

A Percolation Model for Calculating SSB- and DSB-yield



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- **Problem:** basic assumption in microdosimetry: $E_{\text{deposited}} \propto (\text{number of ionisations})$.
... is violated in nanometre-sized volumes (number of ionisations is too small!).
- **Way out** (Bernd Grosswendt, RPD 115 (2005), pp. 1 – 9):

Ionisation-cluster size “v” (i. e. number of ionisations [in the volume] per primary particle) should be measured instead of $E_{\text{deposited}}$ •

$$P_1(Q; d) = \sum_{k=0}^{\infty} [f_1^{(1)}(Q; d)]^{*k} \frac{\langle k \rangle^k(Q)}{k!} \exp(-\langle k \rangle(Q)) = \text{Probabil. to cause } v = 1 \text{ at } d$$

$$F_2 = \sum_{v=2}^{\infty} \sum_{k=0}^{\infty} [f_v^{(1)}(Q; d)]^{*k} \frac{\langle k \rangle^k(Q)}{k!} \exp(-\langle k \rangle(Q)) = \text{Probabil. to cause } v \geq 2 \text{ at } d$$

- Bernd Grosswendt's hypothesis (cf. B. Grosswendt, **From Macro to Nanodosimetry** lecture, Bad Honnef, 2008; B. Grosswendt, RPD 115 (2005), pp. 1-9):

P_1 ↔ single-strand break (SSB)

F_2 ↔ double-strand break (DSB)

- However, an ionisation cluster with $\nu \geq 2$ can also refer to single ionisations caused anywhere in the volume.
- Thus, an ionisation-cluster model would be of advantage!

- There has been developed a highly sophisticated realistic DNA target model by [Friedland et al. \(Radiat. Res. 150 \(1998\) pp. 170 – 182\)](#) up to now which can be used, among many others, for calculating the SSB- and DSB-yield.
- In the following, I propose an alternative (percolation) model which is
 - very simple,
 - very quick,
 - and easy to use.

The model is by far not as powerful as the one of Friedland et al. (see above), but may be used (among others)

→ to analyse the geometry dependence of the cluster distribution.

➤ General remarks about percolation models:

➤ percolation → percolare (Latin) ⇔ „to trickle through“

E. g.: liquid trickles through sand (→ clusters arise).

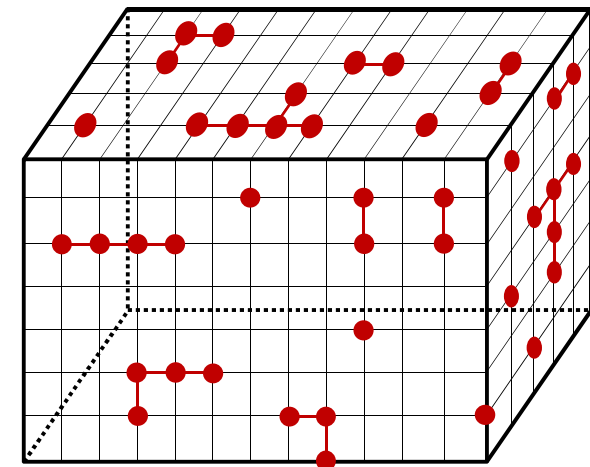
➤ (simple) statistical models

➤ known in statistical/solid-state/nuclear/heavy ion physics, polymer chemistry, ...

➤ basic idea:

– site is occupied with occupation probability „ p “

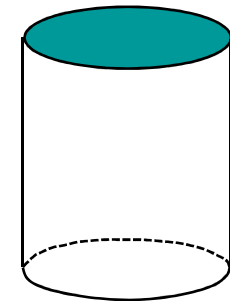
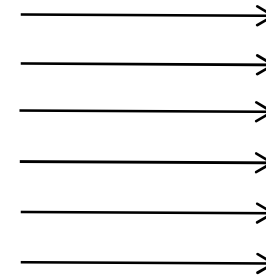
– occupied neighboured sites are connected with bound probability „ q “



➤ Model formulation :

➤ Scenario (cf. Bernd Grosswendt, RPD 115 (2005), pp. 1 – 9) :

Electron beam
(homogeneous,
monoenergetic)



Cylinder

- Volume: Height as well as diameter: 2.0 nm.

Liquid water, density: 0.998203 g/cm³

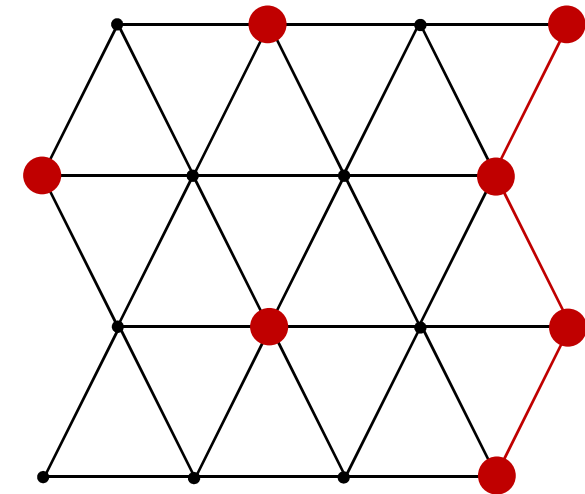
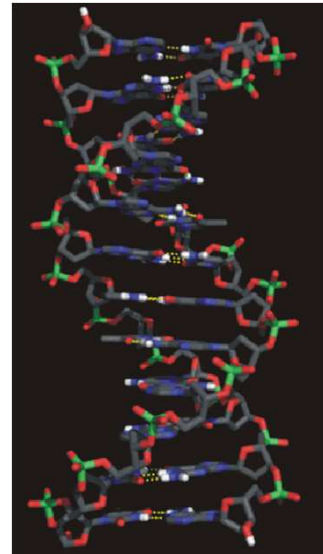
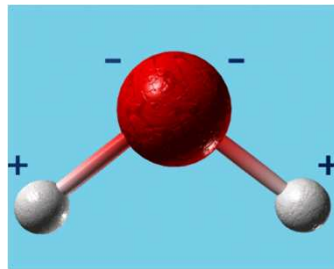
Molar masses: $m_a(\text{H}) = 1.00794 \text{ u}$

$m_a(\text{O}) = 15.9994 \text{ u}$

⇒ Number of atoms within the cylinder: **≈ 629**

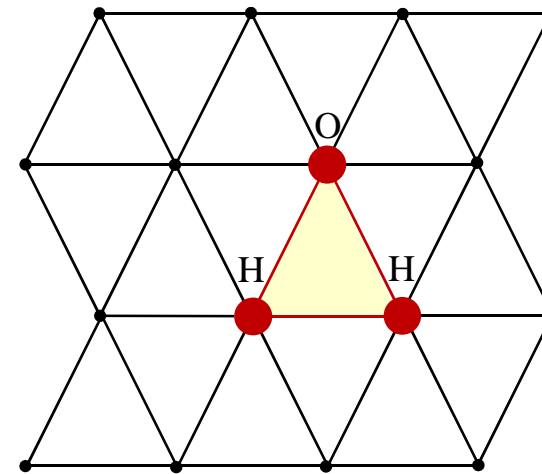
- Assumptions: - triangular lattice structure

... motivated by H₂O molecule and DNA double helix.



- Clustering is dominated by lattice structure
→ 3-dim. lattice can be approximated by a 2-dim. one (25x25 sites)
- DNA molecule can be substituted by H₂O molecules.

- Further assumptions: - SSB if 1, 2, or 3 ionisations of the same H₂O molecule took place.



- DSB if ionisations belong to 2 or more molecules

- $q = 1$

- $p \Leftrightarrow$ ionisation probability W ; $W = \omega \cdot \sigma_{\text{ion}}$

↑
number of atoms (sites) per area

- Cross section for single ionisation of molecules:

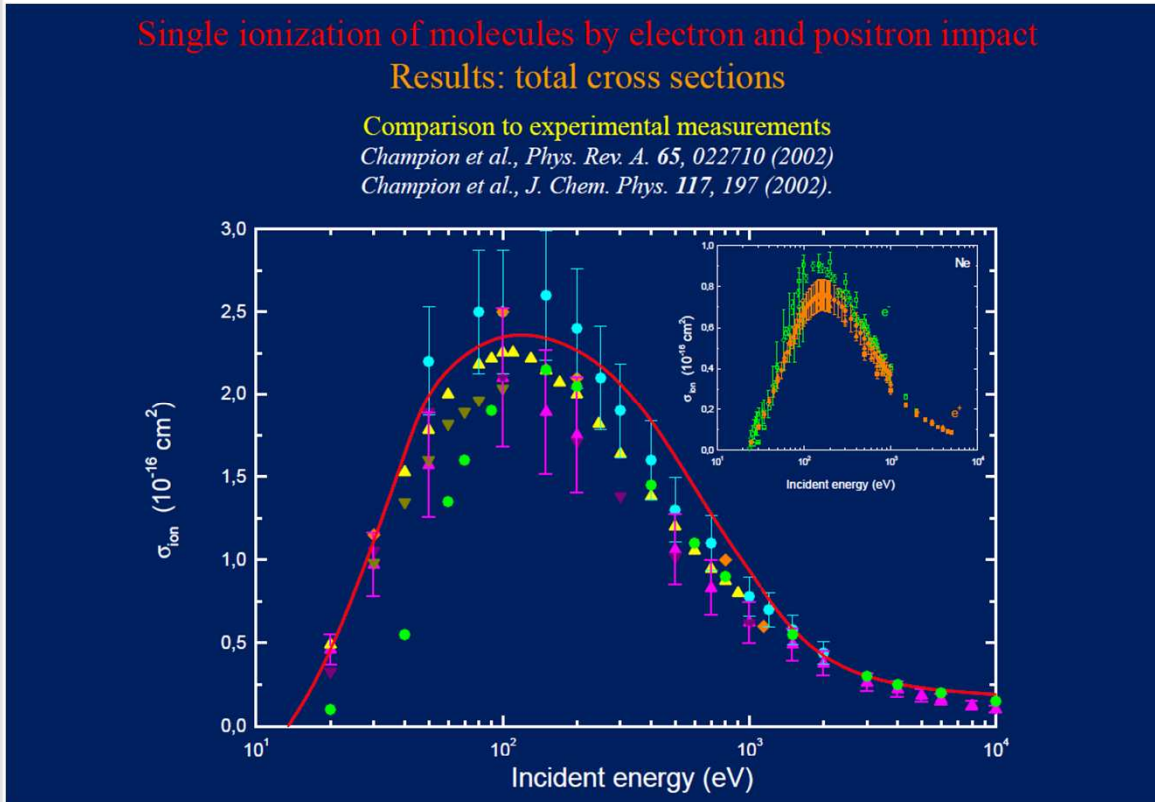
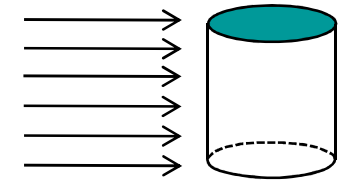


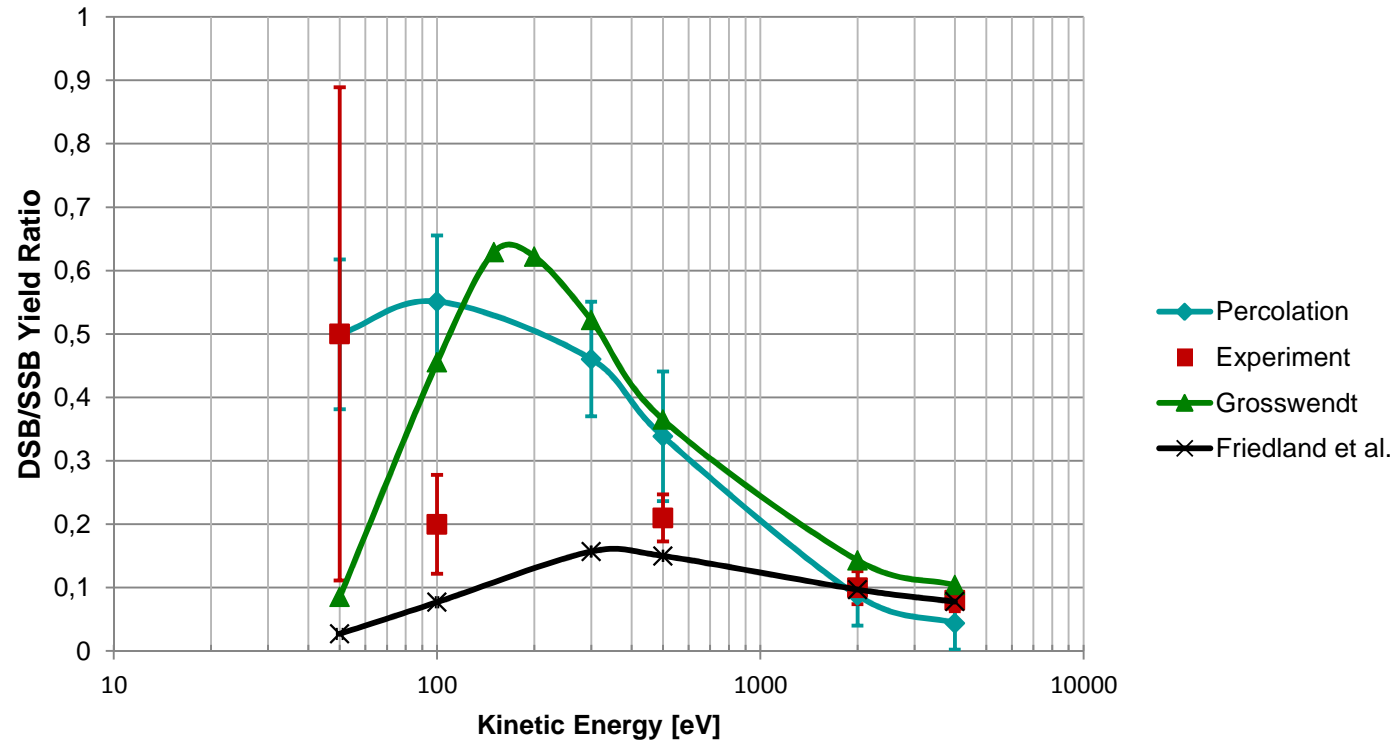
Figure taken from Ch. Champion, **GEANT4-DNA, New physics models, from cell to DNA**, lecture, KIT - Basic Training Course For Micro- and Nanodosimetry, Oct. 2011.

Kinetic energy [MeV]	Occupation probability	Cross section [10^8 b]
0.05	0.1711	2.0
0.10	0.1996	2.3
0.30	0.1800	2.1
0.50	0.1392	1.6
2.00	0.0365	0.4
4.00	0.0228	0.3

➤ Result:



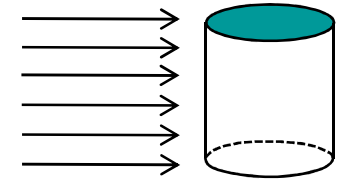
Electrons



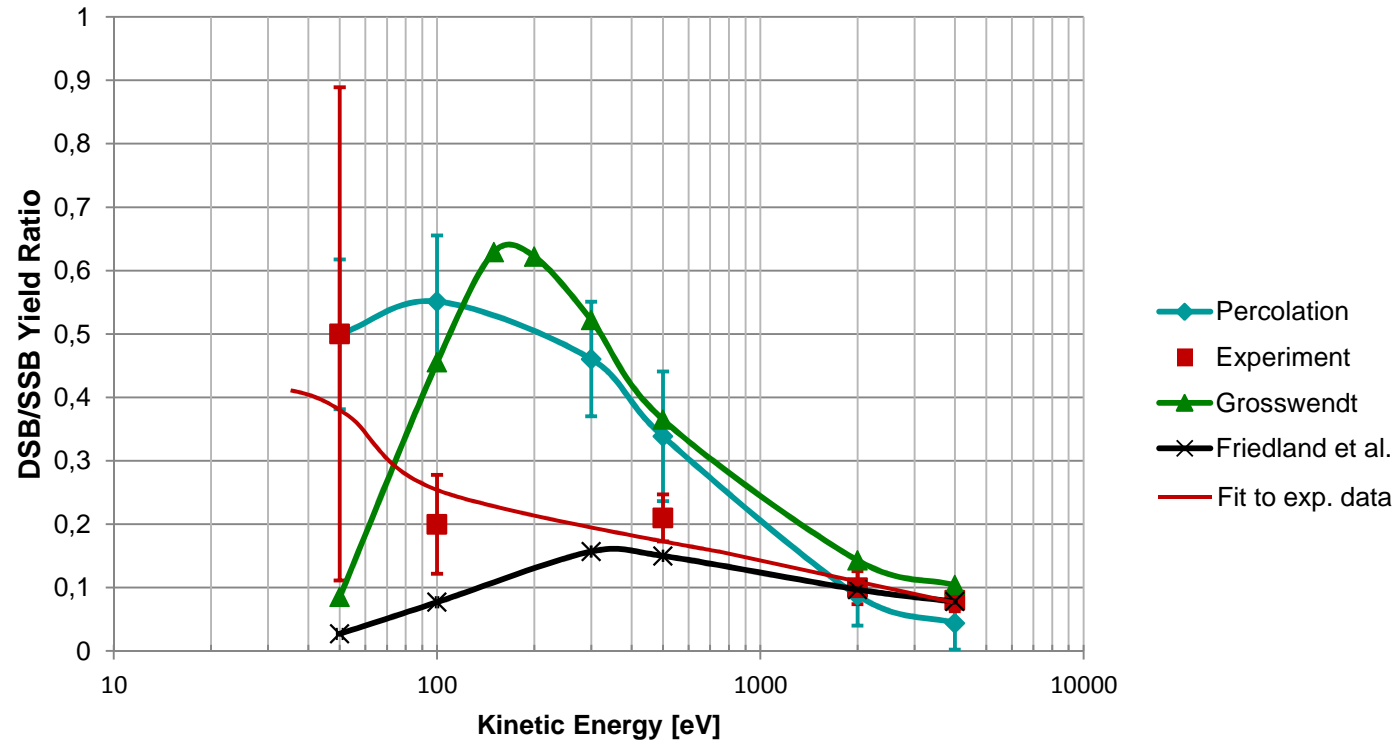
Except for the percolation model, all values above were taken from **Bernd Grosswendt, RPD 115 (2005), pp. 1 – 9).**

Experiment (irradiation of pBR322 plasmid DNA) was done by **Folkard et al., Int. J. Radiat. Biol. 64 (1993), pp. 651 - 658.**

➤ Result :



Electrons



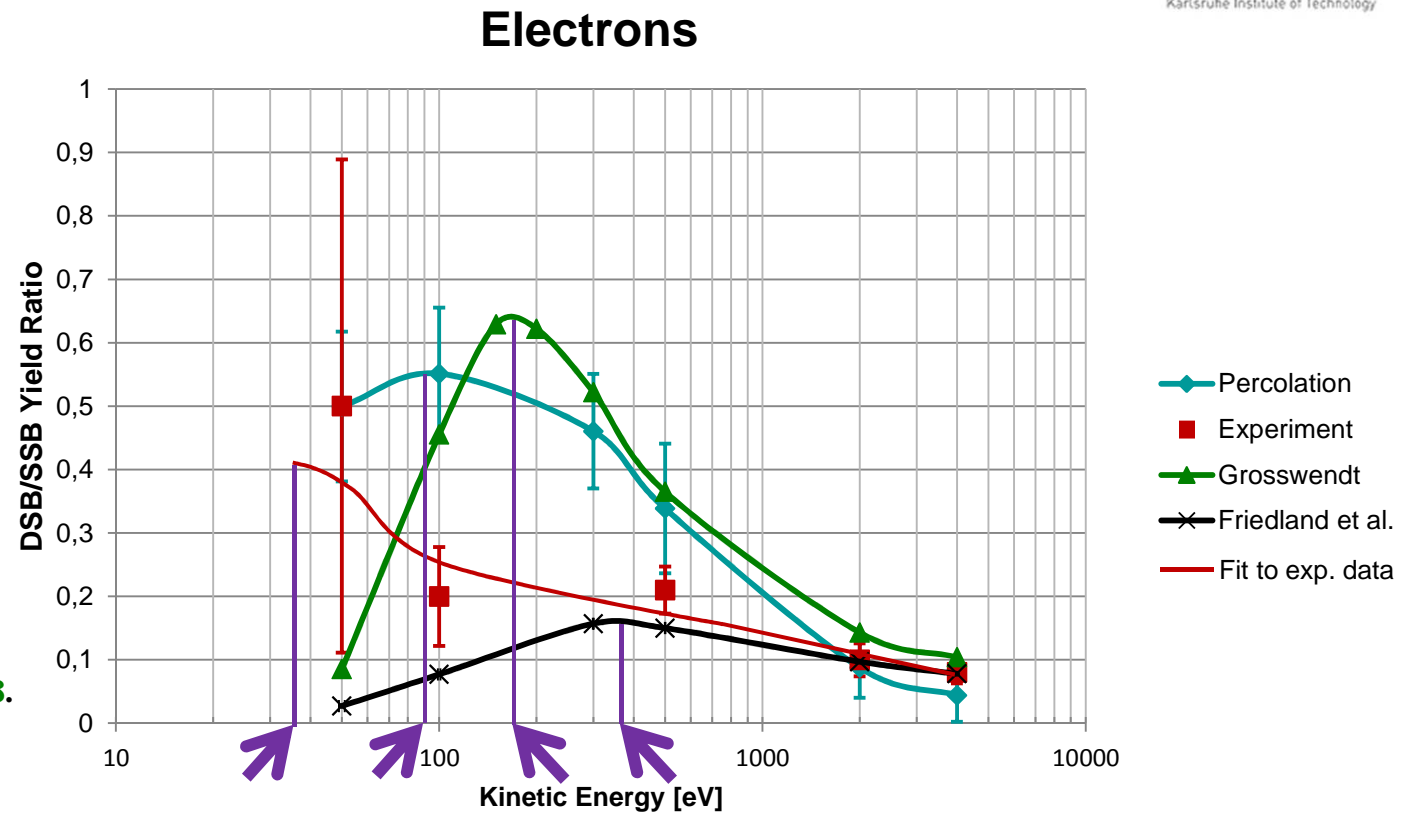
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➤ Result and Conclusion :

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➤ Percolation model values agree similarly well with the experimental values like that of Grosswendt or Friedland et al.

Essential input of the percolation model only was: **geometry** and $p \leftrightarrow \sigma_{ion}$.

CAUTION: Percolation model has not sufficiently been tested up to now!

Thank you!

Ant Nebula (Mz 3)

