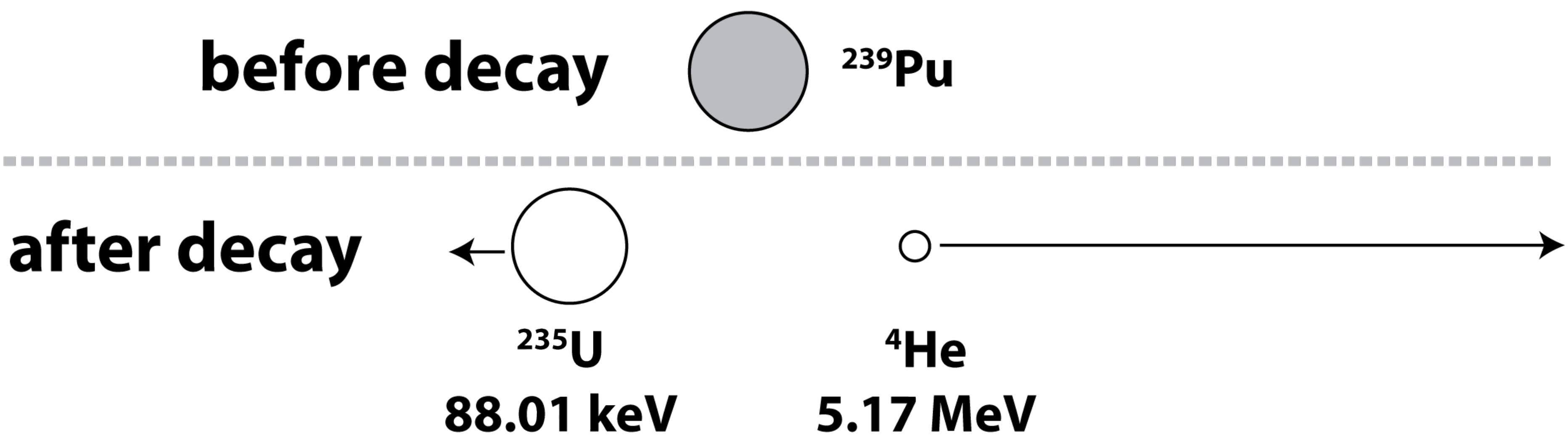
Phase Transformation Rate Theory – Semiconductors and Ceramics



before decay
^{239}Pu
after decay
^{235}U
88.01 keV
^{4}He
5.17 MeV

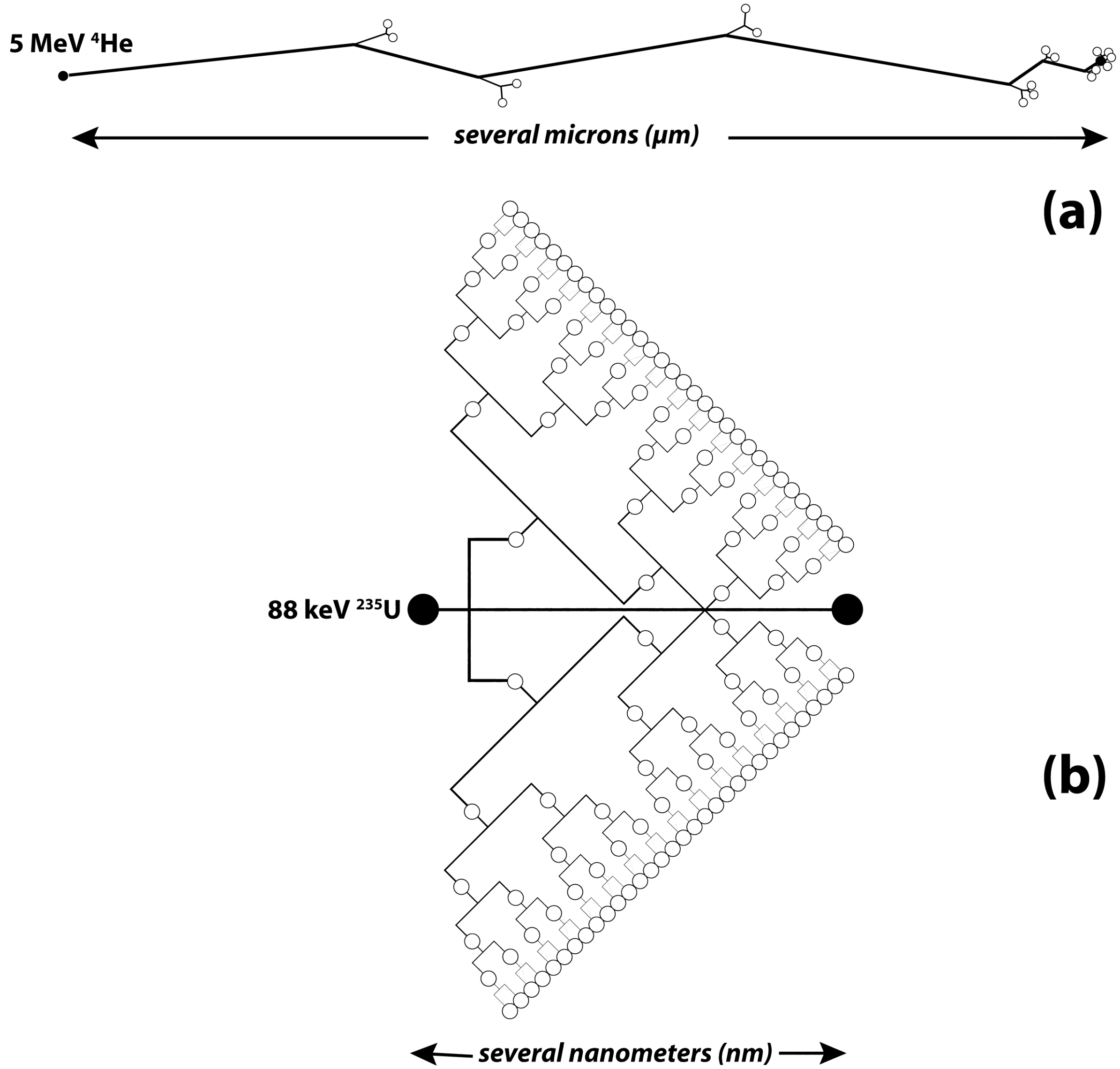
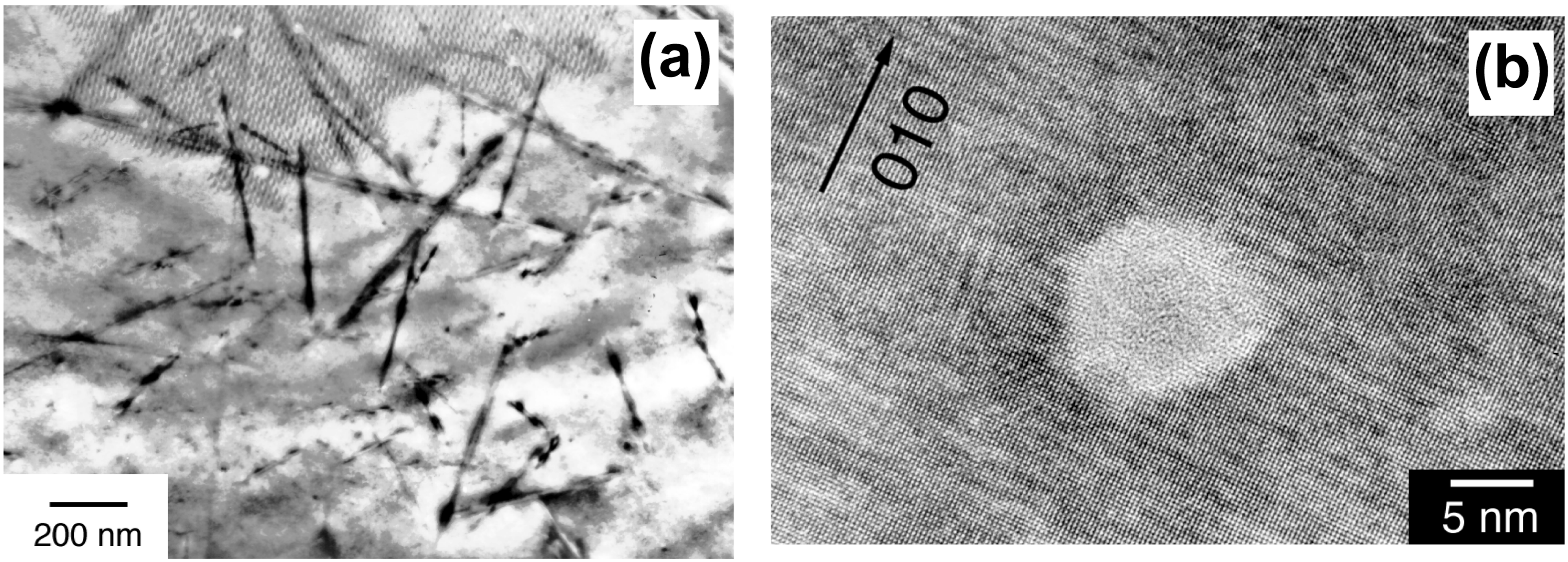
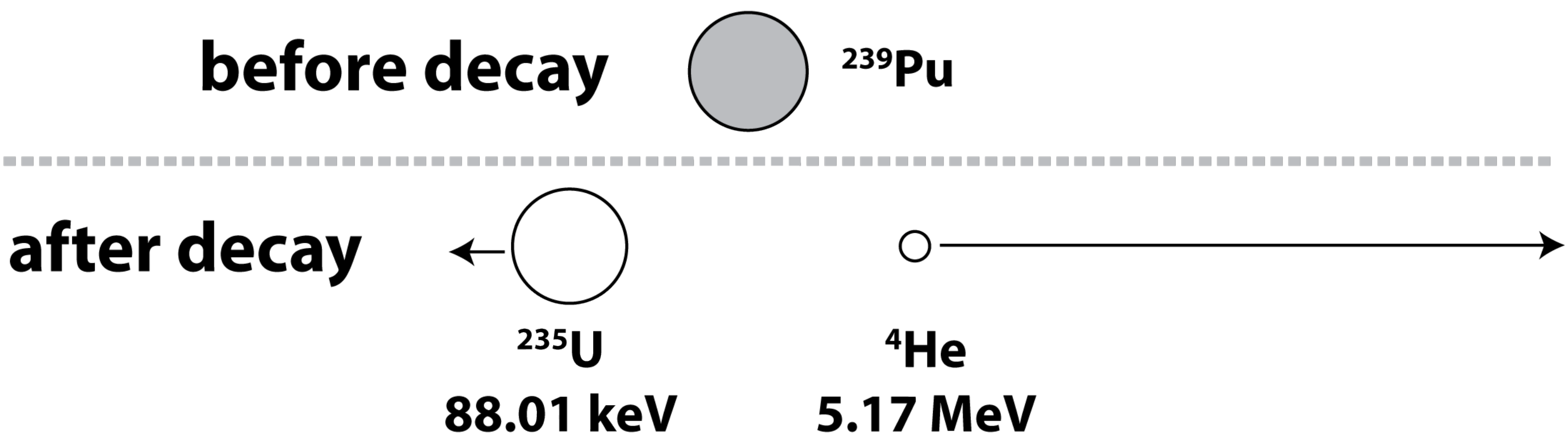


Figure 5.4. Schematic drawings of cascade geometries for **(a)** a high-energy light ion such as a 5 MeV ^{4}He ion and **(b)** a moderate energy heavy ion such as an 88 keV ^{235}U ion. The light ion (a) produces a *dilute* displacement cascade with a characteristic "pearls-on-a-string" geometry. The heavy ion (b) produces a *dense* cascade in which all the atoms in the interior of the cascade are set in motion in a process known as a *displacement spike*.



(a)
200 nm
(b)
010
5 nm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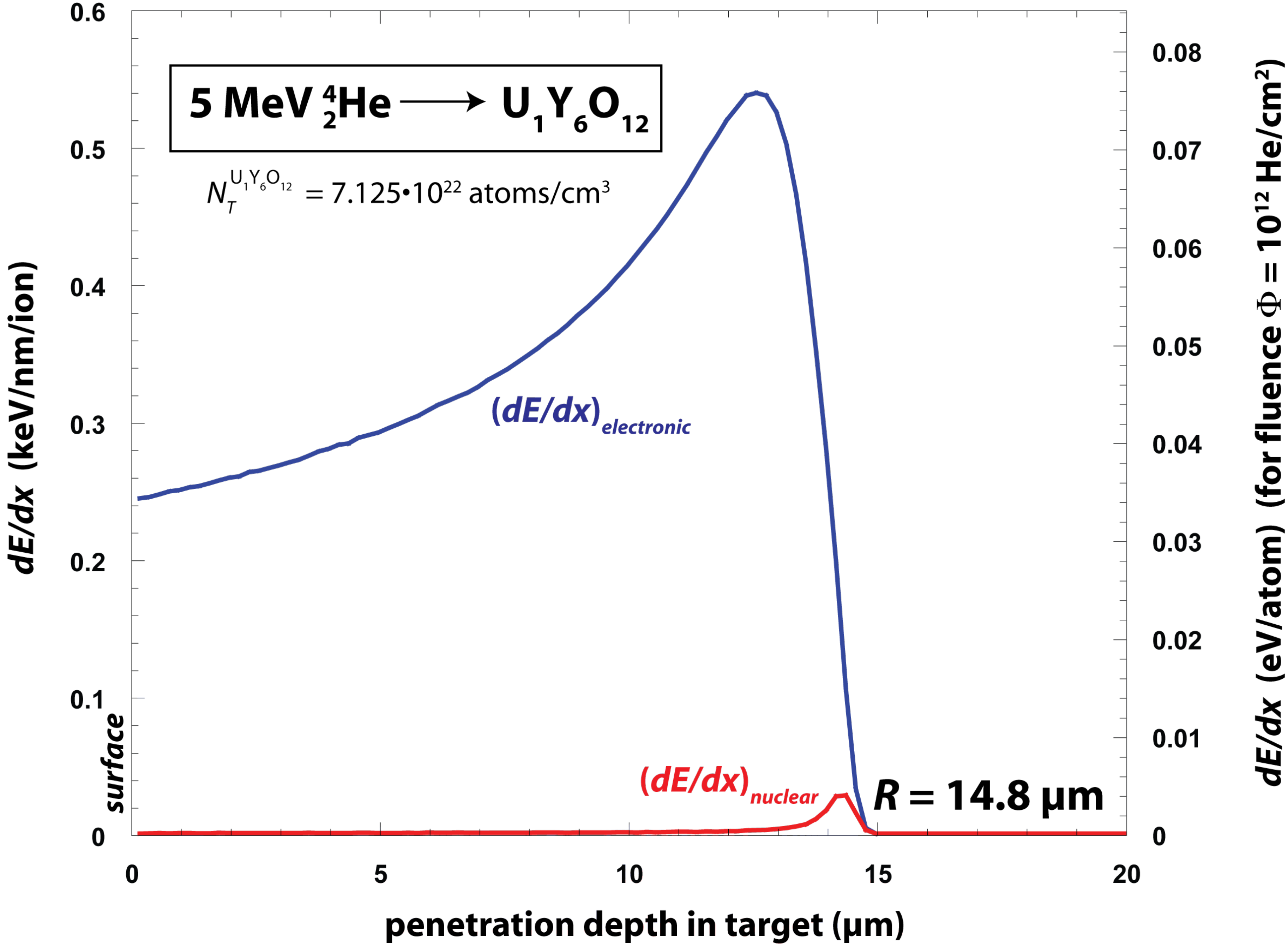
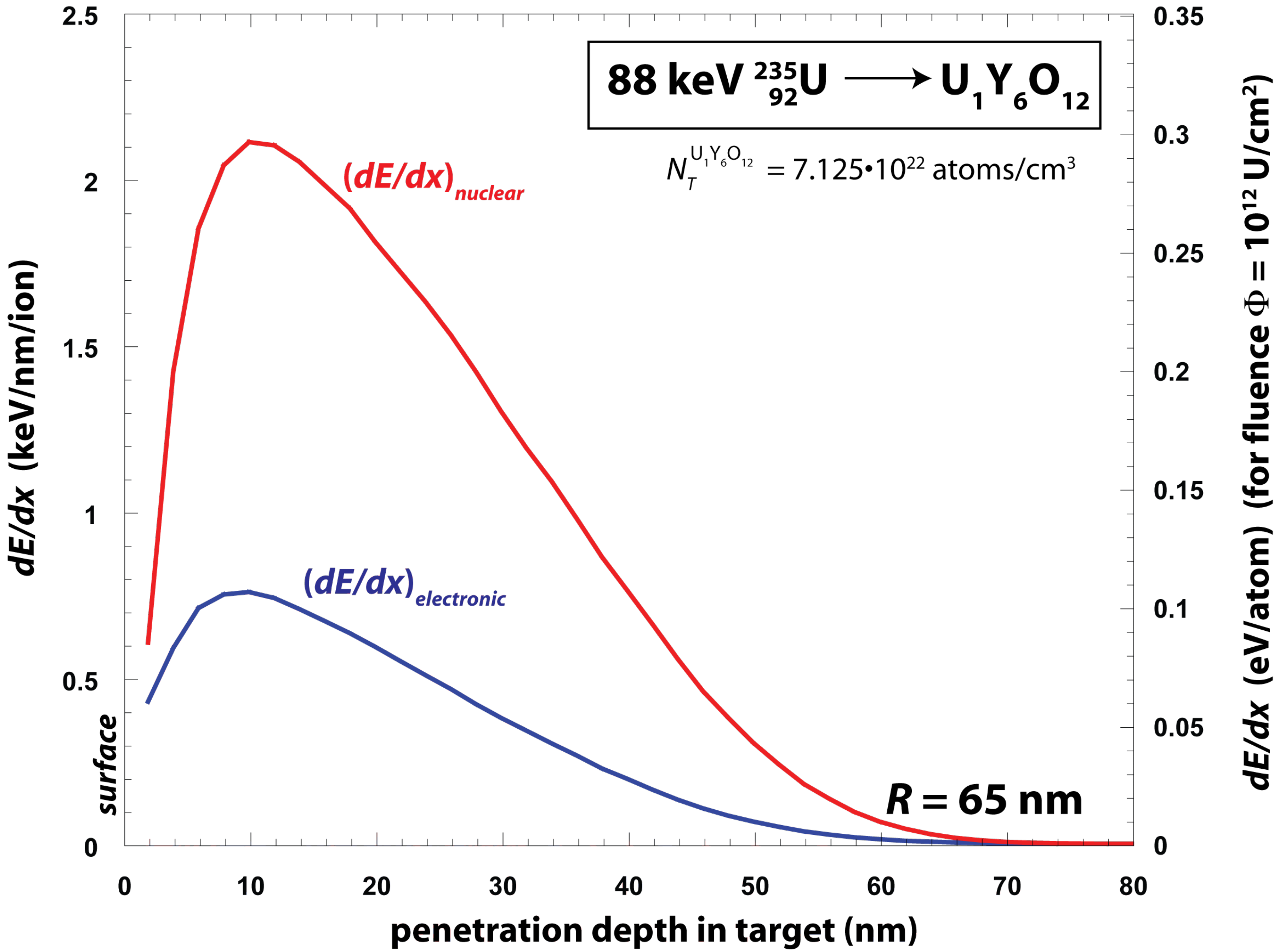
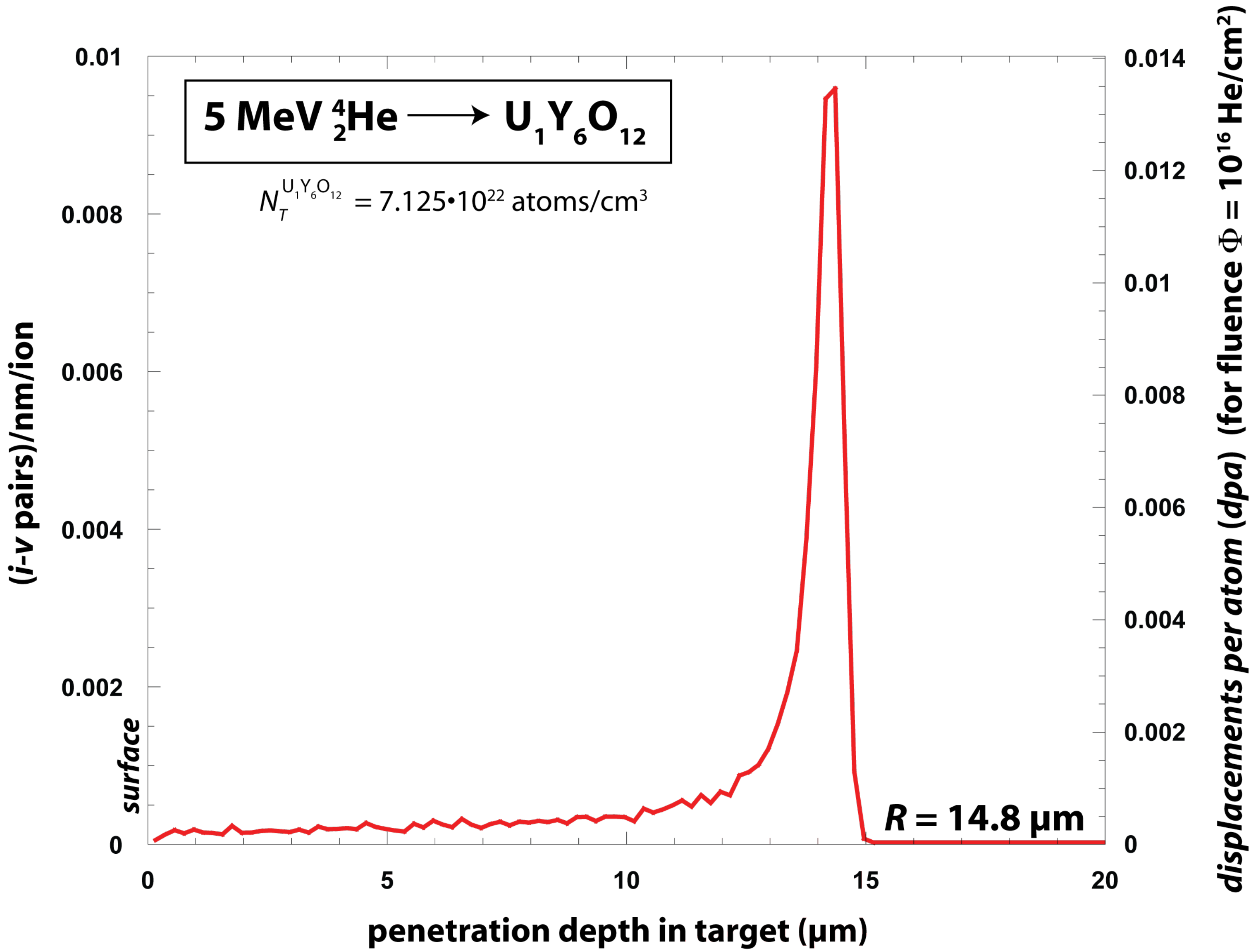


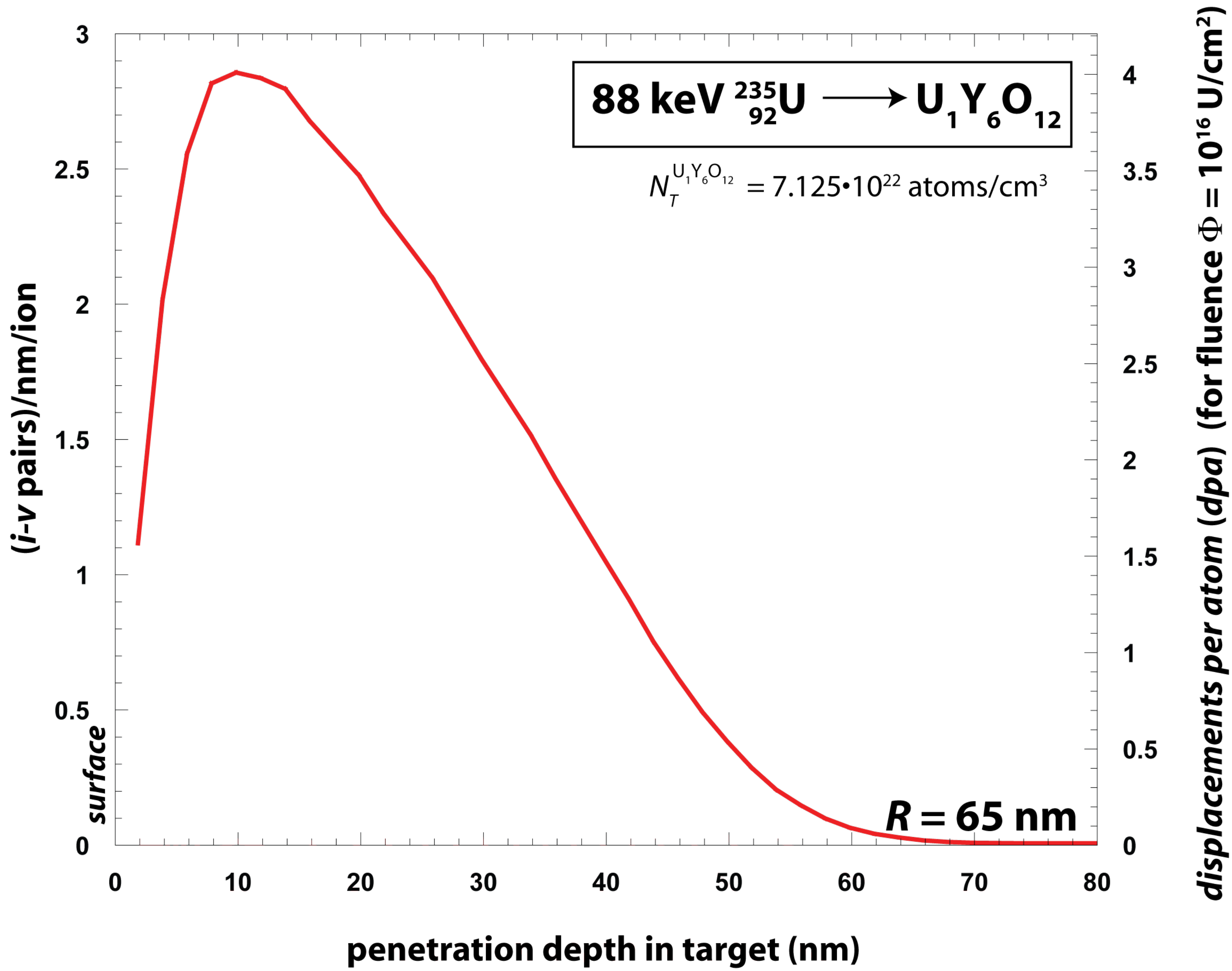
5 MeV $^4_2He \longrightarrow U_1Y_6O_{12}$
$N_T^{U_1Y_6O_{12}} = 7.125 \cdot 10^{22}$ atoms/cm^3
$(dE/dx)_{electronic}$
$(dE/dx)_{nuclear}$
$R = 14.8$ μm
surface
dE/dx (keV/nm/ion)
dE/dx (eV/atom) (for fluence $\Phi = 10^{12}$ He/cm^2)
penetration depth in target (μm)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
5
10
15
20



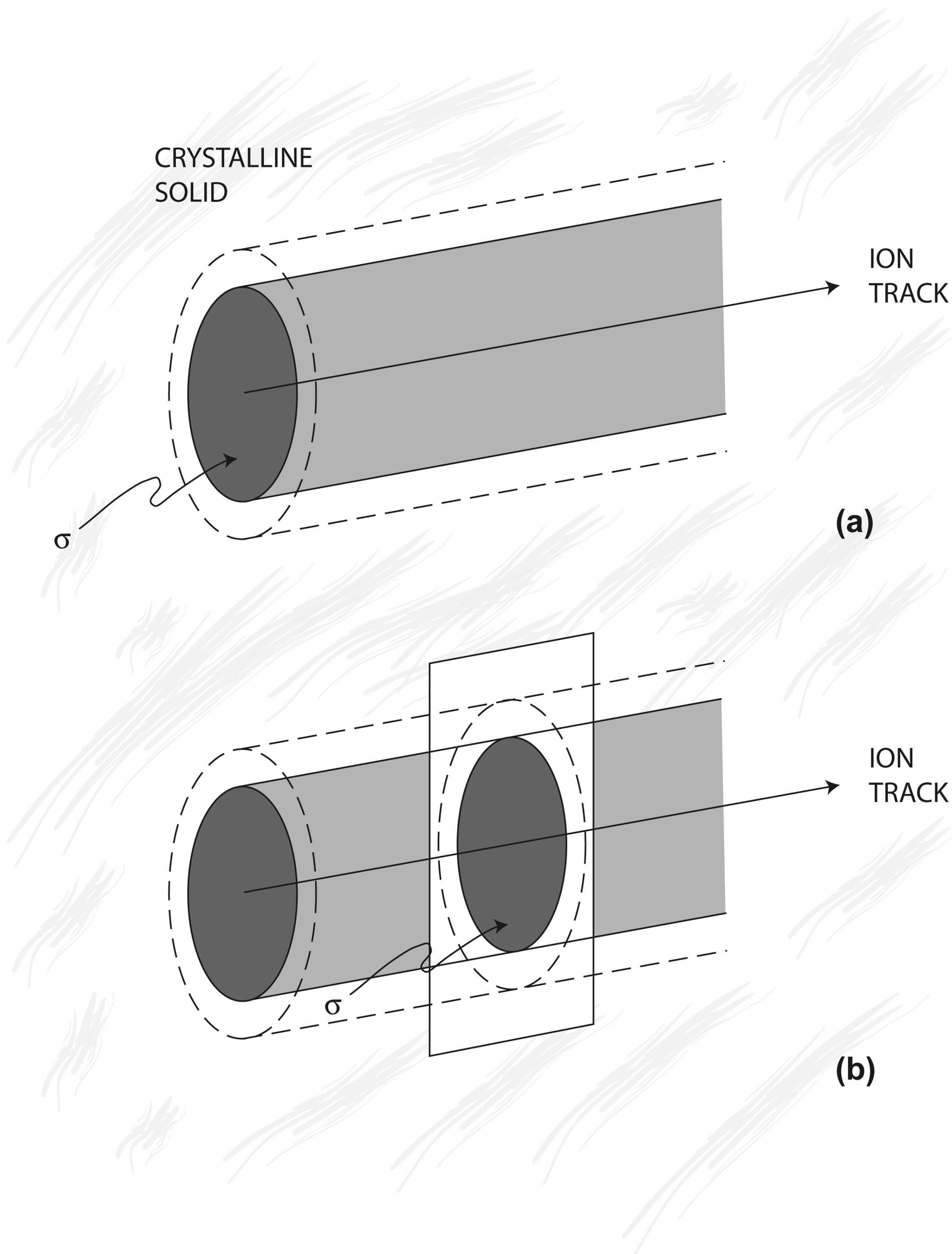
88 keV $^{235}_{92}U \longrightarrow U_1Y_6O_{12}$
$N_T^{U_1Y_6O_{12}} = 7.125 \cdot 10^{22}$ atoms/cm^3
$(dE/dx)_{nuclear}$
$(dE/dx)_{electronic}$
$R = 65$ nm
surface
dE/dx (keV/nm/ion)
dE/dx (eV/atom) (for fluence $\Phi = 10^{12}$ U/cm^2)
penetration depth in target (nm)
0
0.5
1
1.5
2
2.5
0.05
0.1
0.15
0.2
0.25
0.3
0.35
10
20
30
40
50
60
70
80

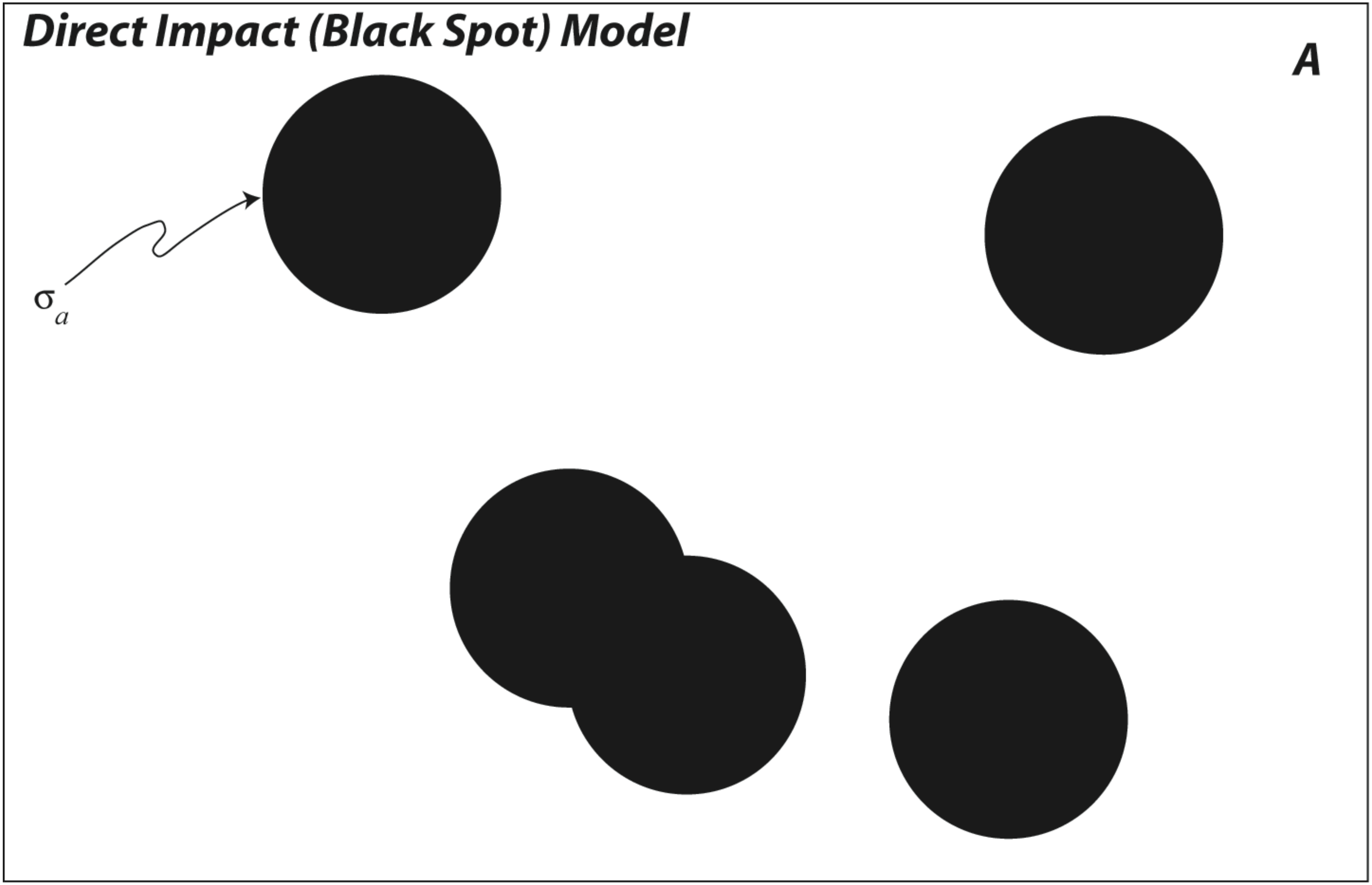


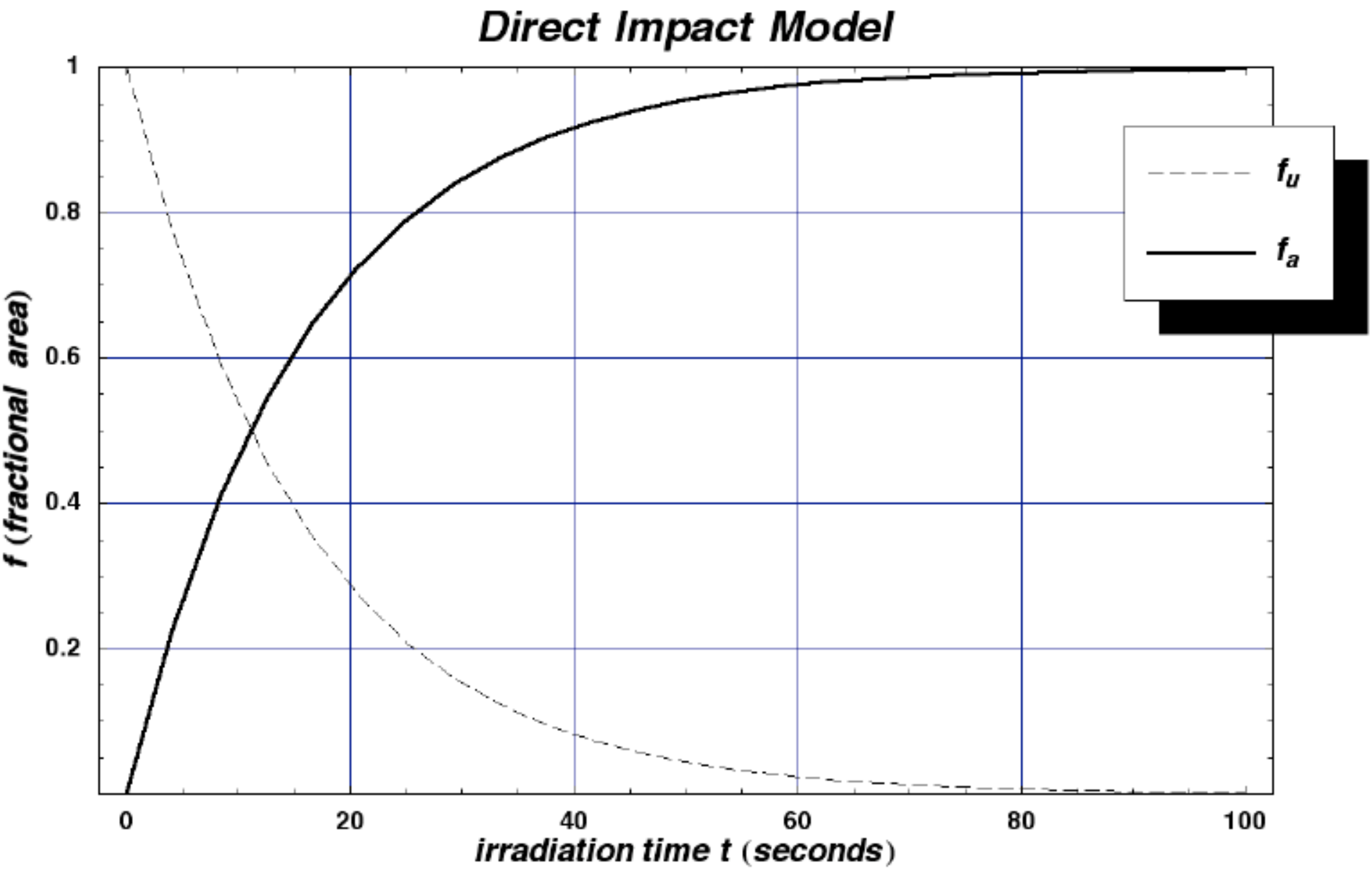
5 MeV ^4_2He → $U_1Y_6O_{12}$
$N_T^{U_1Y_6O_{12}}$ = 7.125•10^{22} atoms/cm^3
(i-v pairs)/nm/ion
displacements per atom (dpa) (for fluence Φ = 10^{16} He/cm^2)
penetration depth in target (μm)
surface
R = 14.8 μm
0.01
0.008
0.006
0.004
0.002
0
0.014
0.012
0.01
0.008
0.006
0.004
0.002
0
0
5
10
15
20



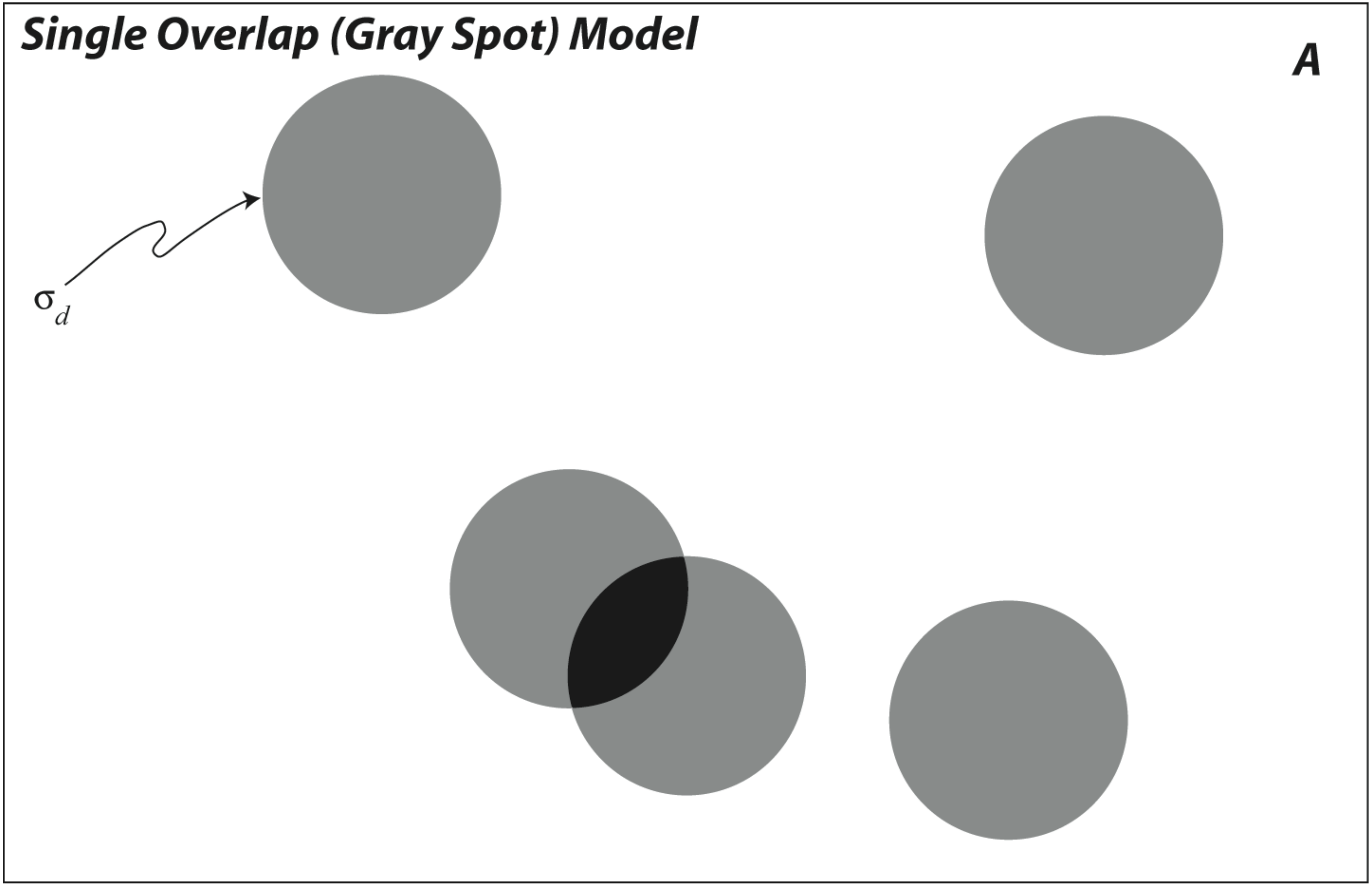
88 keV $^{235}_{92}U \longrightarrow U_1Y_6O_{12}$
$N_T^{U_1Y_6O_{12}} = 7.125 \cdot 10^{22}$ atoms/cm^3
R = 65 nm
surface
(*i-v* pairs)/nm/ion
displacements per atom (*dpa*) (for fluence $\Phi = 10^{16}$ U/cm^2)
penetration depth in target (nm)
0
10
20
30
40
50
60
70
80
0.5
1
1.5
2
2.5
3
3.5
4

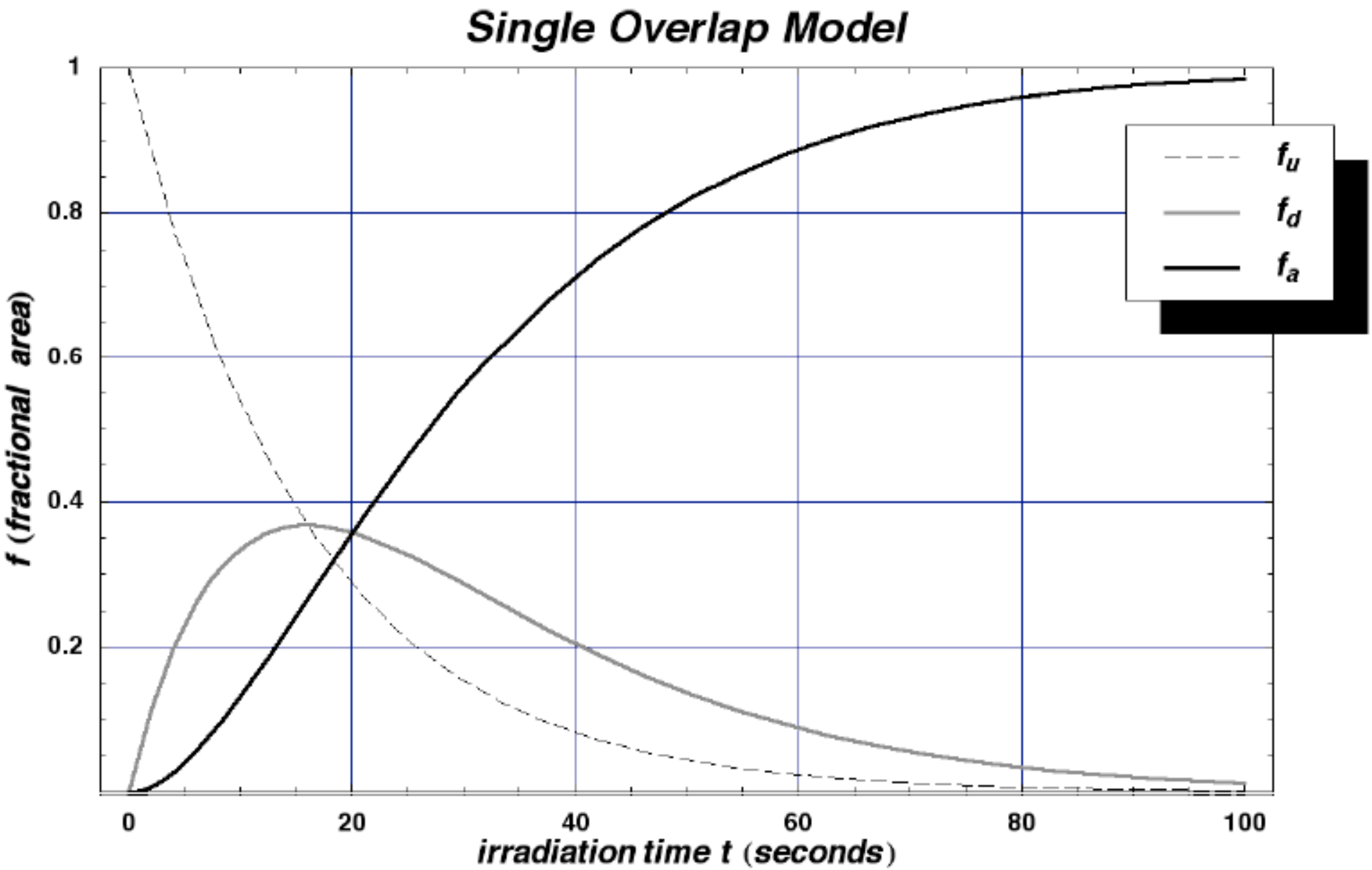

CRYSTALLINE
SOLID
ION
TRACK
σ
(a)
ION
TRACK
σ
(b)


Direct Impact (Black Spot) Model
A
σ a

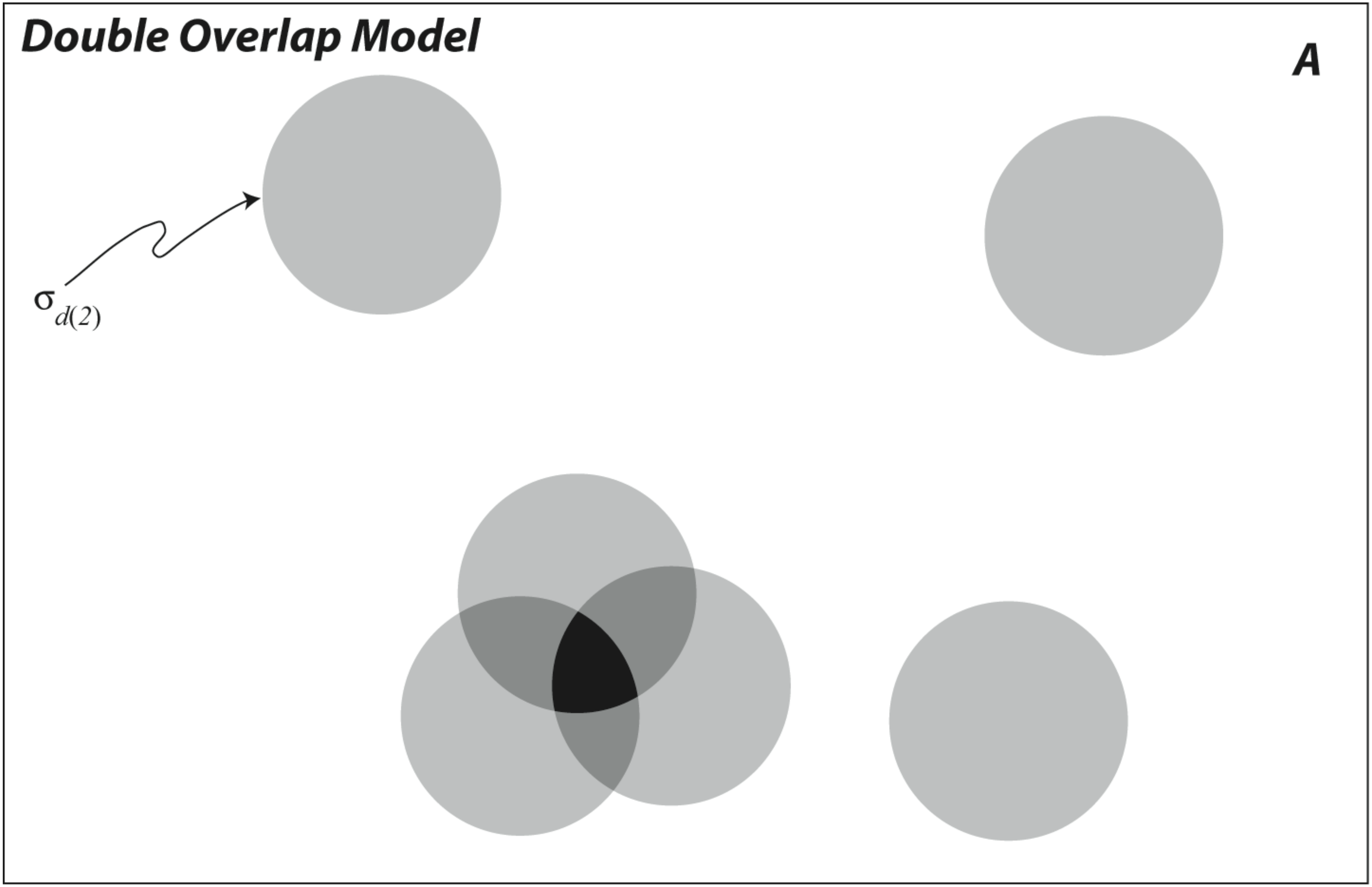


Direct Impact Model
f (fractional area)
irradiation time t (seconds)
1
0.8
0.6
0.4
0.2
0
20
40
60
80
100
f_u
f_a

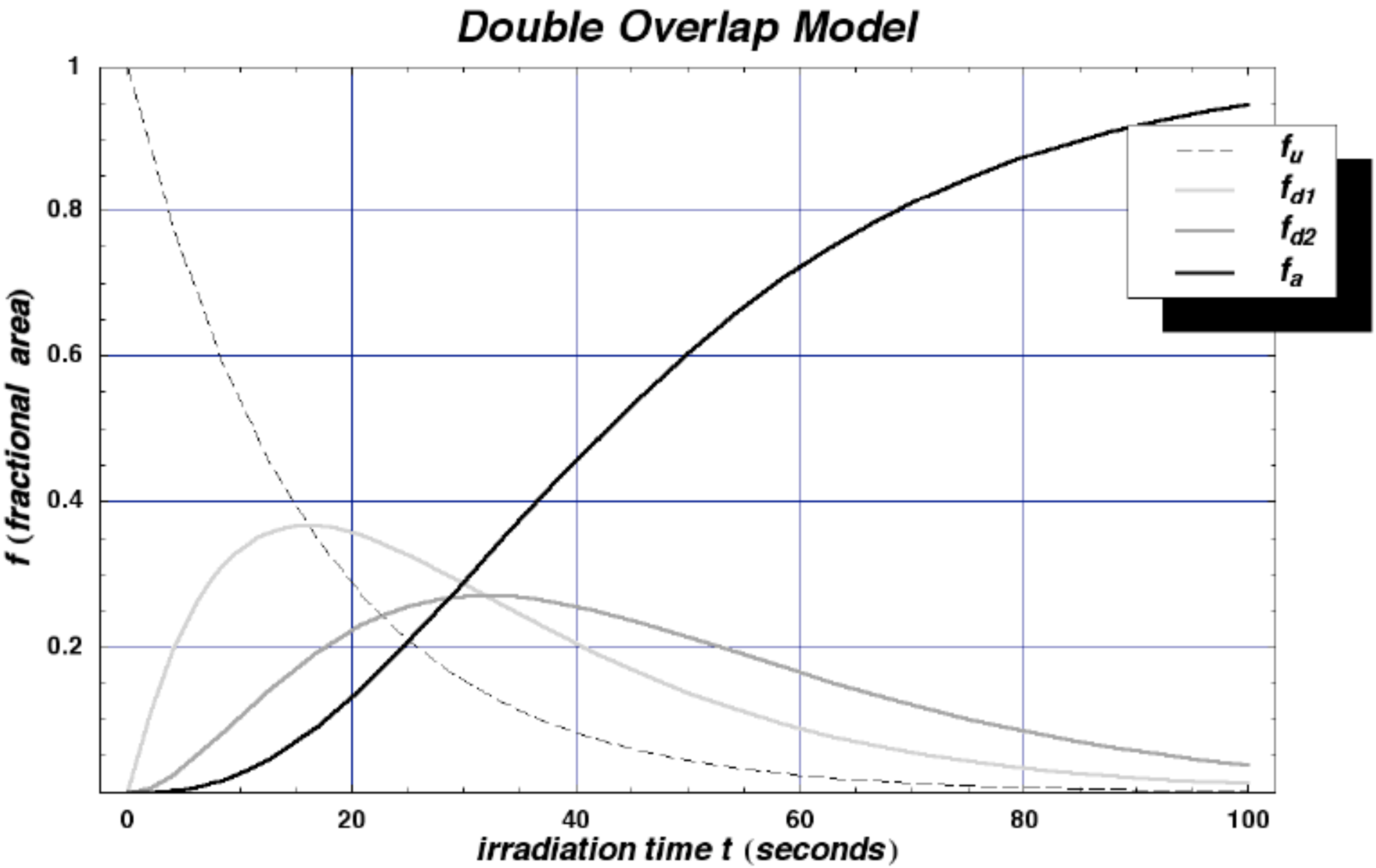

Single Overlap (Gray Spot) Model
A
σ d



$$\sigma_d = 6.25 \cdot 10^{-14}\ \text{cm}^2 \quad ; \quad \varphi = 10^{12}\ \text{ions}/\text{cm}^2 \cdot \text{s}$$

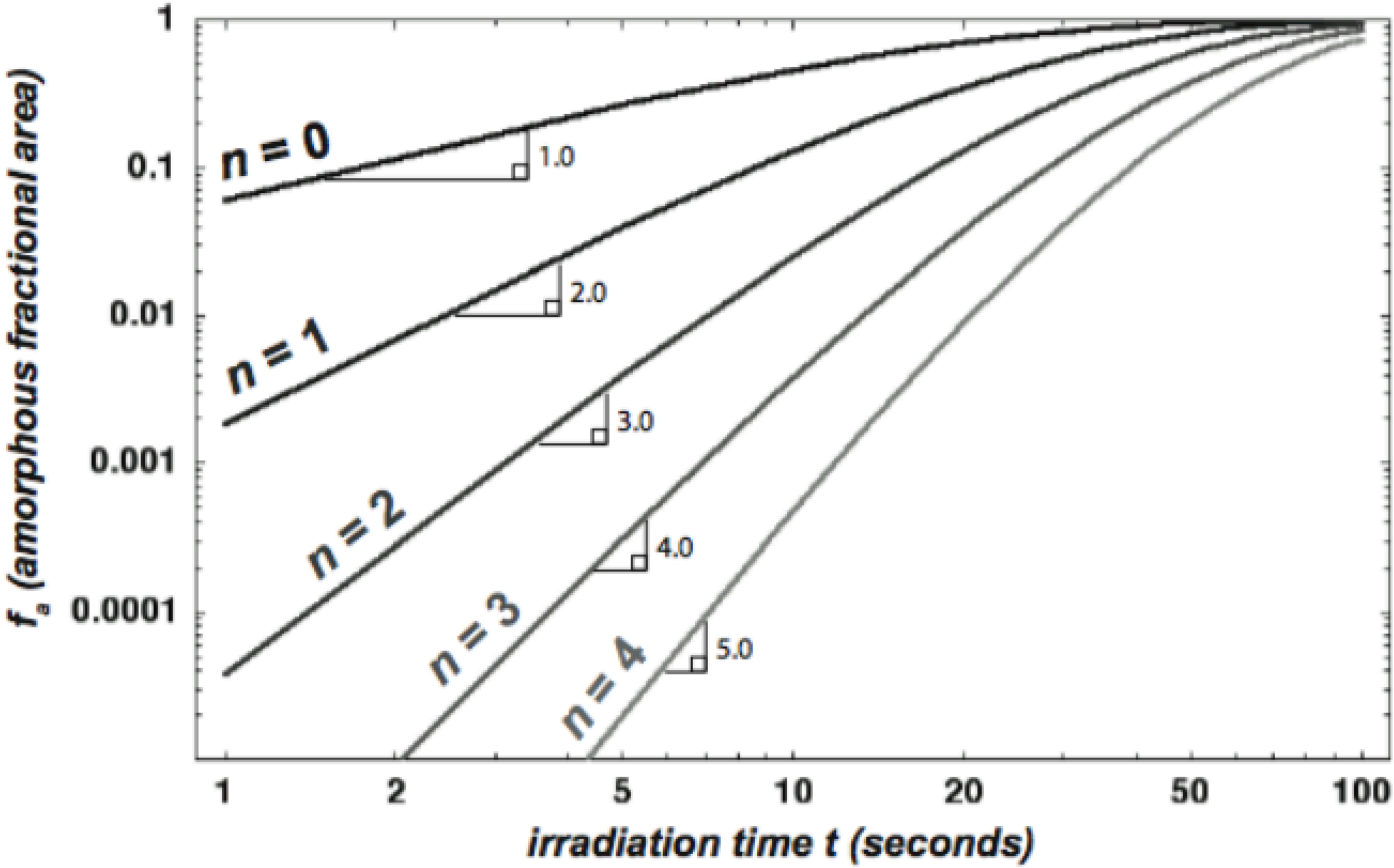


Double Overlap Model
A
$\sigma_{d(2)}$

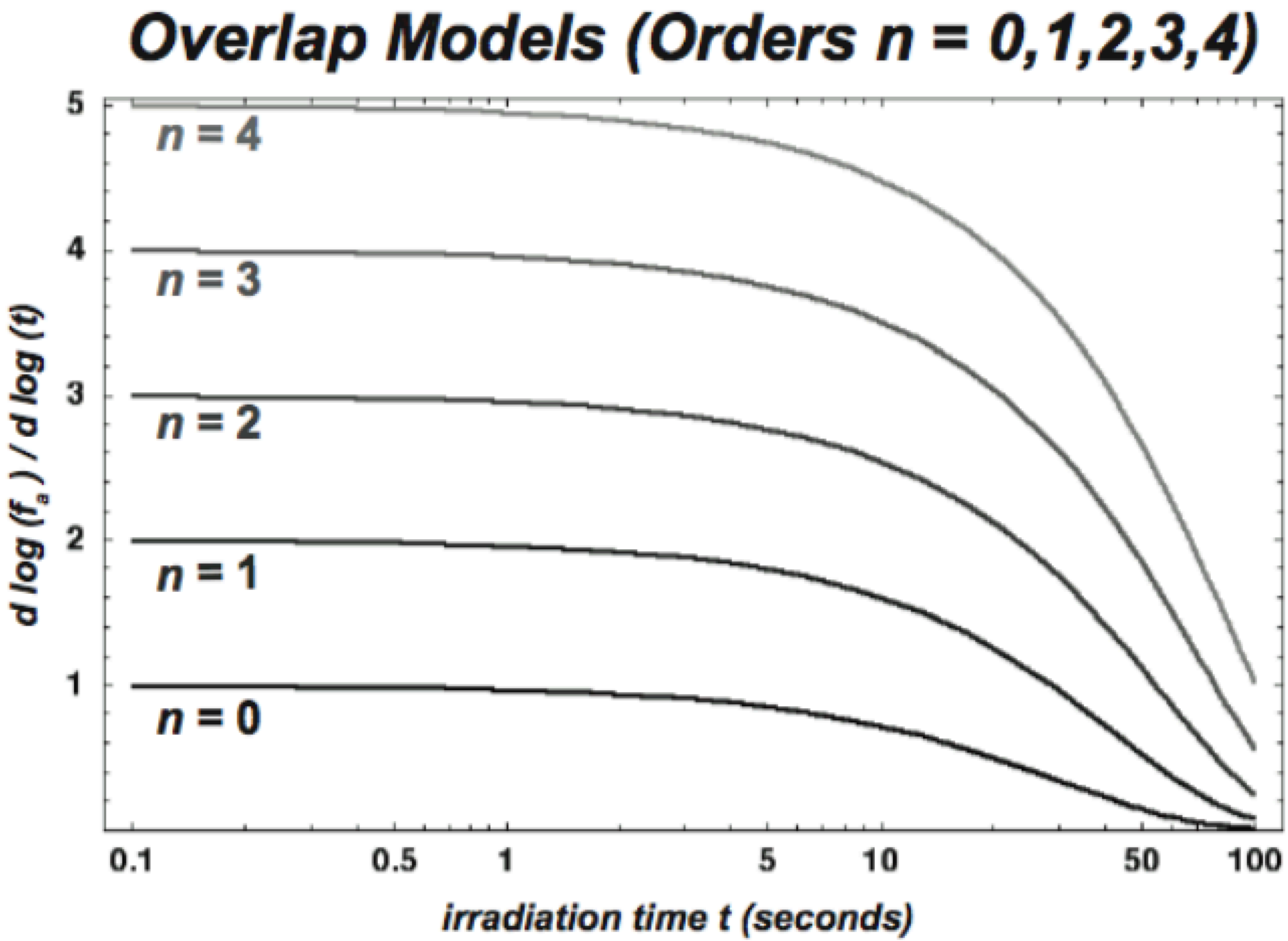


$$\sigma_d = 6.25 \cdot 10^{-14}\ \text{cm}^2 \quad ; \quad \varphi = 10^{12}\ \text{ions}/\text{cm}^2 \cdot \text{s}$$

Overlap Models (Orders n = 0,1,2,3,4)

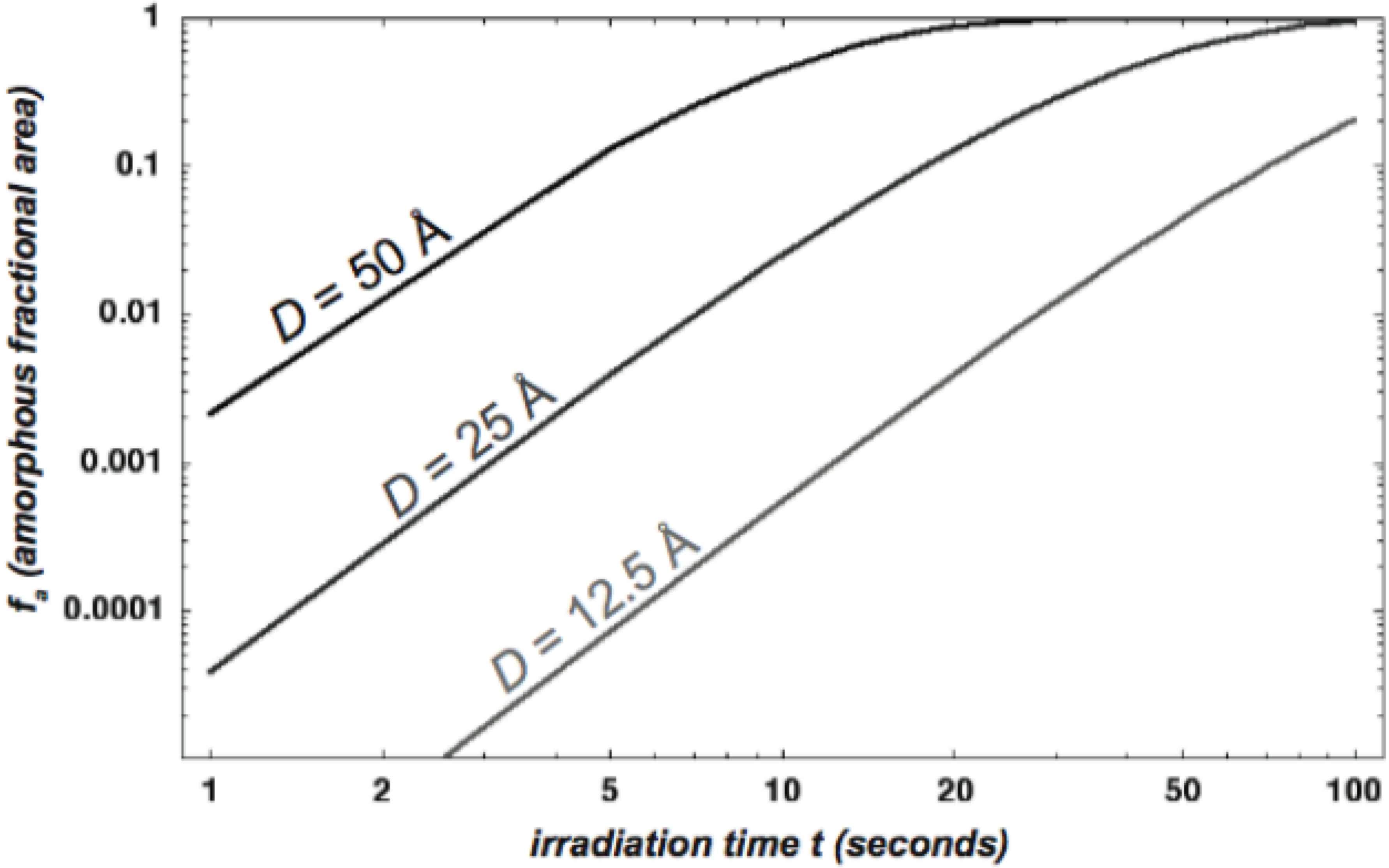


$$\sigma_d = 6.25 \cdot 10^{-14}\ \text{cm}^2 \quad ; \quad \varphi = 10^{12}\ \text{ions}/\text{cm}^2 \cdot \text{s}$$



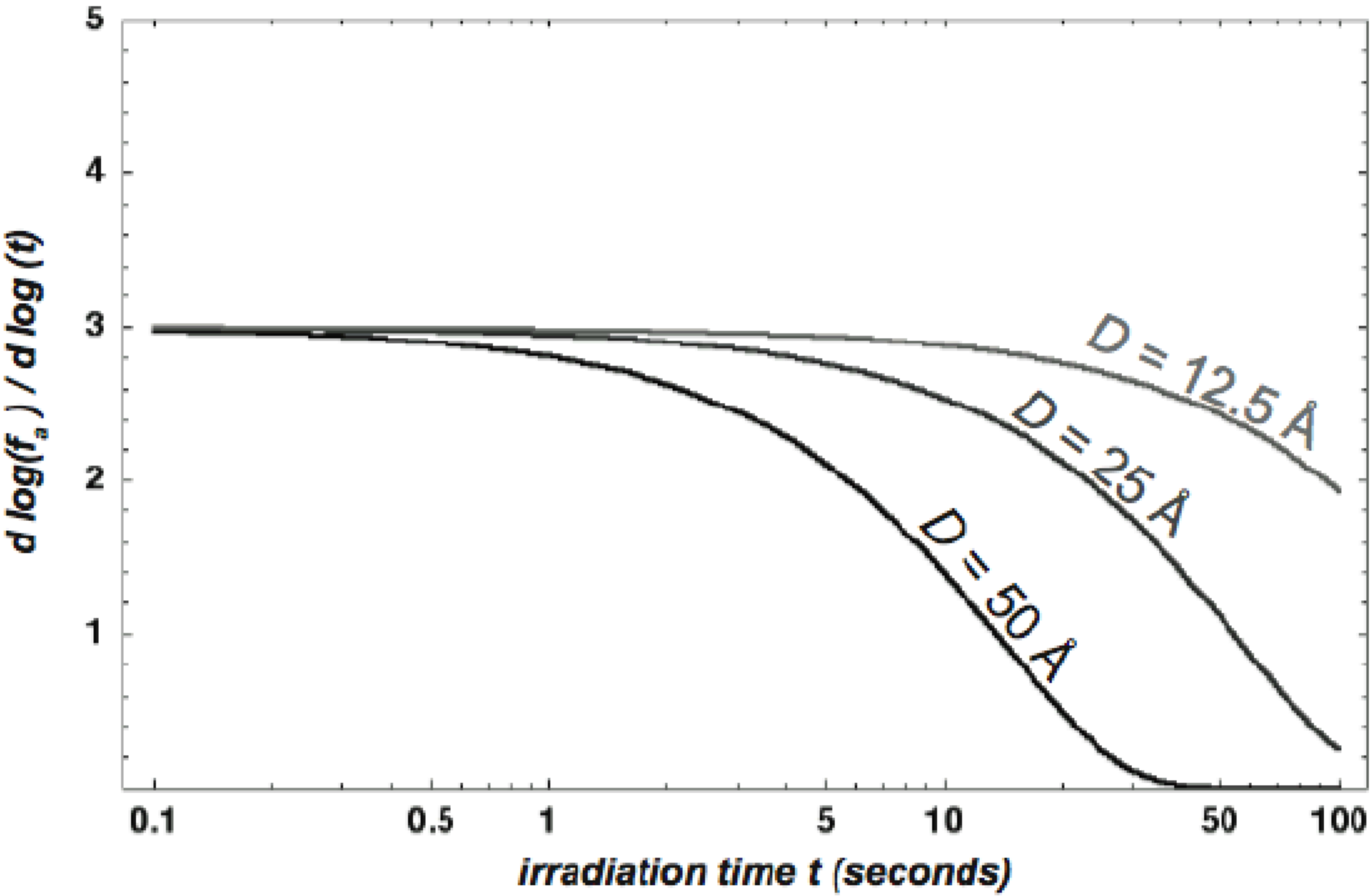
$$\sigma_d = 6.25 \cdot 10^{-14}\ \mathrm{cm}^2 \quad ; \quad \varphi = 10^{12}\ \mathrm{ions}/\mathrm{cm}^2 \cdot \mathrm{s}$$

Double Overlap Model, Different Size Cascades

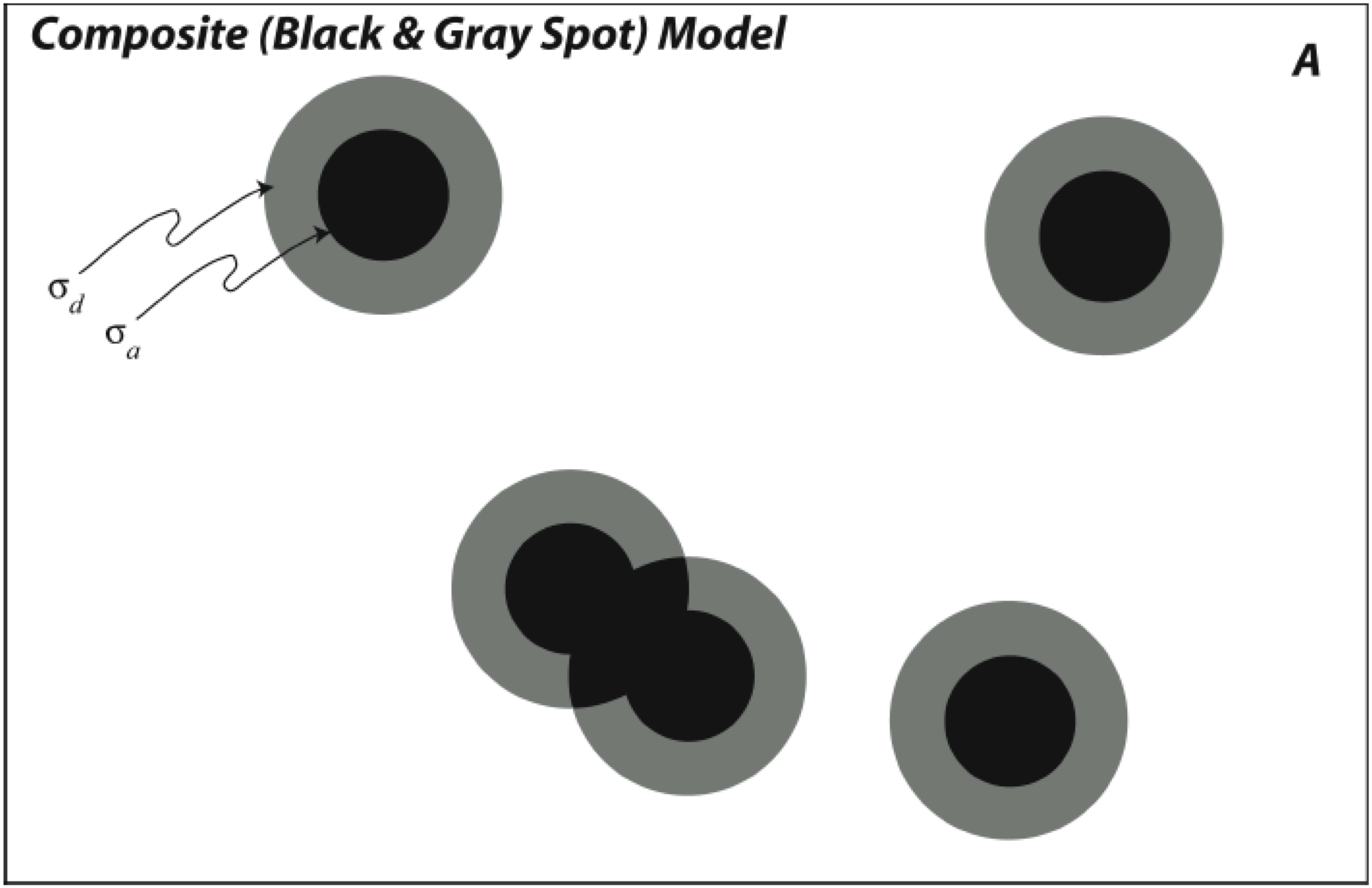


$$\sigma_d = \{1.5625, 6.25, 2.5\} \cdot 10^{-14}\ \mathrm{cm}^2 \quad ; \quad \varphi = 10^{12}\ \mathrm{ions}/\mathrm{cm}^2 \cdot \mathrm{s}$$

Double Overlap Model, Different Size Cascades



$$\sigma_d = \{1.5625, 6.25, 2.5\} \cdot 10^{-14}\ \text{cm}^2 \quad ; \quad \varphi = 10^{12}\ \text{ions}/\text{cm}^2 \cdot \text{s}$$


Composite (Black & Gray Spot) Model
A
σd
σa

$$\frac{df_u}{dt} = -\left(P_d + P_a\right) f_u$$

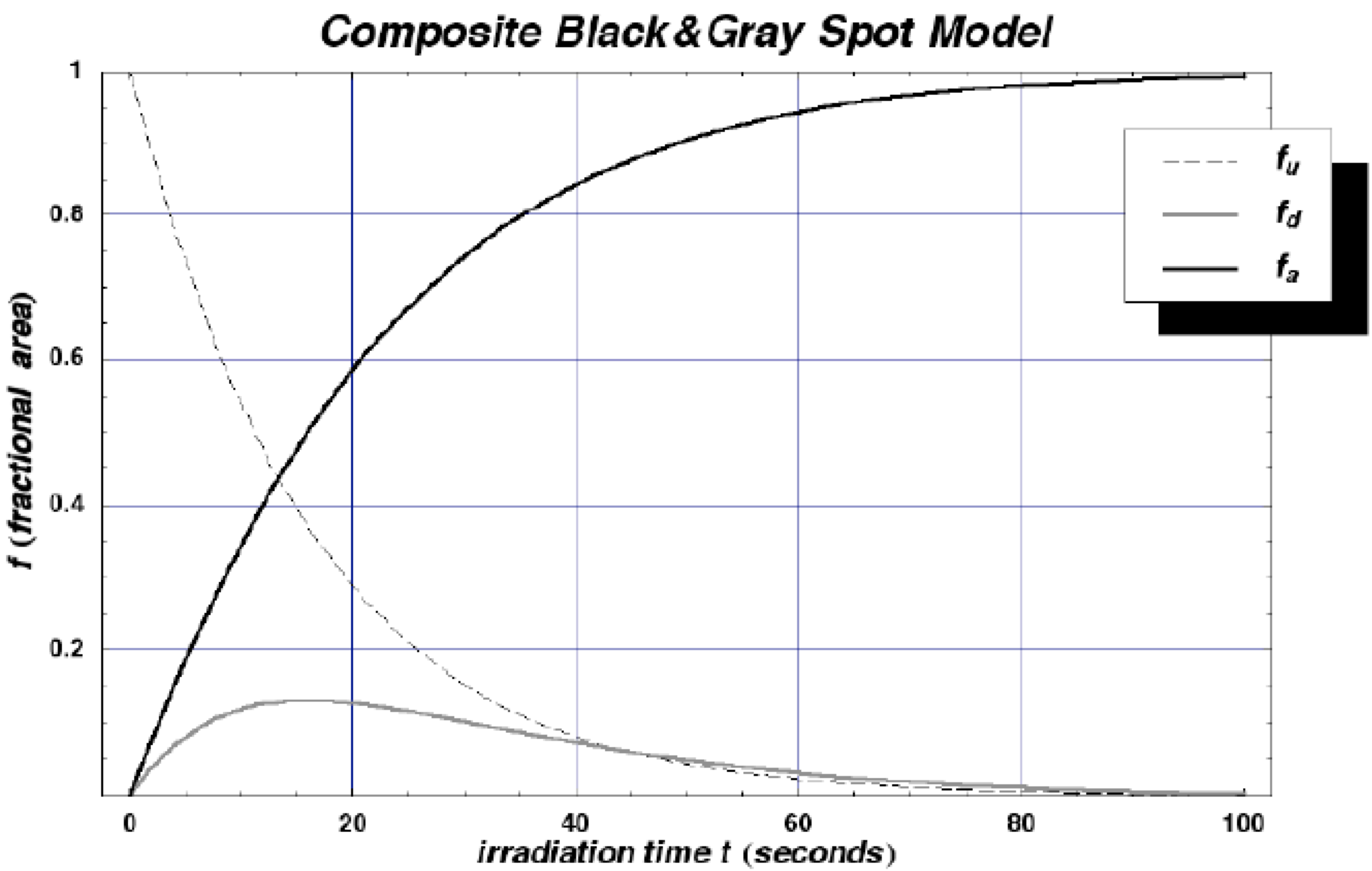
$$\frac{df_d}{dt} = +P_d\ f_u - \left(P_d + P_a\right) f_d$$

$$\frac{df_a}{dt} = +P_a\ f_u + \left(P_d + P_a\right) f_d$$

$$f_u(t) = e^{-\left(P_d + P_a\right)t}$$

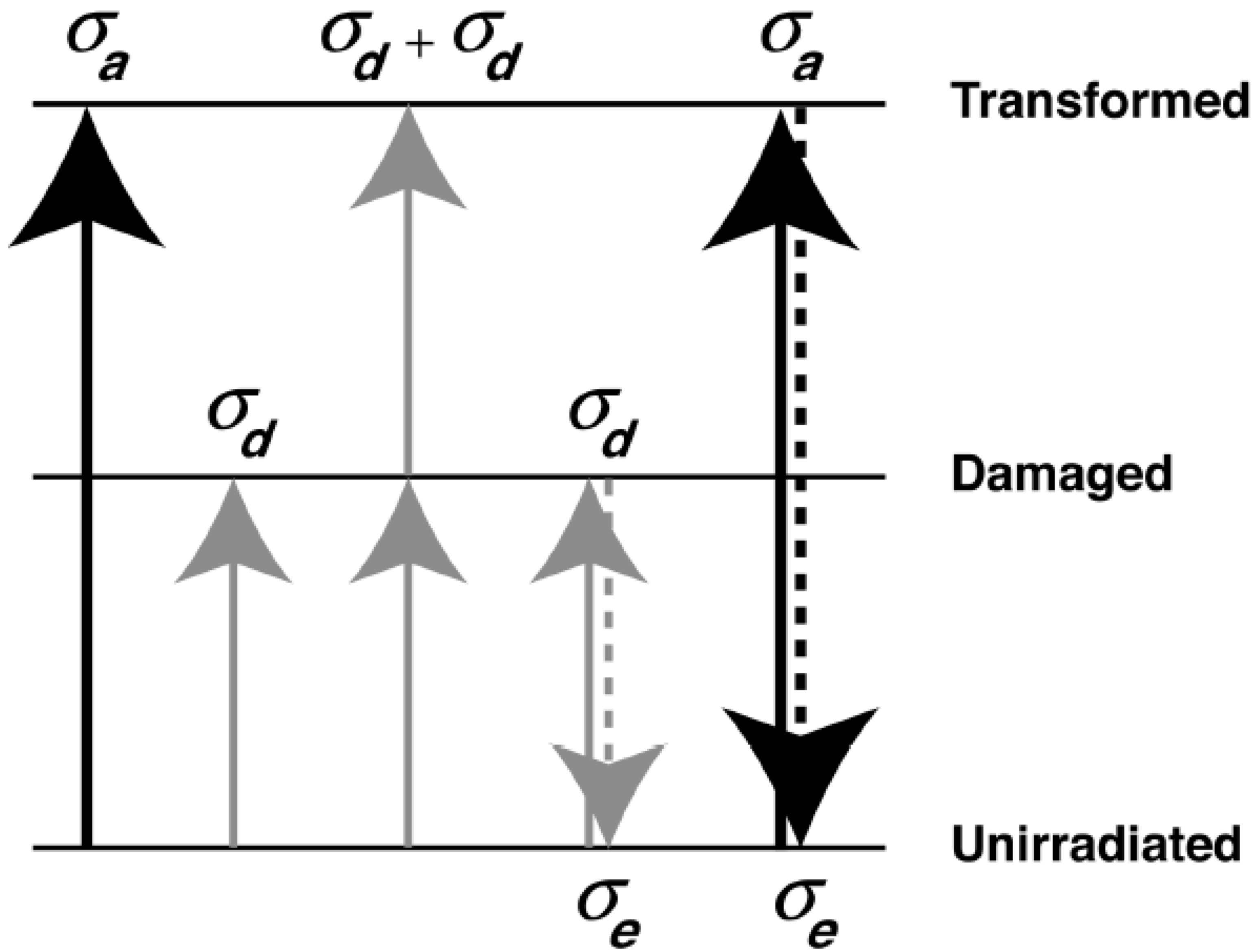
$$f_d(t) = P_d\ t\ e^{-\left(P_d + P_a\right)t}$$

$$f_a(t) = 1 - e^{-\left(P_d + P_a\right)t} - P_d\ t\ e^{-\left(P_d + P_a\right)t}$$



Composite Black&Gray Spot Model
f (fractional area)
irradiation time t (seconds)
f_u
f_d
f_a
1
0.8
0.6
0.4
0.2
0
20
40
60
80
100

Black & Gray Spot Model with an Eraser



$$\frac{df_u}{dt} = -P_c\, f_u + P_e\, f_d + P_e\, f_a$$

$$\frac{df_d}{dt} = +x\, P_c\, f_u - \left(P_c + P_e\right) f_d$$

$$\frac{df_a}{dt} = +\left(1 - x\right) P_c\, f_u + P_c\, f_d - P_e\, f_d$$

$$f_u(t) = \frac{P_e}{P_c + P_e}\left(1 + \frac{P_c}{P_e} e^{-(P_c + P_e)t}\right)$$

$$f_d(t) = x\,\frac{P_c\, P_e}{\left(P_c + P_e\right)^2}\left[1 - e^{-\left(P_c + P_e\right)t}\left(1 - \left(P_c + \frac{P_c^{\,2}}{P_e}\right) t\right)\right]$$

$$f_a(t) = \frac{P_c\,\left(P_c + (1-x)\, P_e\right)}{\left(P_c + P_e\right)^2}\left[1 - e^{-\left(P_c + P_e\right)t}\left(1 + \frac{x\, P_c\,\left(P_c + P_e\right)}{P_c + (1-x)\, P_e}\, t\right)\right]$$

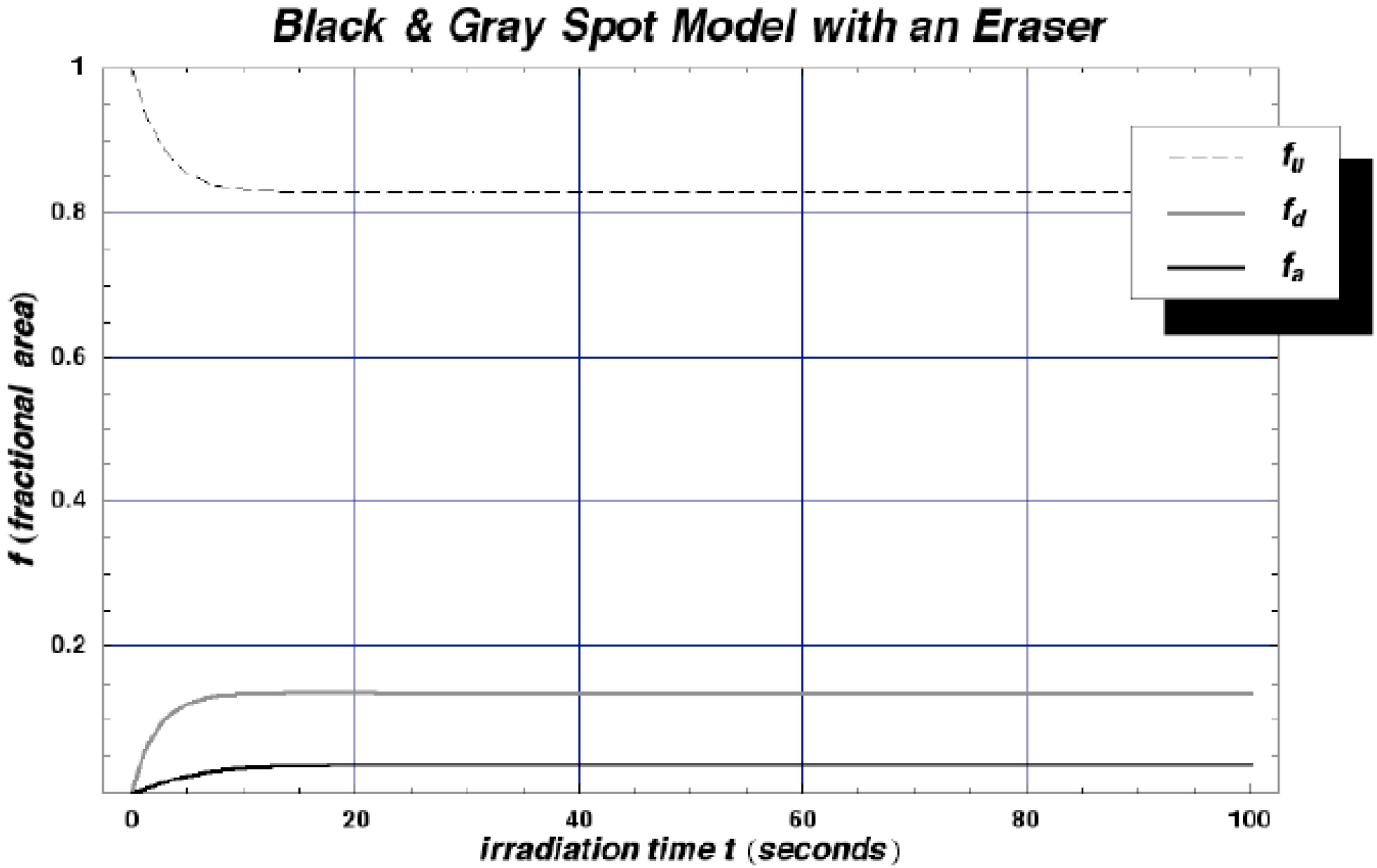
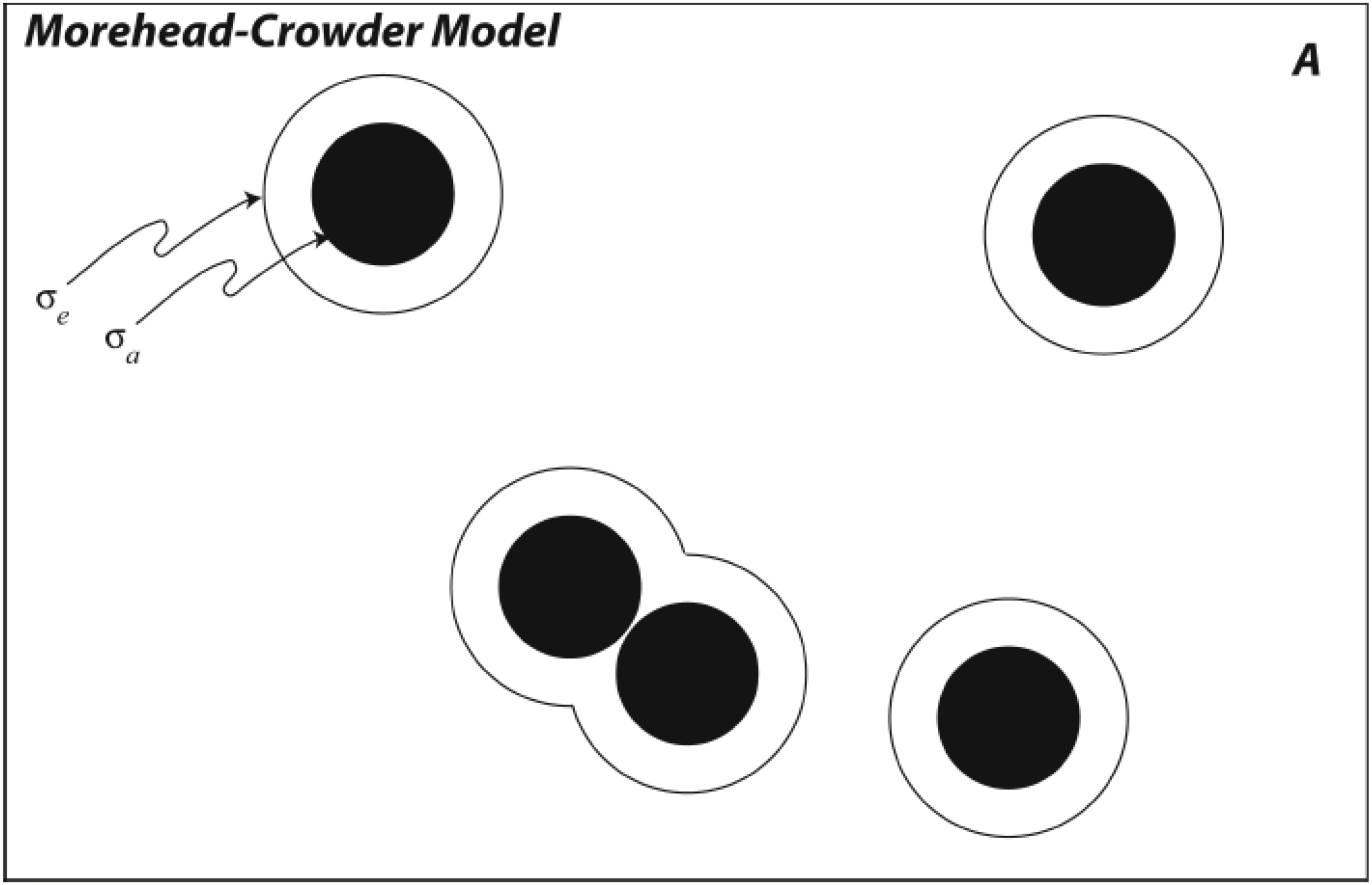


Figure 18. Plot of the dependence of fractional areas f_u, f_d and f_a on irradiation time, t, based on Eqn. (24). For this calculation, we assumed $P_c = 0.0625\ s^{-1}$, $P_e = 0.3\ s^{-1}$, and $x = 0.95$. These are close to the values used by Abe et al. [5] to fit this model to amorphization rate data for germanium (Ge) irradiated concurrently with 30 keV Xe^+ ions at an ion flux of 3.0×10^{15} ions/m^{2}s and 1 MeV electrons at a flux of 2.2×10^{23} e/m^{2}s.


Morehead-Crowder Model
A
σe
σa

$$\frac{df_u}{dt} = -\left(P_{a0} - P_e(T)\right) f_u + 0\ f_a$$

$$\frac{df_a}{dt} = +\left(P_{a0} - P_e(T)\right) f_u + 0\ f_a$$

$$f_u(t) = e^{-\left(P_{a0} - P_e(T)\right)t}$$

$$f_a(t) = 1 - e^{-\left(P_{a0} - P_e(T)\right)t}$$

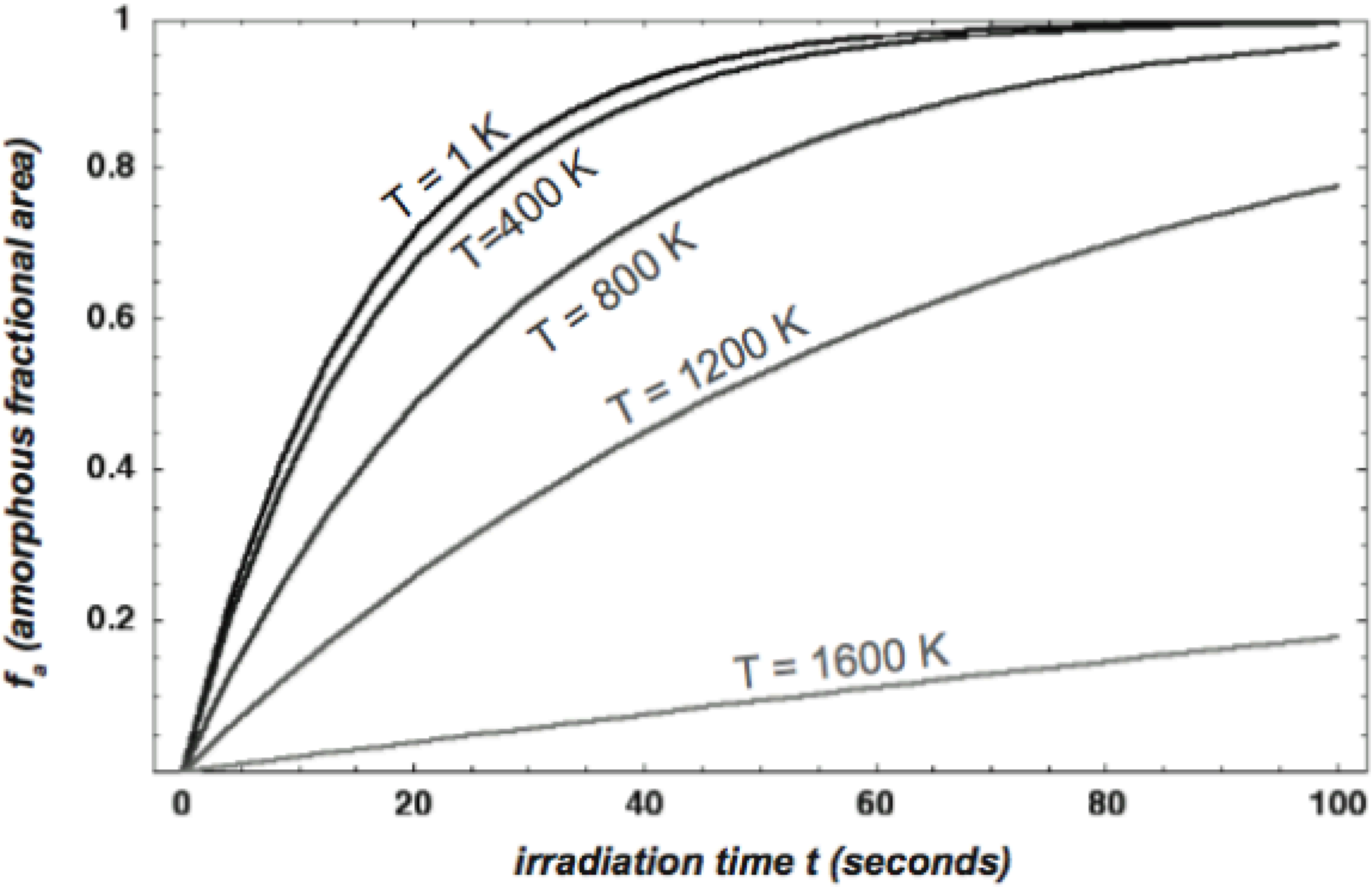
$$P_e(T) = P_{e0}\ e^{\frac{-E_a}{kT}}$$

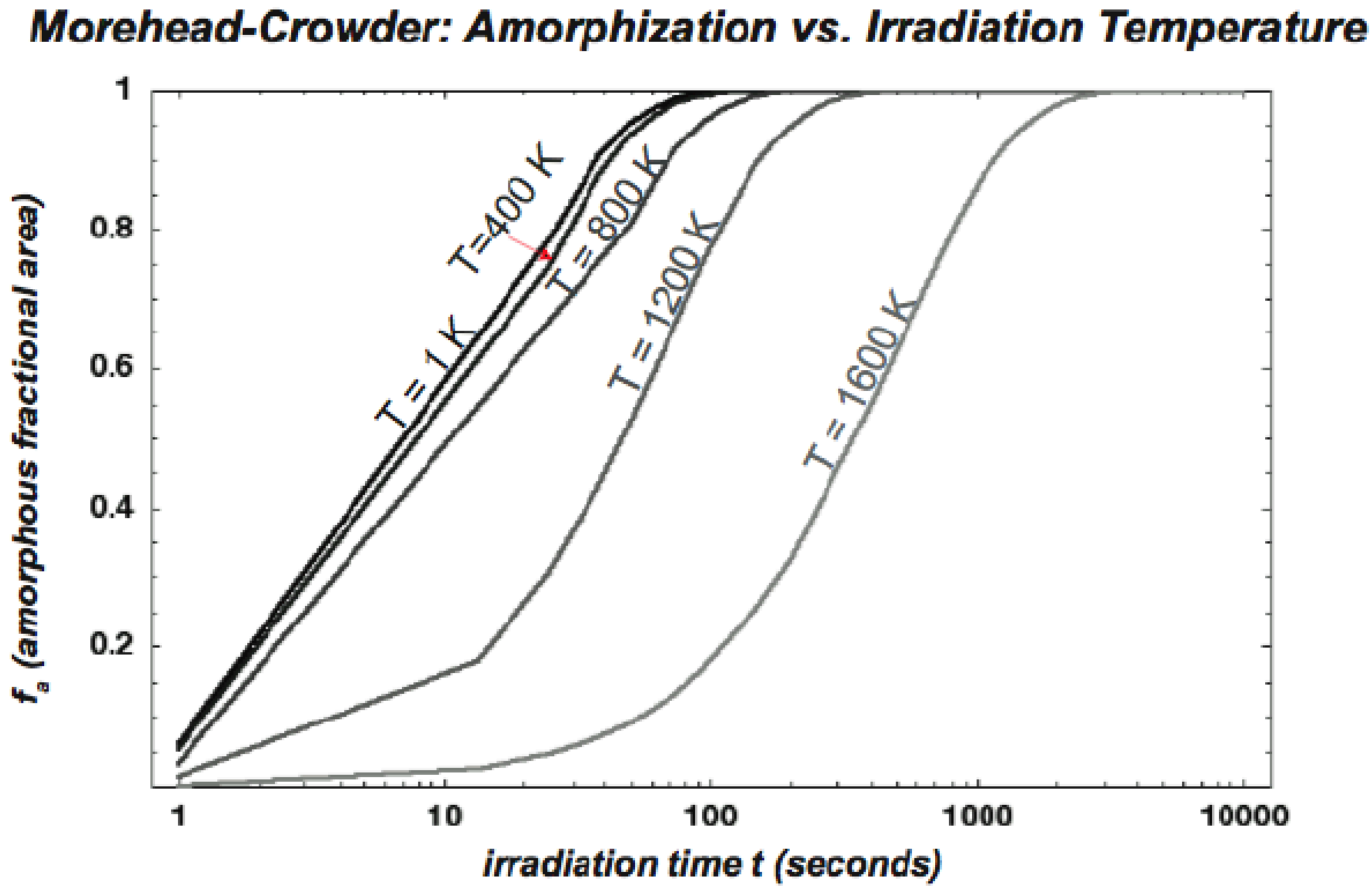
$$f_u(t) = e^{-\left(P_{a0} - P_{e0}\, e^{-\frac{E_a}{kT}}\right)t}$$

$$f_a(t) = 1 - e^{-\left(P_{a0} - P_{e0}\, e^{-\frac{E_a}{kT}}\right)t}$$

$$T_C = \frac{E_a}{k \ln\left(\frac{P_{e0}}{P_{a0}}\right)}$$

Morehead-Crowder: Amorphization vs. Irradiation Temperature




Morehead-Crowder: Amorphization vs. Irradiation Temperature
1
0.8
0.6
0.4
0.2
f_a (amorphous fractional area)
1
10
100
1000
10000
irradiation time t (seconds)
T = 1 K
T=400 K
T = 800 K
T = 1200 K
T = 1600 K