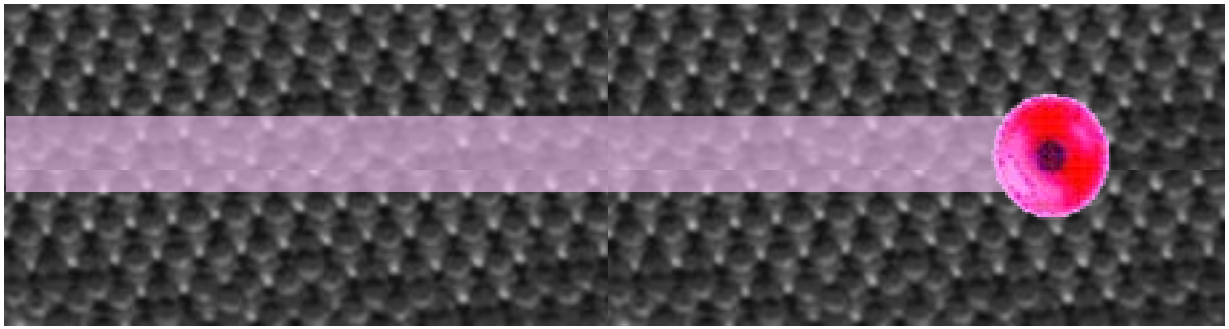
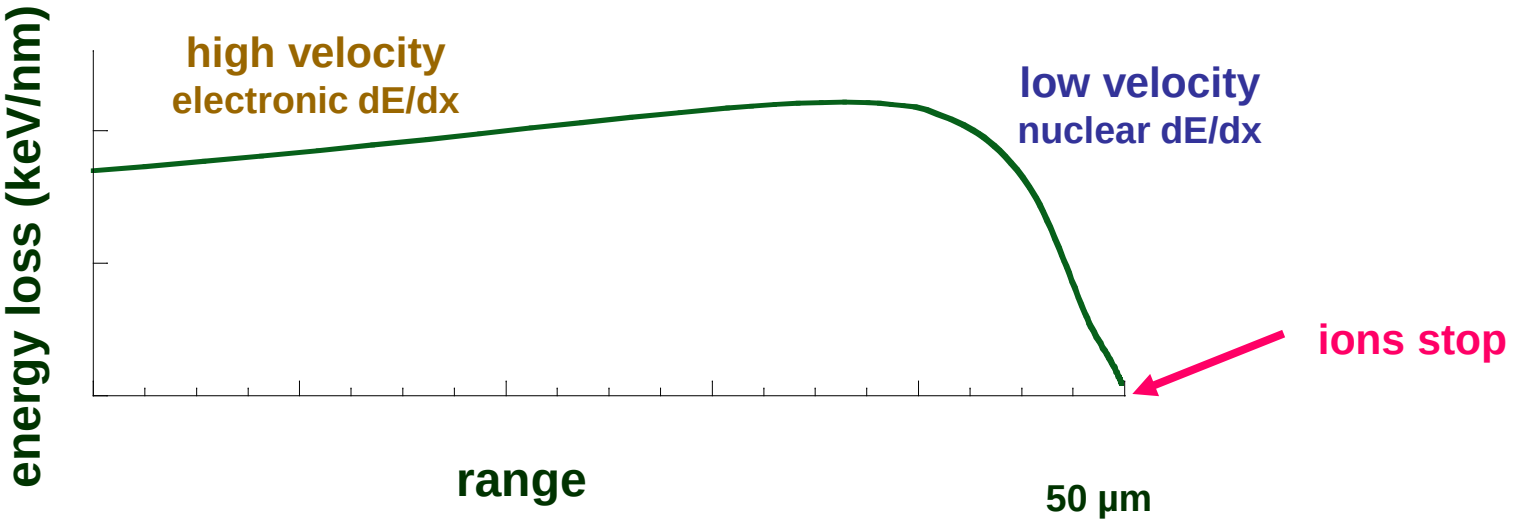
Energy loss along ion trajectory

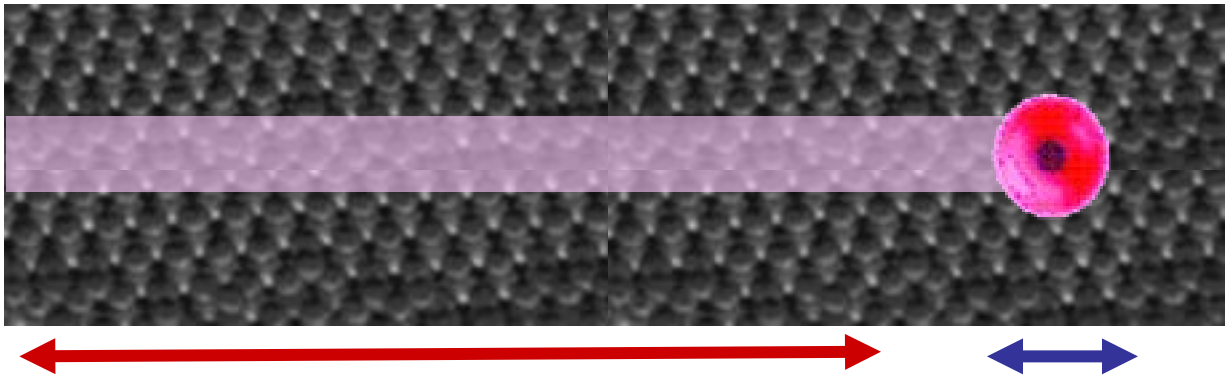
1000-MeV Xe v = 10% c range ~50 µm flight time ~10^{-12} s





Ion - solid interaction

1-GeV Xe ion **v = 10% c** **range ~50 µm** **flight time ~10^{-12} s**

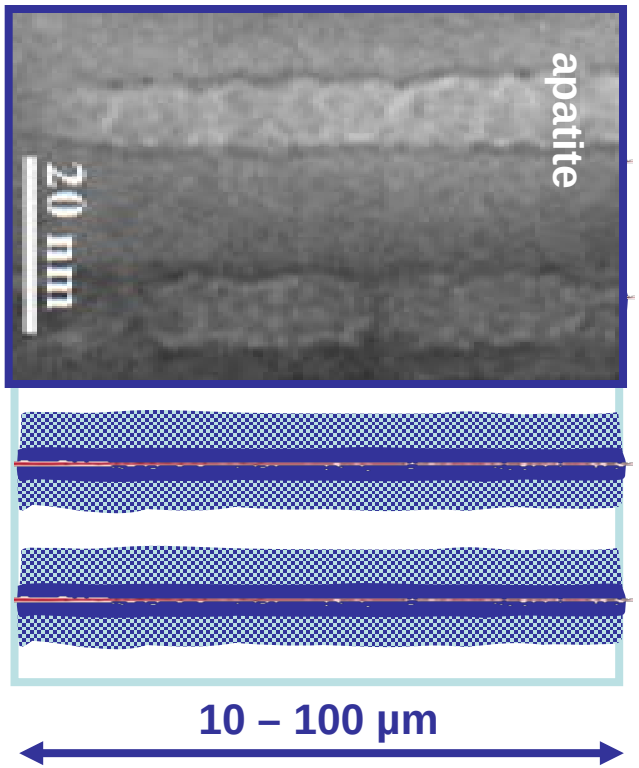


49 µm
collisions with electrons
excitation and ionization

1 µm
elastic collisions
with atoms

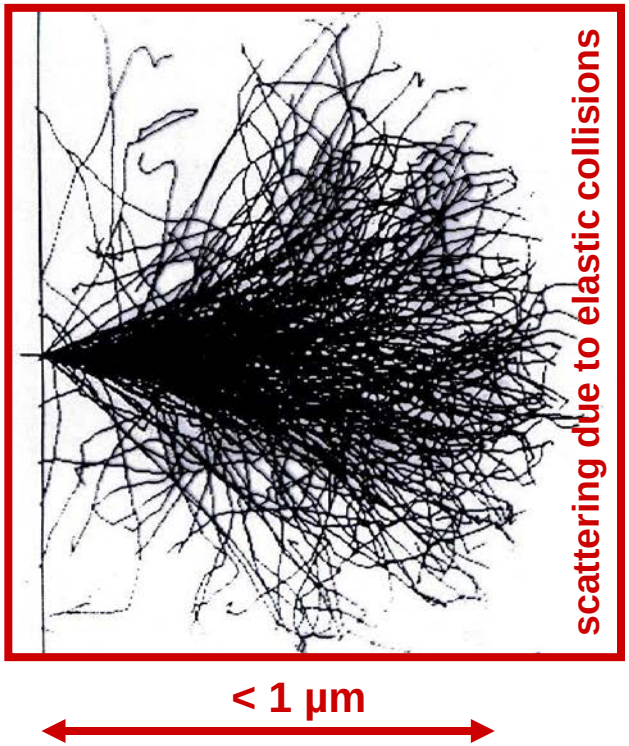
electron cascade

high energies (MeV-GeV)



- minimal scattering → parallel tracks
- each ion produces cylindrical track
- track size scales with dE/dx
- track formation depends on material

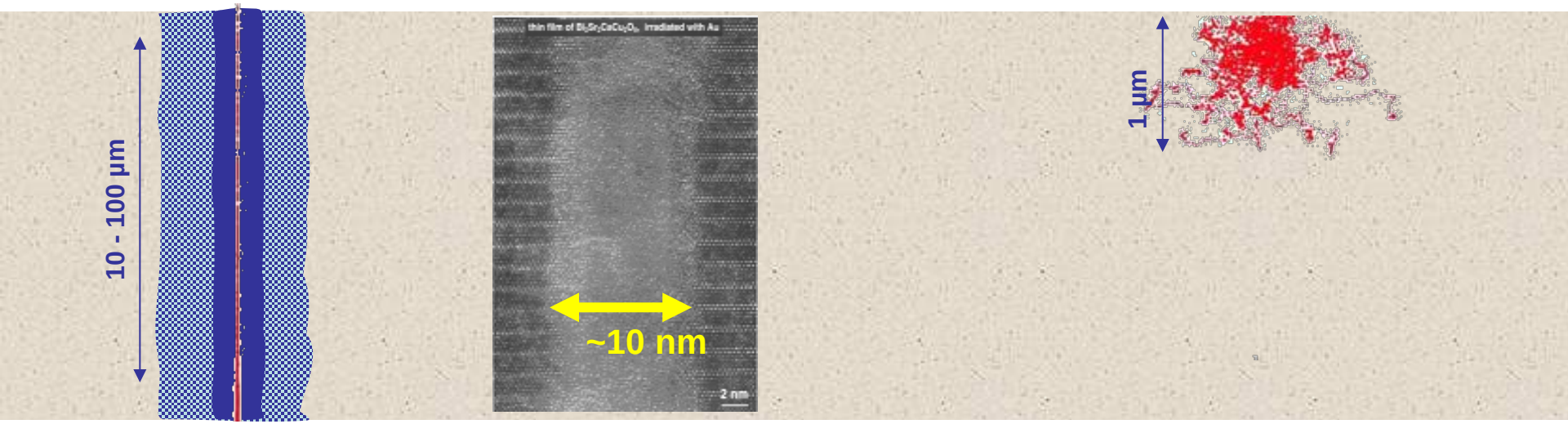
low energies (keV)



- elastic collision cascade
(energy & momentum conservation)
- weak materials dependence
- important parameter → displacement energy E_d

electronic stopping

nuclear stopping



target electrons
↓
electron cascade
↓
coupling to lattice
↓
lattice disorder
↓
track

step 1

step 2

energy transfer from electronic to atomic system
→ material sensitivity

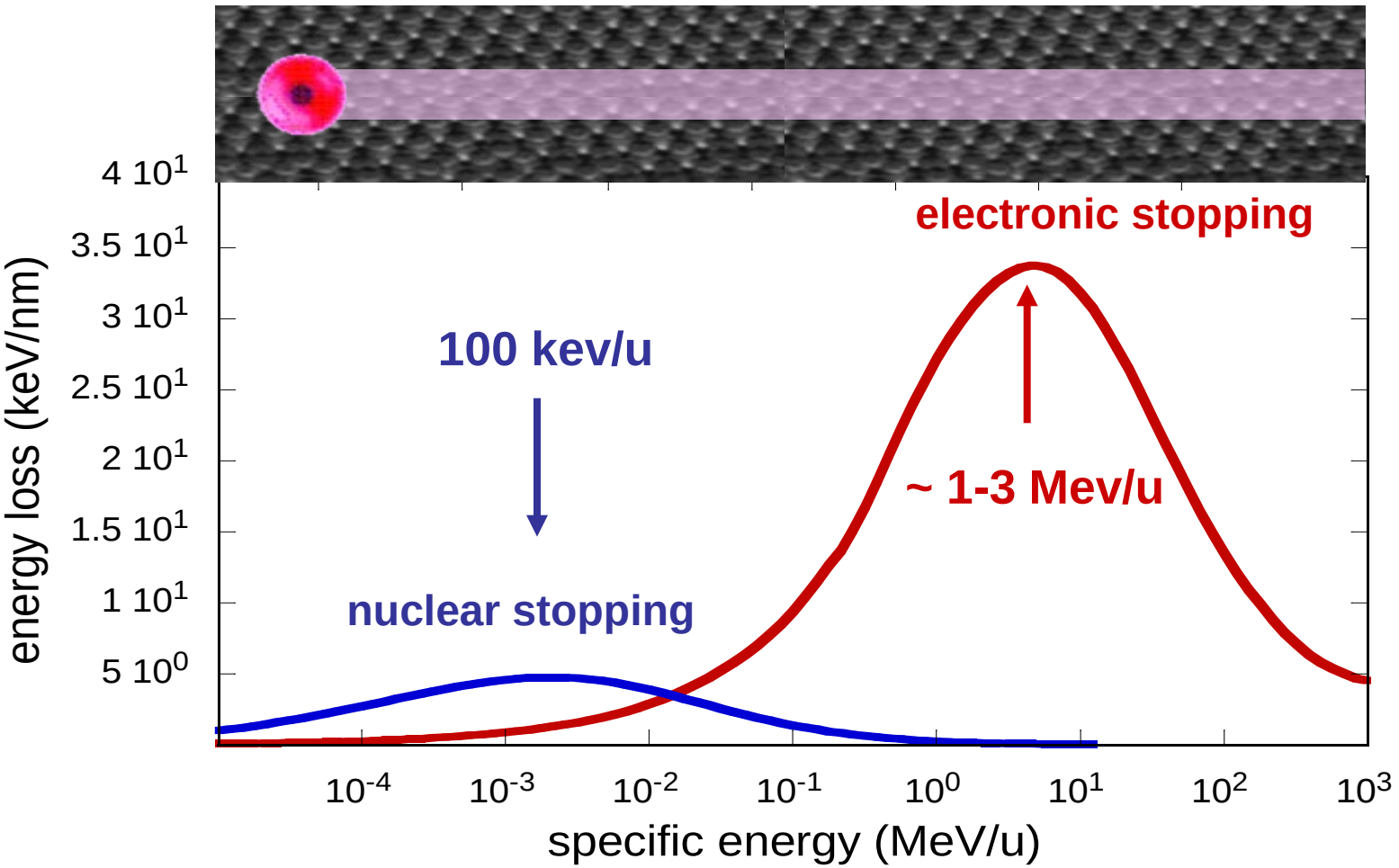
direct process

target atoms
↓
atomic collision cascade

damage scales with dpa
(displacement per atom)

Warning: dpa is no helpful parameter for damage creation with MeV-GeV ions!!

Nuclear and electronic energy loss



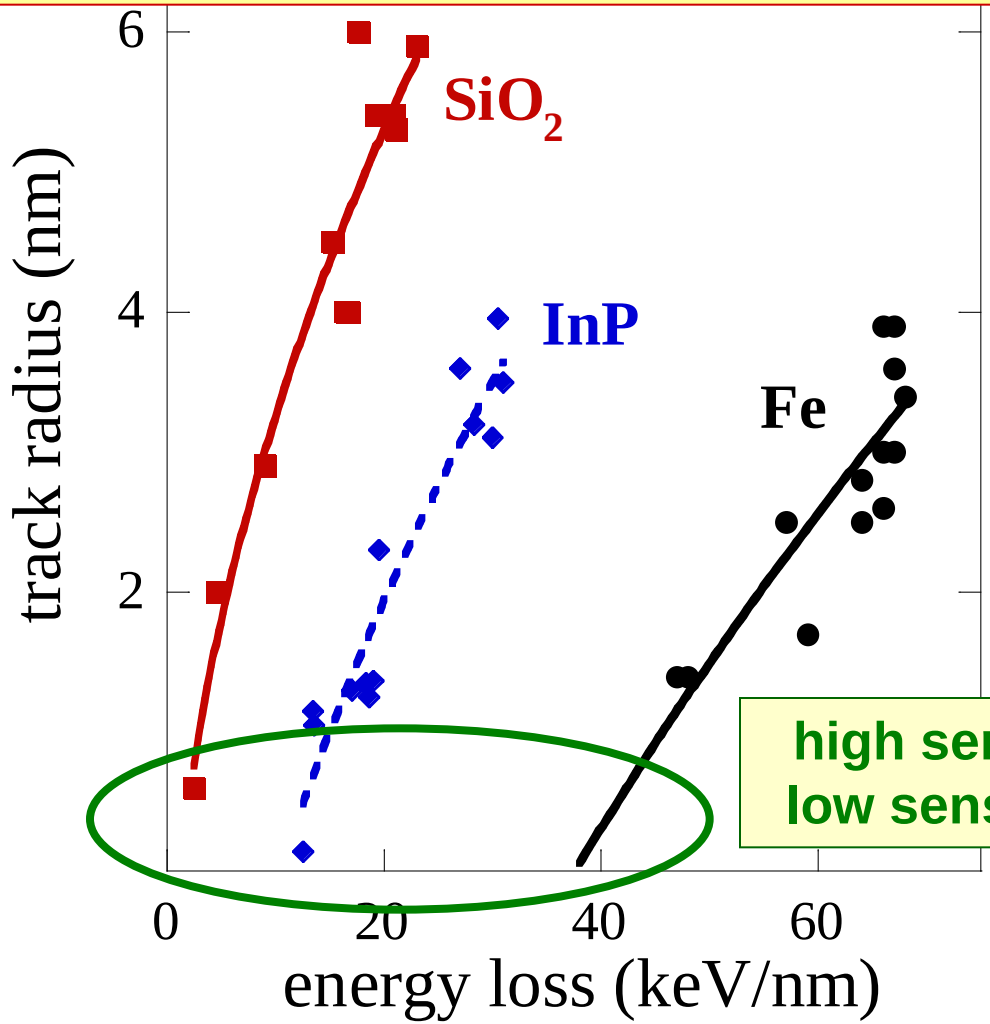
elastic collisions
projectile – target atom

inelastic processes
projectile – target electrons

1) Track size increases with electronic stopping power

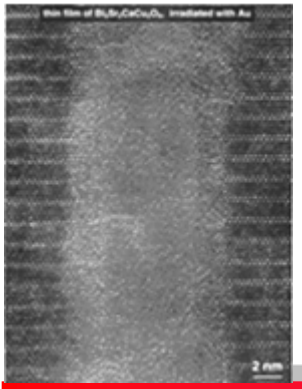
2) Track size insulators > semiconductors > metals

3) Materials sensitivity scales with dE/dx threshold



recapitulate

high sensitivity → low threshold
low sensitivity → large threshold



Track formation depends on materials nature

high sensitivity — **low sensitivity**

dE/dx threshold	~1 keV/nm	~20 keV/nm	~50 keV/nm

insulators

- polymers
- oxides, spinels
- ionic crystals
- ~~diamond~~

semi-conductors

- amorphous Si, Ge
- GeS, InP, $Si_{1-x}Ge_x$
- ~~Si, Ge~~

metals

- amorphous alloys
- Fe, Bi, Ti, Co, Zr
- ~~Au, Cu, Ag,~~

~~no tracks~~

Track formation in metals

metals are rather insensitive due to

- large number of conduction electrons
- very mobile electrons
- large thermal conductivity

no tracks:

Nb, Cu, Ni, Nb, Pd, W, Ag, Pt, Au

tracks:

pure metals: Fe, Ti, Co, Zr, Bi

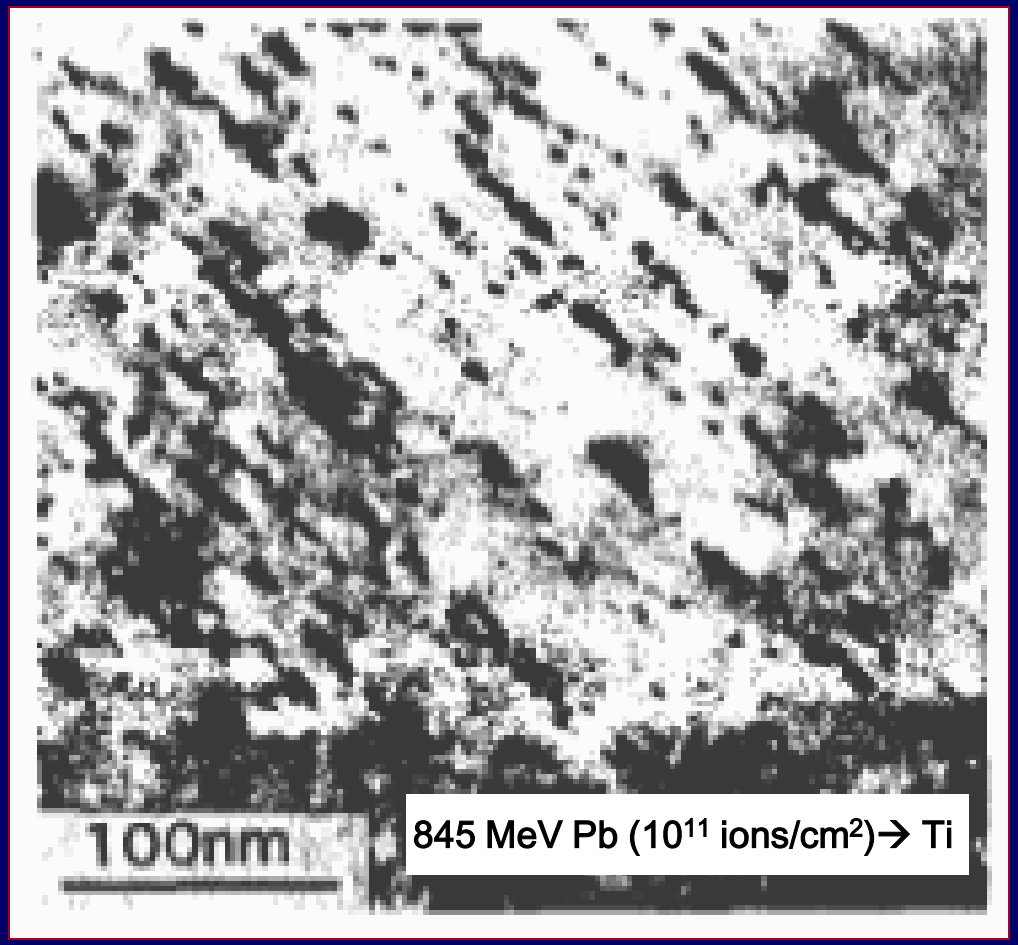
compounds: NiB, FeCrNi, TiNi, etc

metallic glasses: PdSi, FeB, etc

track observation in metals rather difficult
(no amorphisation, no optical defects,...)

Tracks in metals (Ti)

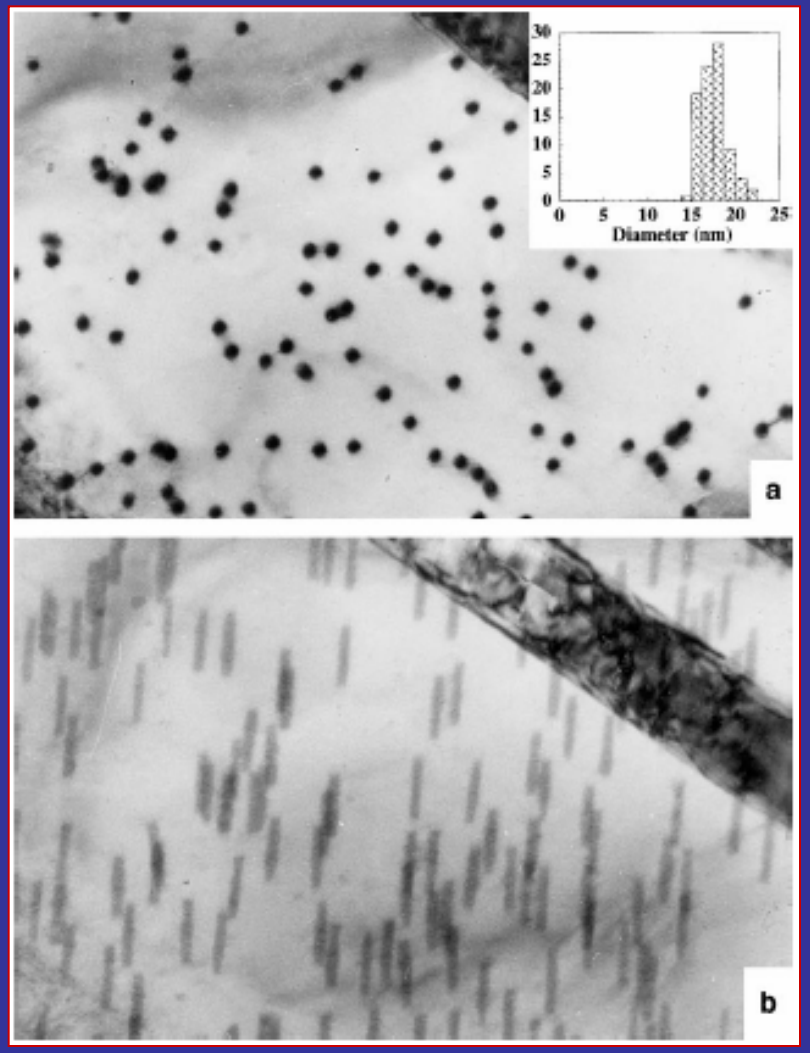
transmission electron microscopy



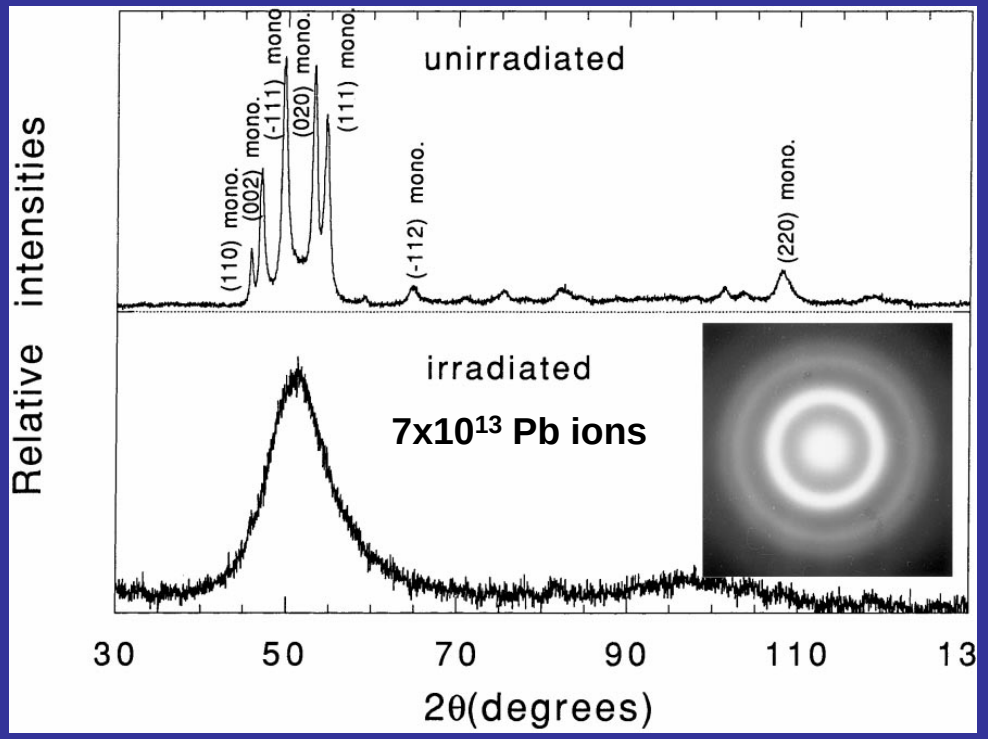
dotted tracks in Ti

Dunlop et al. NIM B 112 (1996)

Tracks in metals (NiTi)



Barbu et al., NIMB 145 (1998)



homogeneous cylindrical tracks

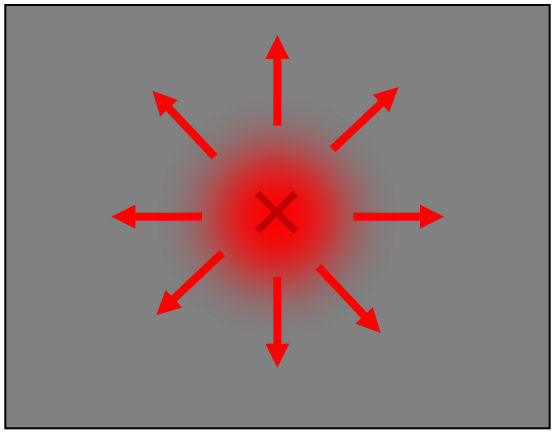
amorphization of martensitic NiTi phase

no tracks induced in austenitic phase

Thermal spike model

inelastic thermal spike or two-temperature model

sudden temperature rise in a cylinder around ion trajectory



1) energy diffusion within electron system

2) energy transfer to atoms

3) energy diffusion within atomic system

description in cylindrical geometry
with z-axis = ion trajectory

thermalisation in space and time!

Track formation & thermal spike model

two differential equations coupled via *g*

electrons

$$C_e(T_e)\frac{\partial T_e}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[rK_e(T_e)\frac{\partial T_e}{\partial r}\right] - g(T_e - T_a) + A(r[\alpha_R], t)$$

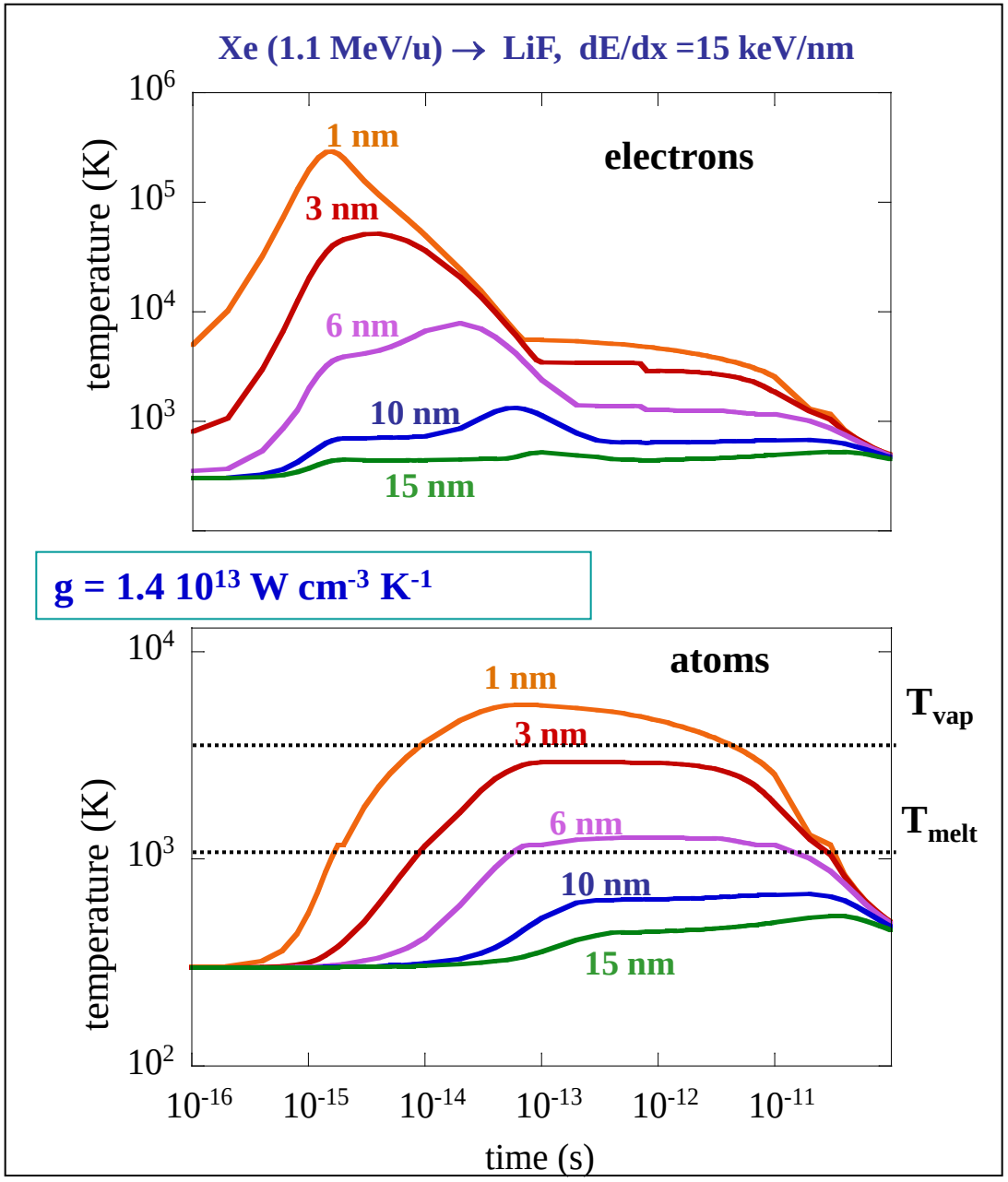
atoms

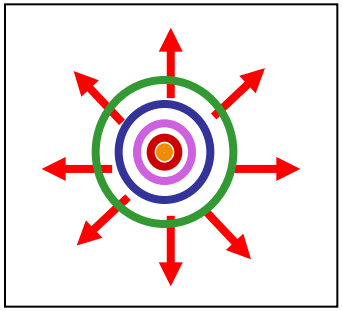
$$C_a(T_a)\frac{\partial T_a}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[rK_a(T_a)\frac{\partial T_a}{\partial r}\right] + g(T_e - T_a)$$

important parameters

- specific heat $C_e(T)$ and thermal conductivity $K_e(T)$ of electron system
- specific heat $C_a(T)$ and thermal conductivity $K_a(T)$ of atomic system
- g electron phonon coupling
- latent heat

track formation → melting depends on $C_{e,a}(T)$, $K_{e,a}(T)$, g, T_m





track formation criteria:

molten radius = track

S_e in metals under sw η > 1 → melting is possible 6745

Table 4. Prediction of S_e sensitivities for some selected metals. ΔH_f is the energy required to melt a metal, S_e is the maximum value that can be …ched in irradiations. The e–p coupling factor is a mean value and λ is the electron mean f… path. The S_e^* values are the maximum S_e values that have been used in experiments.

Metal	ΔH_f ($J\ cm^{-3}$)	S_e (TRIM91) ($keV\ nm^{-1}$)	g ($\times 10^{11}$) ($W\ cm^{-3}\ K^{-1}$)	λ (10^{-7} cm)	η	S_e effect	Measured S_e effect
Be	9368	23	293	3.92	5.2	Yes	
Mg	2270	20	6.82	21.6	0.61	No	
Al	3275	28	8.14	20.9	0.63	No	No [38] $S_e^* \leq 15$ keV/nm
Ti	6701	42	92.8	6.14	5.4	Yes	Yes [22]
V	8907	52	66.4	7.56	3.3	Yes	
Cr	9075	63	94.0	6.51	5.3	Yes	
Mn	7042	63	444	2.98	32	Yes	
Fe	10 977	70	49.8	8.97	2.6	Yes	Yes [13]
Co	12 199	75	34.5	10.9	1.7	Yes	Yes [22]
Ni	10 529	77	40.5	10.1	2.2	Yes	No [13, 17] $S_e^* \leq 67\ keV\ nm^{-1}$
Cu	6895	73	4.94	28.5	0.42	No	No [13] $S_e^* \leq 65\ keV\ nm^{-1}$
Ga	1061	46	19.6	13.1	8.1	Yes	Yes [23]
Zr	4873	48	35.0	9.55	3.5	Yes	Yes [22]
Nb	9074	63	15.0	15.2	0.97	No	No [13] $S_e^* \leq 62\ keV\ nm^{-1}$
Pd	7616	81	13.9	16.4	1.3	Yes?	No [17] $S_e^* \leq 75\ keV\ nm^{-1}$
Ag	4118	70	1.26	53.1	0.19	No	No [13, 17] $S_e^* \leq 68\ keV\ nm^{-1}$
Sn	1184	45	3.69	28.7	1.5	Yes	
W	14 011	93	12.4	17.0	0.74	No	No [17] $S_e^* \leq 80\ keV\ nm^{-1}$
Pt	9003	109	10.3	18.9	1.1	No	No [13] $S_e^* \leq 96\ keV\ nm^{-1}$
Au	4443	99	0.91	62.5	0.18	No	
Pb	1109	55	1.56	43.3	0.85	No	
Bi	1136	50	8.20	18.4	4.2	Yes	Yes [illegible]
U	3149	95	12.4	16.3	3.7	Yes	

Thermal Spike calculations

experiments

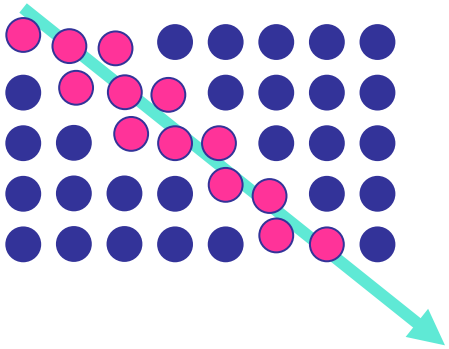
Wang et al., J. Phys. : Condens. Matter 6 (1994) 6733

Thermal spike model

Criticism and limitations:

- short time scales → no equilibrium conditions
- short length scales → macroscopic material parameters
- assumes free electron diffusion for insulators
- ignores holes
- neglects recrystallization processes

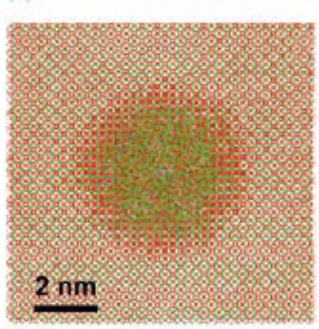
Combine thermal spike model & MD calculations

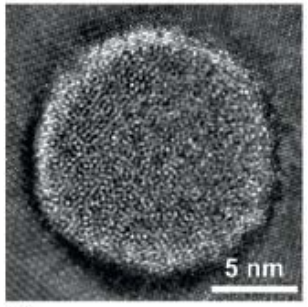


thermal spike: energy deposited to electrons

electron-phonon coupling

temperature profile around ion trajectory





MD: ab initio lattice calculations

solves Newton's equations of atomic motion

electron subsystem included via heat input

How to estimate radiation damage due to high-energy ion beams

- model temperature increase along ion path due to electronic stopping
- use temperature as input to MD code
- model damage creation / track formation by combining nucl & elec stopping
- simulate defect annealing processes at elevated temperature