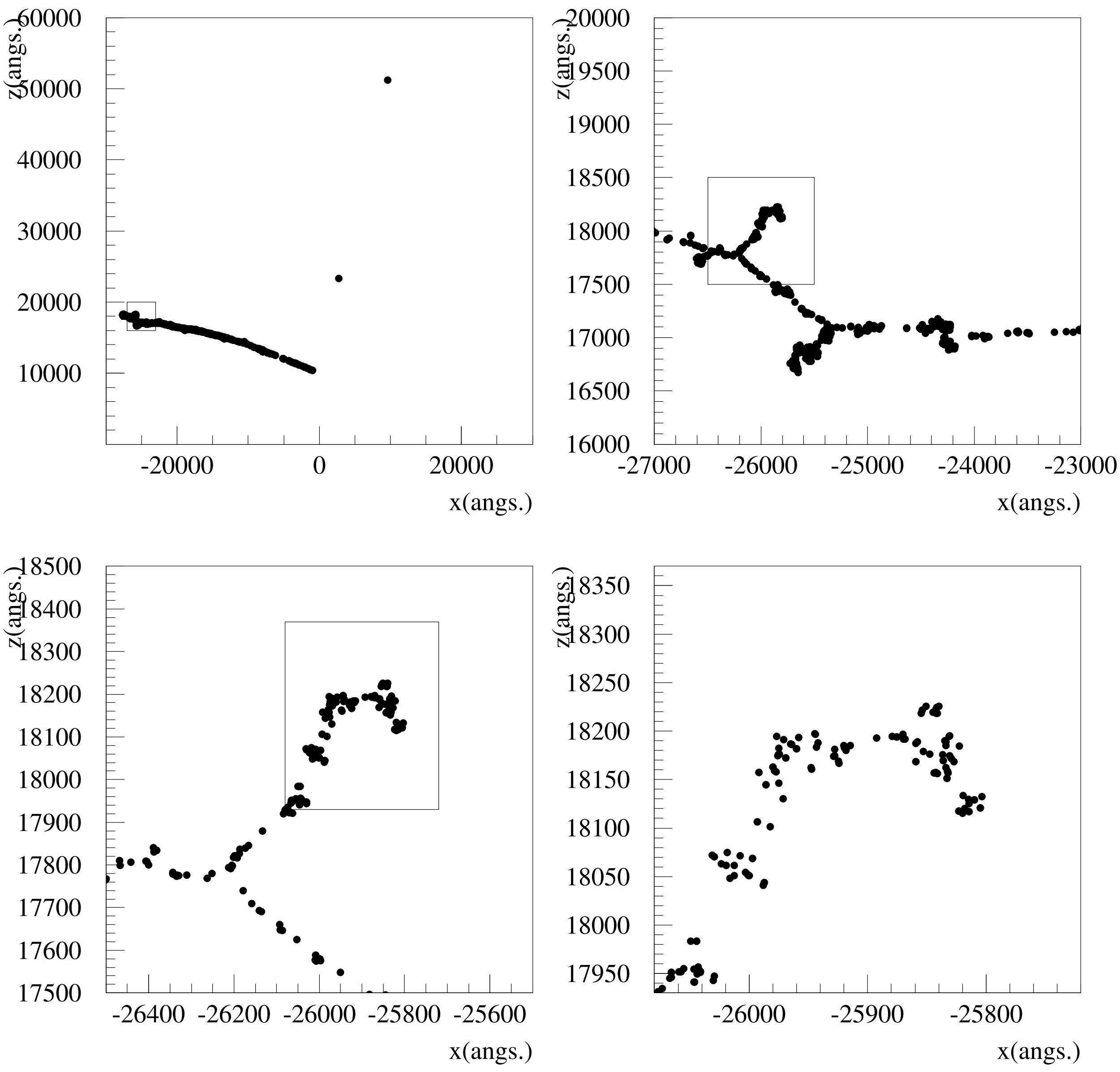
(Usually assumed value ∼50 MeV mb)

XZ-projection of initial Interstitial positions for 4 proton events



19 GeV protons – A closer look

Zoomed XZ-projection of a 19 GeV proton event (Interstitials)



NIEL scaling – or not ?

If V2 are responsible for I_{leak}, then single vacancies should not count as much as clustered ones

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!!!! Remove NIEL of point defects !!!!

NIEL type	1 MeV n	20 GeV p	n/p ratio
Usually used values	95	∼50	∼1.9
Total NIEL	102	66	1.55
Dislocation NIEL	69.4	43.6	1.59
>0 neighbours	51.3	28.4	1.81
>1 neighbours	29.95	15.6	1.91
>2 neighbours	14.9	7.6	1.96
>3 neighbours	6.7	3.4	1.97
>4 neighbours	2.77	1.41	1.96

↓

Dislocation NIEL proportional to NIEL (about 67%)

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NIEL scaling restored if NIEL due to point defects is removed

Defect migration

Difference to Davies model: $\boxed{\textbf{dense initial clusters}}$

thus
I and V reactions are not independent

$\Downarrow$

MORE INPUT NEEDED THAN IN DAVIES MODEL:

R(I,V)
R(I,V2)
absolute values of the capture radii

Molecular dynamics simulations → R(V,V) = 7.7 Å

Fix this and fit R(I,V) and R(I,V2) by requiring reproduction of experimental VO, VV/VO and VO/(CC+CO) introduction rates

Does not fit very well...

Quantity	Experimental	Best fit
VO	$\sim$0.7 cm^{-1}	0.9 cm^{-1}
VO/(CC+CO)	$\sim$0.4	0.4
VV/VO	$\sim$1.5	0.8

(simulation done with 1 MeV, experimental is 14 MeV NIEL scaled !)

Best fit/guess for capture radii

!!!! These should be taken as very preliminary !!!!

V+V $\longrightarrow$ V2 fixed from MD results

Expt. data used when available to fix ratios

Higher order reactions (e.g. V+V3) mostly pure guesses

Reaction	Capture radius R (Å)
V+V $\longrightarrow$ V2	7.7
V+O $\longrightarrow$ VO	5.0
V+VO $\longrightarrow$ V2O	8.4
V+V2 $\longrightarrow$ V3	3.0
V+V3 $\longrightarrow$ V4	7.7
I+V $\longrightarrow$ Si	15.1
I+V2 $\longrightarrow$ V	11.1
I+V3 $\longrightarrow$ V2	11.1
I+VO $\longrightarrow$ O	6.0
I+V2O $\longrightarrow$ VO	3.6
I+C $\longrightarrow$ Ci	5.2

Would help a great deal to get updated values.....

Simulation of defect migration

Each defect undergoes a random walk (jump to neighbouring lattice site)

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Interstitials diffuse 10000 times faster than vacancies

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If 2 defects come closer than 16.2 Åthey might recombine. The probability for this is $(R/16.2)^3$, where R is the capture radius.

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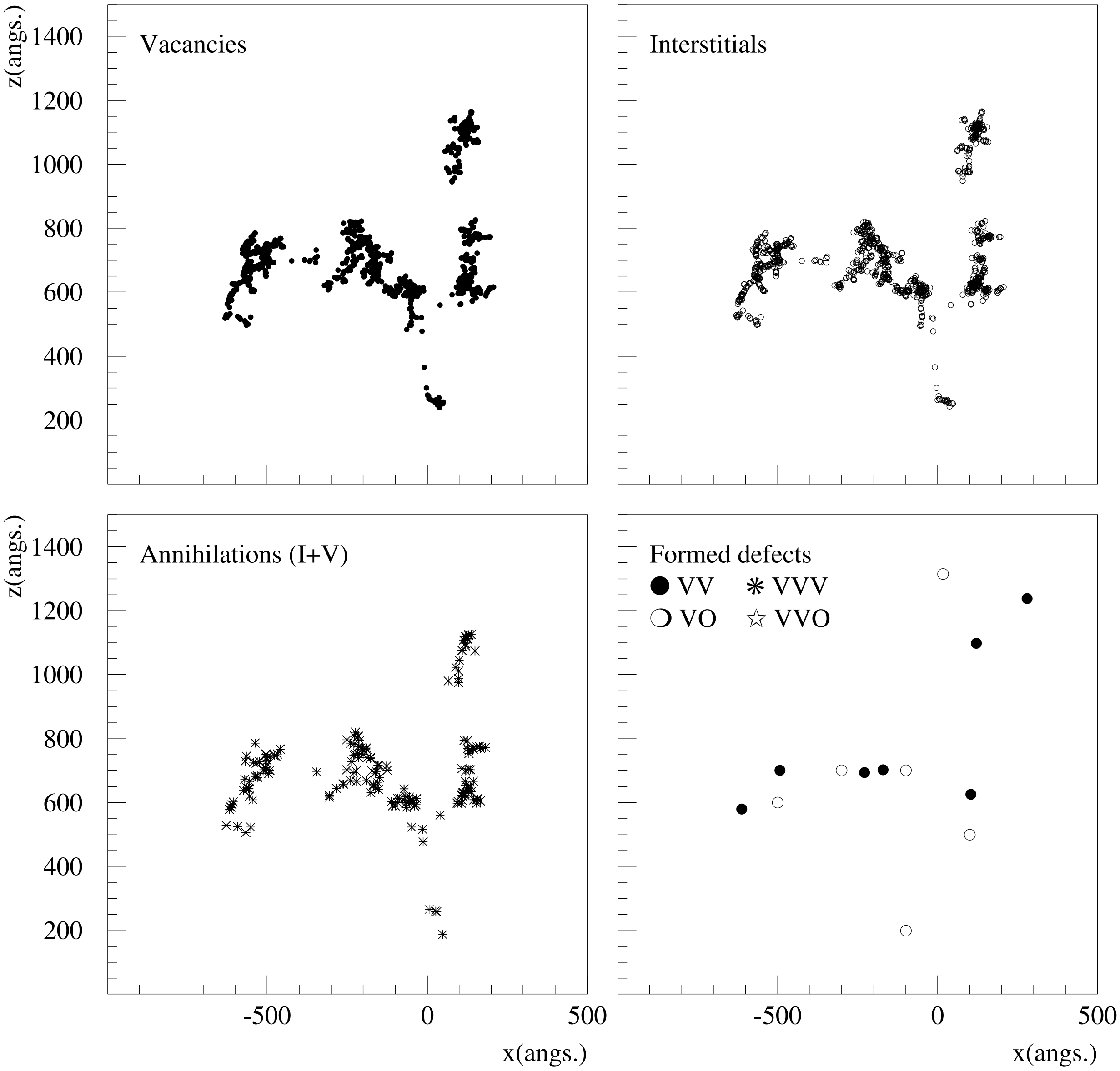
If defects get far (1000 Å) from their initial position and the nearest neighbour is far (200 Å) they are considered free. For these the standard Davies model is applied.

Note: **Contrary to Davies model VV is NOT a primary defect, but introduced by V+V combination.**
Only I and V are primary.

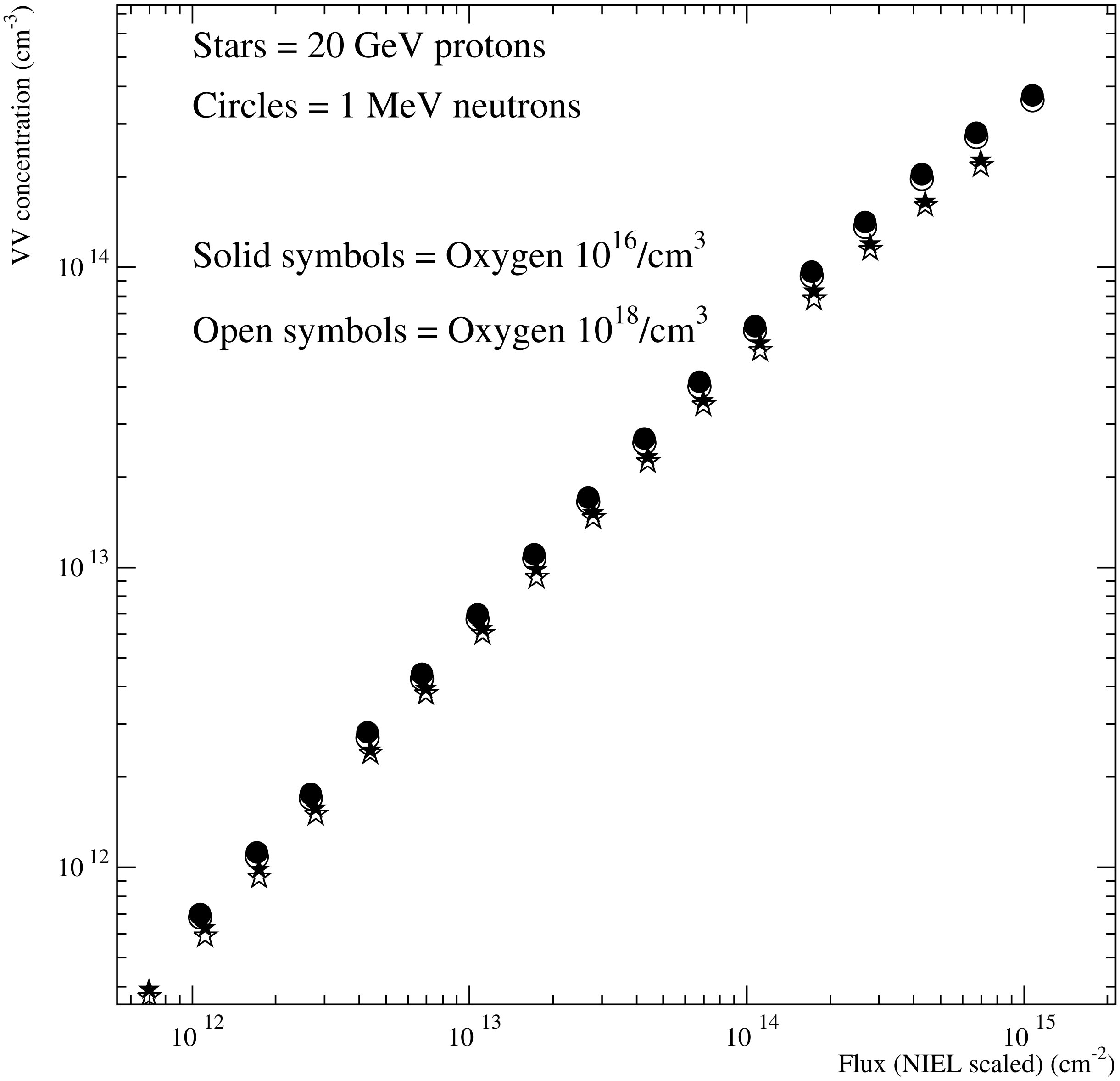
Stable defect formation

Example of 100 keV Si recoil



The large R(I,V) and R(I,V2) values lead to almost total annihilation of the clusters (but only so experimental V2, VO and CC+CO introduction rates can be reproduced)

Evolution of VV



VV scales with NIEL (perfectly if we use 1.9 and not 1.55)

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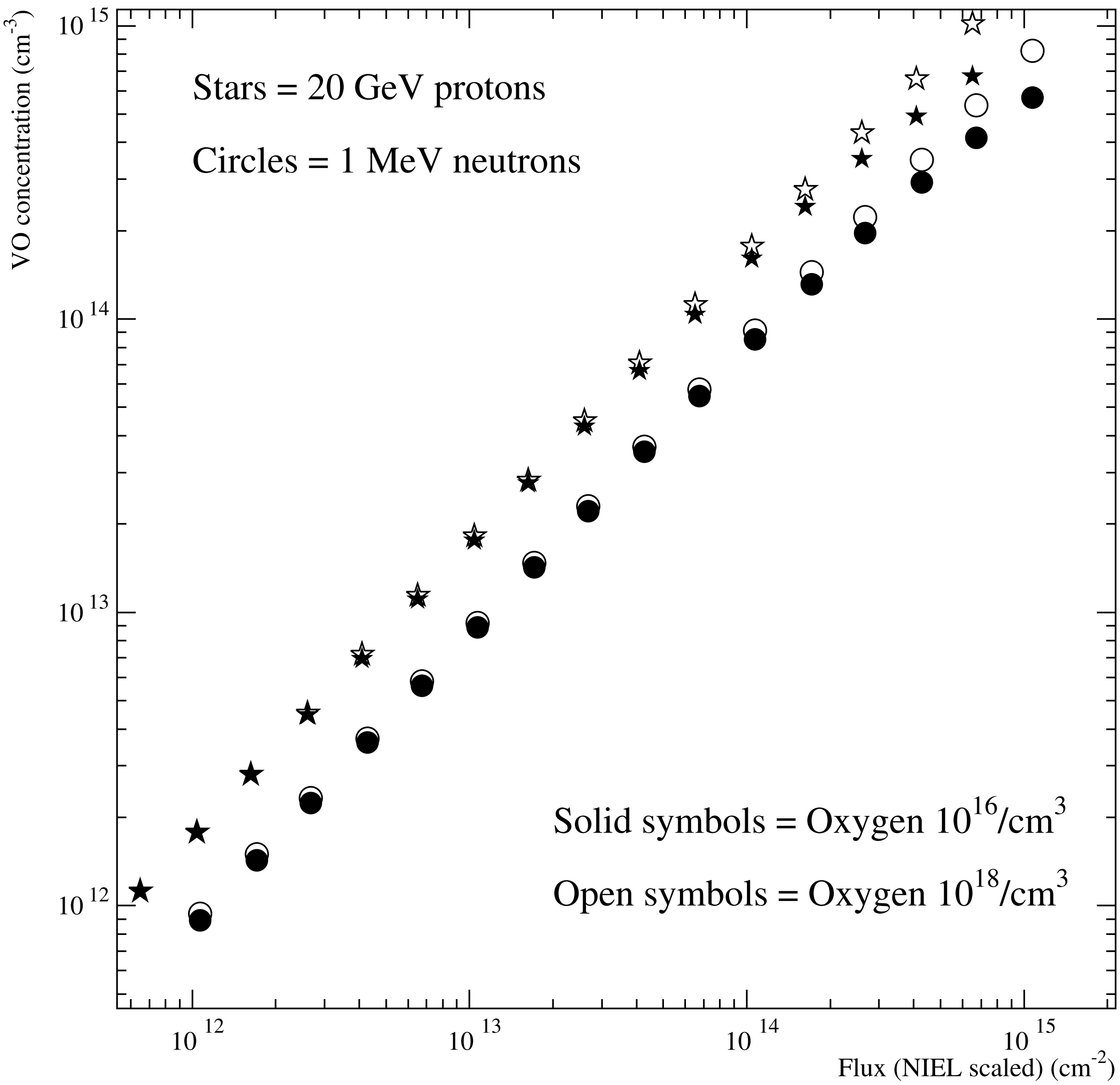
Oxygen has only very minor effect on VV

Evolution of VO



VO does not scale with NIEL

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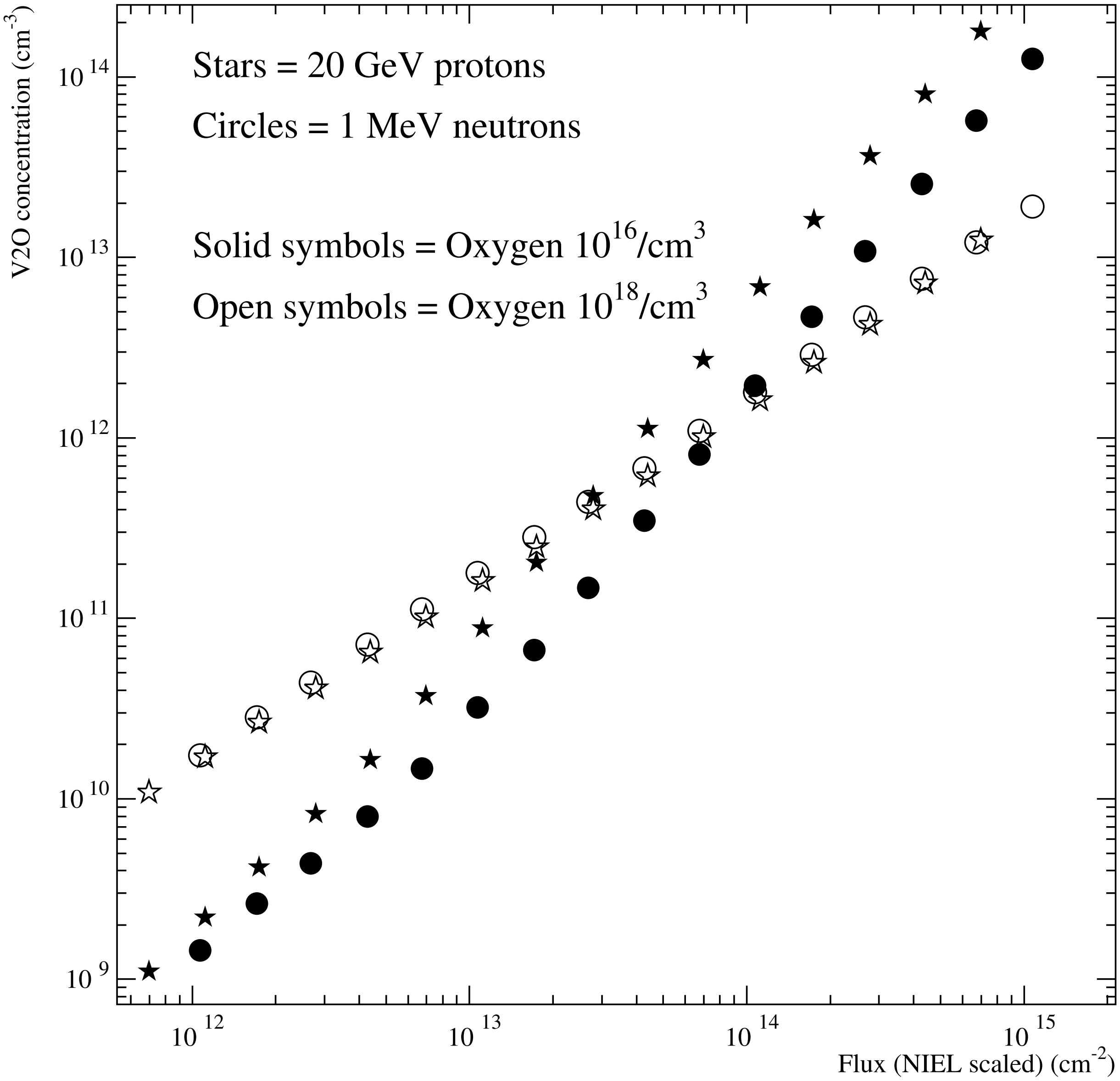
Point defects produce more VO than clusters

Evolution of V2O



V2O does not scale with NIEL if low oxygen

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V2O does scale with NIEL if high oxygen !!!

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Behaviour is consistent with expectation and VO development

BUT if we assume V2O gives N_{eff} changes...

...seems to be in contradiction to experimental data