“THERMAL SPIKE” Model Applied To Thin Targets Irradiated With Swift Heavy Ion Beams (≈MeV/u)

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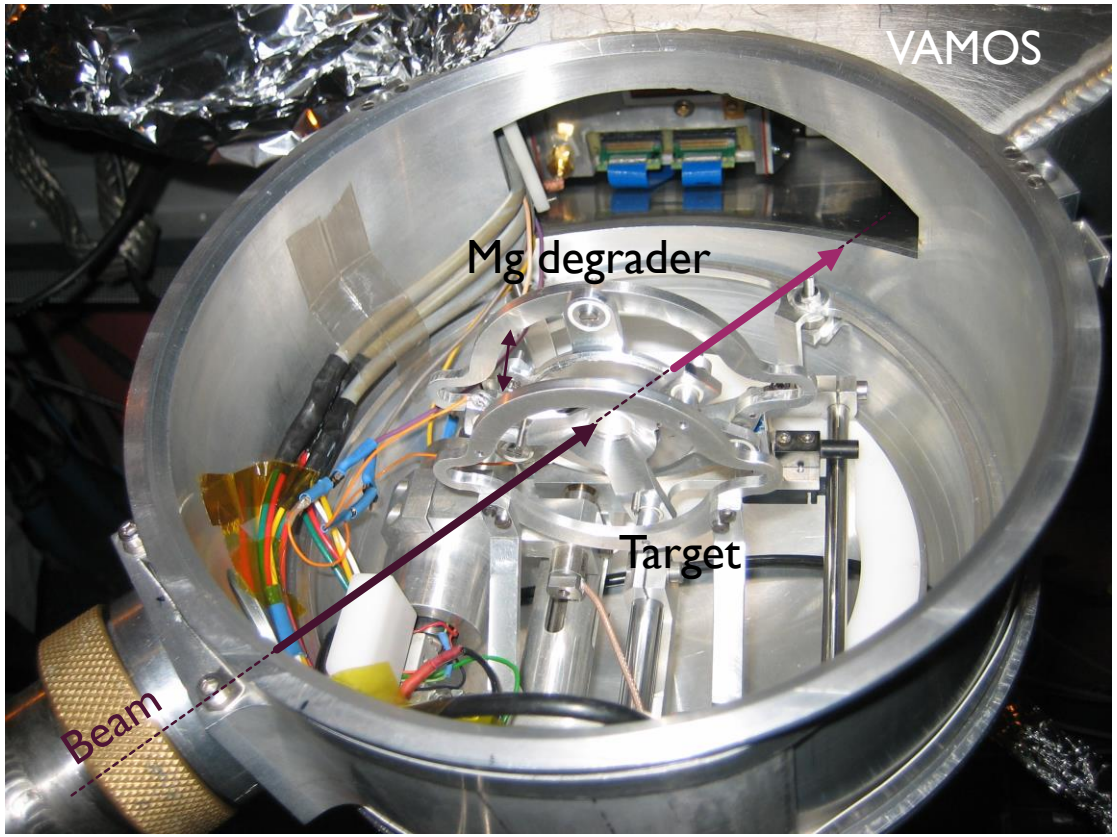
1. Targets’ issues:
   Plunger technique & observations
2. Thermal Spike Model:
   Description & simulations
3. Conclusion

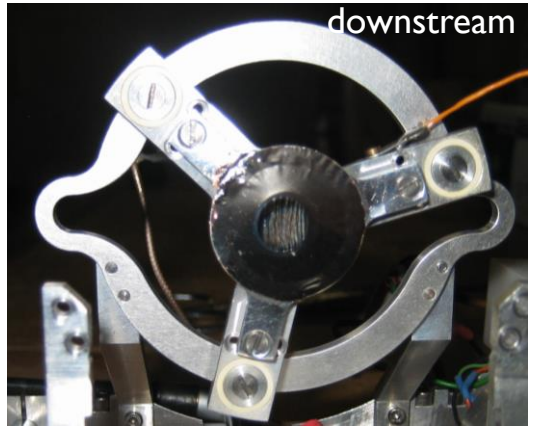
FAST DAMAGE OF TARGETS

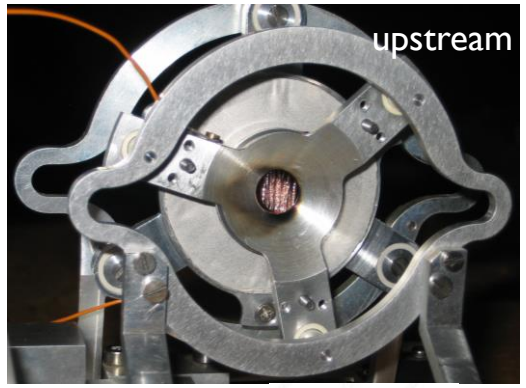
- ^{238}U beam: 6,76 MeV/u; 3 nA
- Target: Cu+ Ti

  dP ~ 10-25 mW

  $\Phi_{beam} \approx \Phi_{target} \approx$ cm
- Degrader: Mg ≈mg/cm²
- Adjustable distance with a precision < 1µm
- Target seriously deformed quickly







Plunger set-up at VAMOS

- No problem with ^{64}Ni targets @ 30 nA (dP=220 mW)
- Thermal calculations at thermodynamically equilibrium: $T_{eq} << T_{fus}$

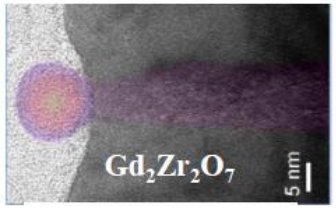
HOW TO EXPLAIN FAST TARGET'S DAMAGE ?

Which Effect ?

- Mechanical → fabrication process, mounting on frame, interlayer interaction…
- Chemical → oxidation, …..
- Equilibrium target heating by the beam → $T=f(P_{in}=P_{rad}(\varepsilon) + P_{cond}(\lambda)) << T_{fus}$?
- Irradiation by individual ions→ Tracks, sputtering ….
- Phase change of the material → T_{limit} ?

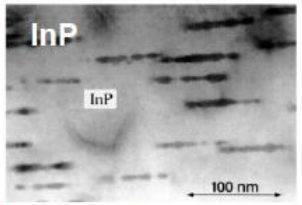
TRACK FORMATION BY SWIFT HEAVY IONS: OBSERVATIONS (METALS & INSULATORS)

A track in a material is a trail of damage resulting from a nanometric, dense and shortly created electronic excitation; first observation by Silk & Barnes, Philos. Mag. 4 (1959) 970 - Review on M.Toulemonde et al, NIM B277 (2012) 28

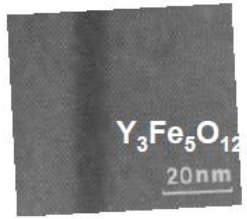


BaJ. Zhang et al. JAP105 (2009) 113510

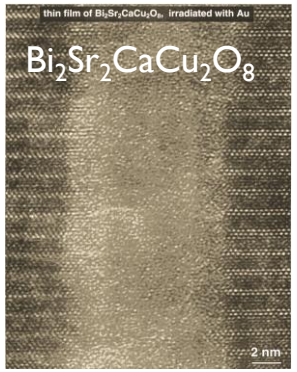
Barbu et al. Europhys. Lett. 15(1991)3713



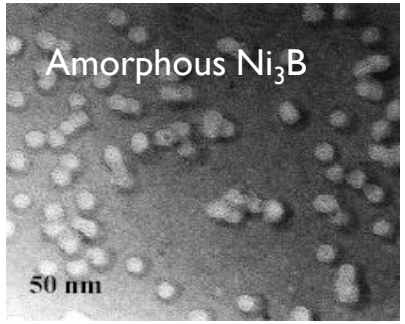
Wesch et al. Nucl. Instr. Meth. B225 (2004) 111



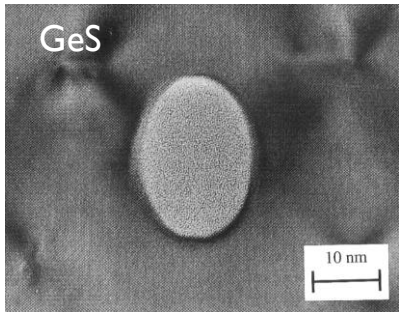
Toulemonde and Studer Phil. Mag. A58 (1988) 799



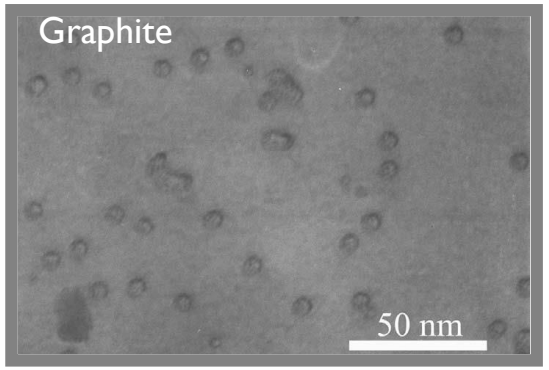
Wiesner et al. Physica C268(1996)161



Dunlop et al. Nucl. Instr. Meth. B146(1998)222



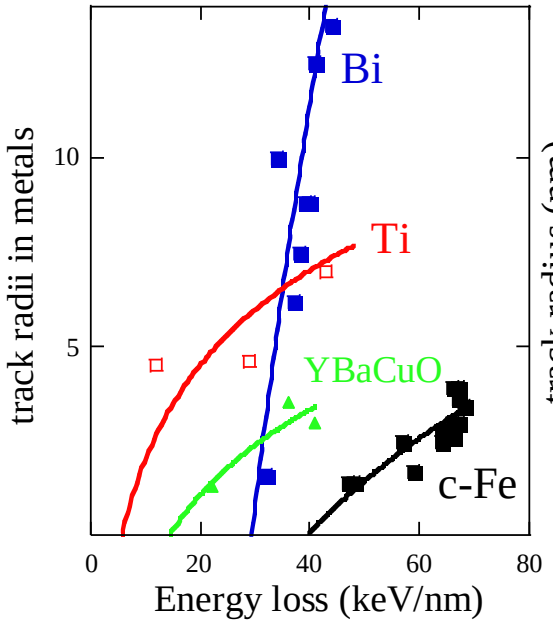
Vetter et al. Nucl. Instr. Meth. B141(1998)747

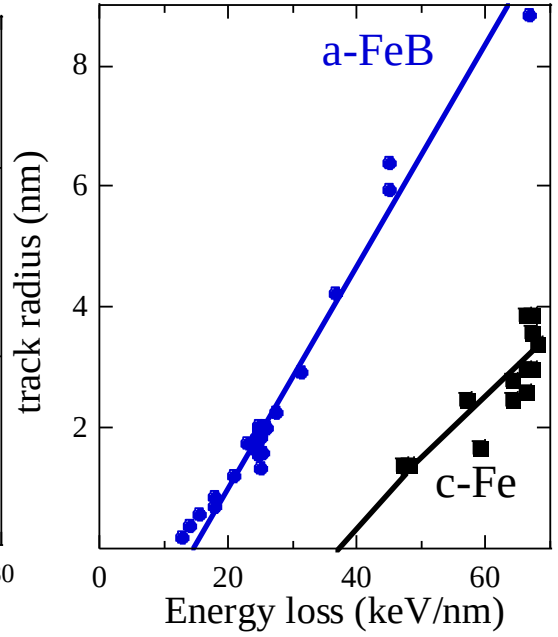


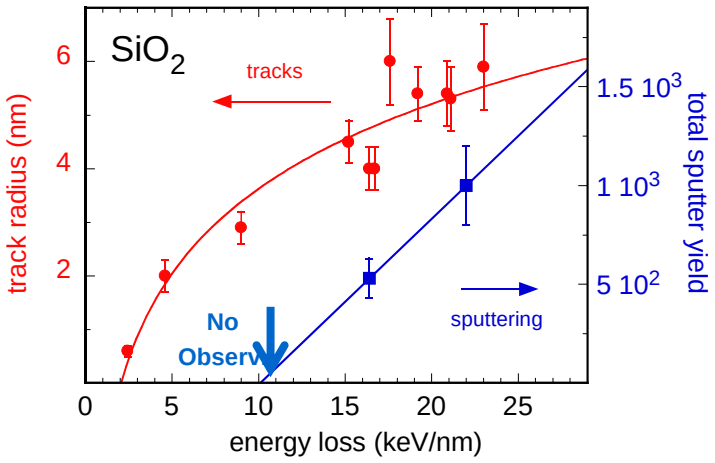
Dunlop et al. Phys. Rev. 76(2007)155403

Are there correlations (track radius, sputtering yield…) with some specific parameters?

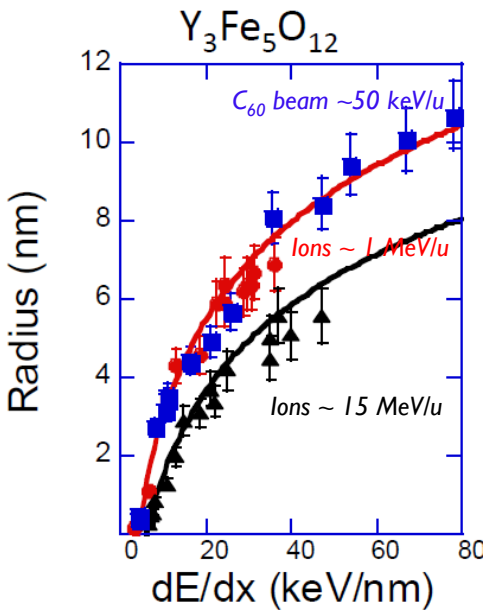
TRACK FORMATION BY SWIFT HEAVY IONS: OBSERVATIONS AND TENDENCIES







Toulemonde et al, Phys. Rev. Lett. 88 (2002) 057602
Meftah et al, Phys. Rev. B 49 (1994) 12457

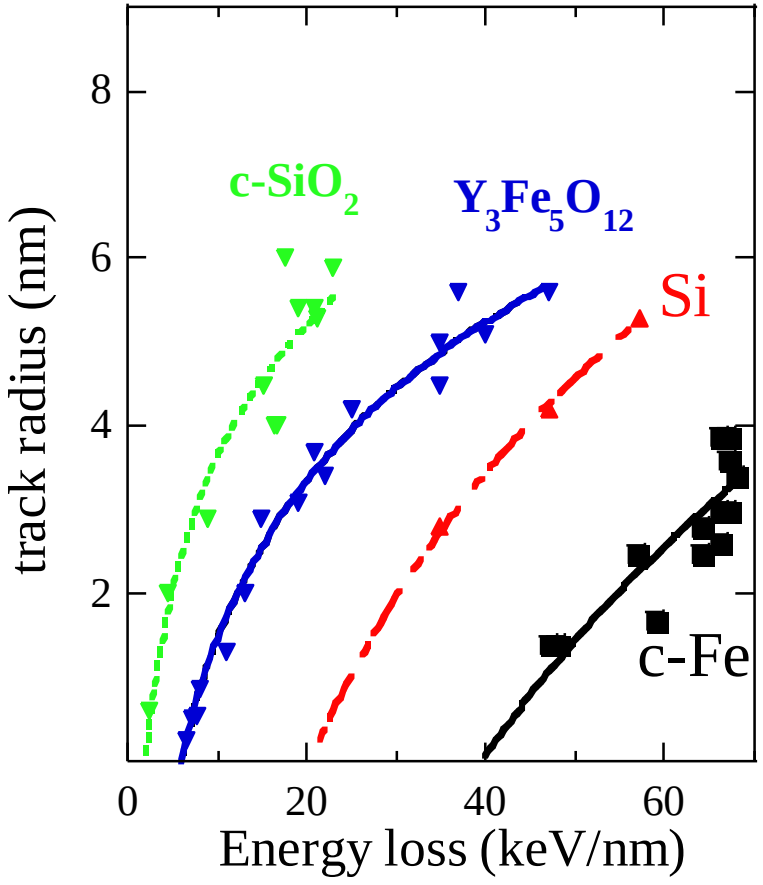


Meftah et al, Phys. Rev. B 48 (1993) 920
Jensen et al, Nucl. Inst. Meth. B 146 (1998) 412

Bi: C. Dufour et al, J. Phys.: Condens. Matter 5 (1993) 4573
Ti: Dammak et al, Rad. Eff. Def. Sol. 126 (1993) 111
a-FeB: Audouard et al, J. Phys. Cond. Matter 5 (1993) 995
$YBa_2Cu_3O_{7-\delta}$: Toulemonde et al. Nucl. Instr.Meth. B91(1994)108

c-Fe: Dunlop et al, C. R. Acad. Sci., Paris II, 309 (1989) 1277 // Nucl. Instr. Meth. B90 (1994) 33

TRACK FORMATION COMPARED WITH METALS, SEMICONDUCTORS AND INSULATORS



metals

NO Cu, Ag, Pt, Ni, Nb

YES **Fe**, Bi, Ti, Co, Zr

YES **amorphous alloys**

semiconductors

NO Si, Ge only with C60

YES GeS, InP, $Si_{0.5}Ge_{0.5}$

YES **amorphous alloys**

insulators

YES polymers, ionic crystals, oxydes (**SiO_2**), etc…

c-SiO_2	Meftah et al. Phys. Rev. B49(1994)12457
$Y_3Fe_5O_{12}$	Meftah et al. Phys. Rev. B48(1993)920
c-Fe	Dunlop et al. Nucl. Instr. Meth. B90(1994)33
Si	Dunlop et al. Nucl. Instr. Meth. B146(1998)302

Need of a macroscopic description of experimental results

REFERENCES

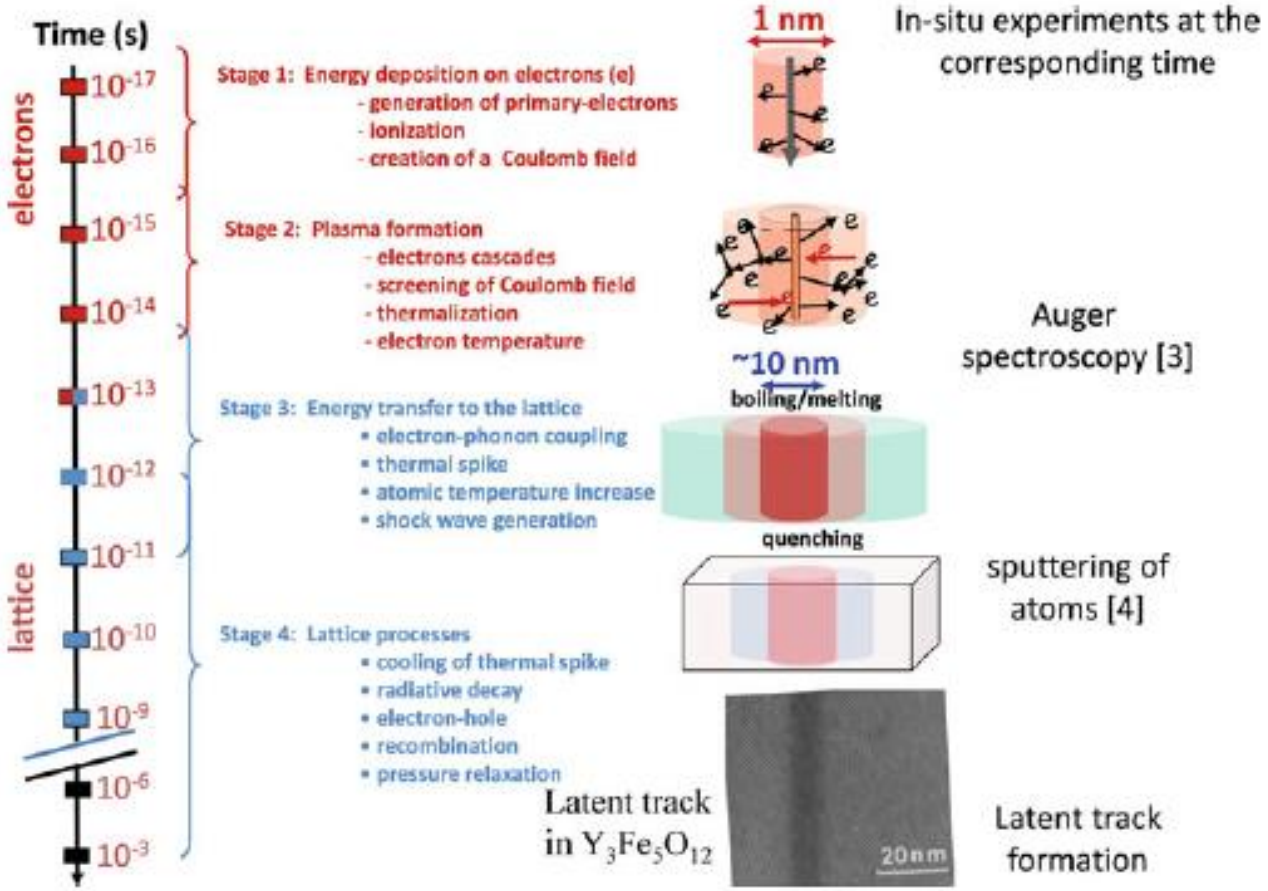
Werner Wesch, Elke Wendler, Editors, "Ion Beam Modification of Solids, Ion-Solid Interaction and Radiation Damage" Springer Series in Surface Sciences 61 (2016) https://www.springer.com/series/409

Chapter 2
Models for the Description of Track Formation

Christian Dufour and Marcel Toulemonde

Abstract The different models developed to describe track formation induced by swift heavy ions will be presented. The macroscopic ones are the Coulomb explosion model, the bond weakening (BW) model, the exciton self-trapping (STX) model, the concept of reduced electronic energy loss, the analytical thermal spike model, the IDEA (Ionization Diffusion-Explosion-Amorphization) model, the inelastic thermal spike model (i-TS) and to finish microscopic descriptions using molecular dynamic (MD) calculations. All the models were applied to describe the track formation in different kinds of materials (metals, semiconductors or insulators), while additionally the i-TS model and MD calculations were used to describe the sputtering yield. It will be shown that the initial energy deposition plays an important role in the different descriptions and that there is no simple link between the energy deposited in the electronic and later in the atomic system. The large number of models presented here shows by itself that we are far away from a complete description of track formation. So the ambition here is just to give a present status of the different models.

A TRANSIENT THERMAL PROCESS



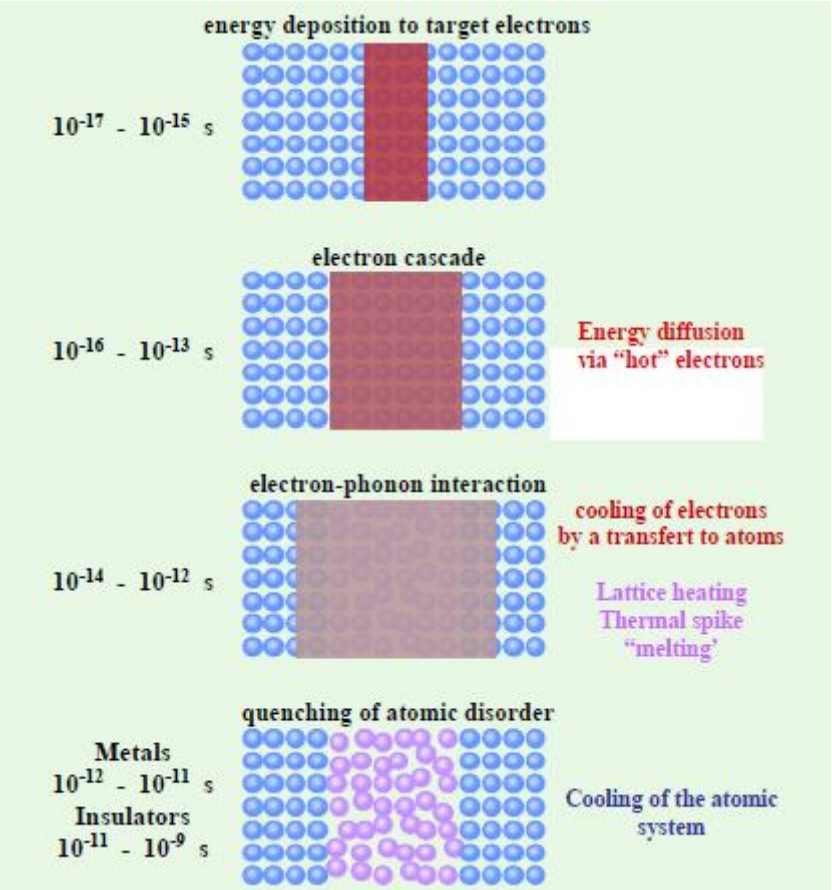
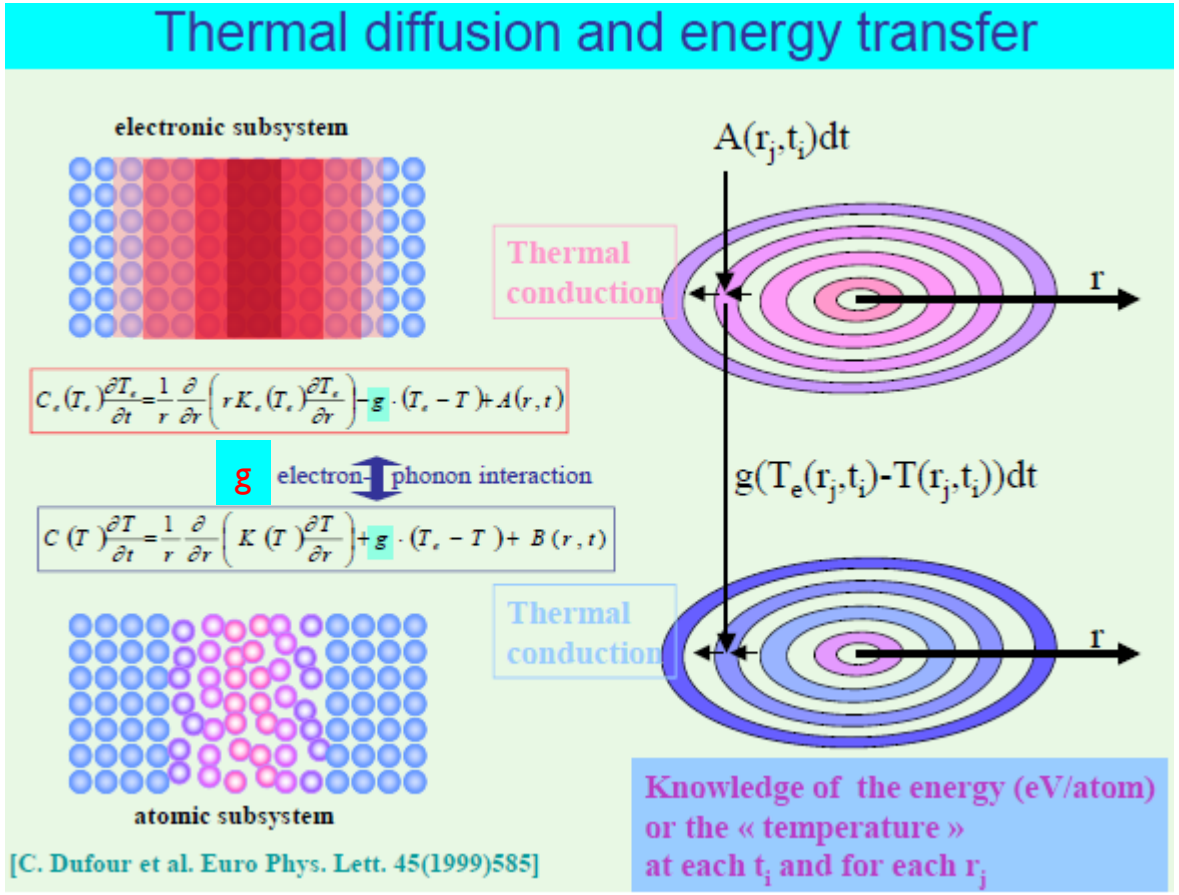


Figure from Chapter 2 p. 64, Springer Series in Surface Sciences 61 (2016)

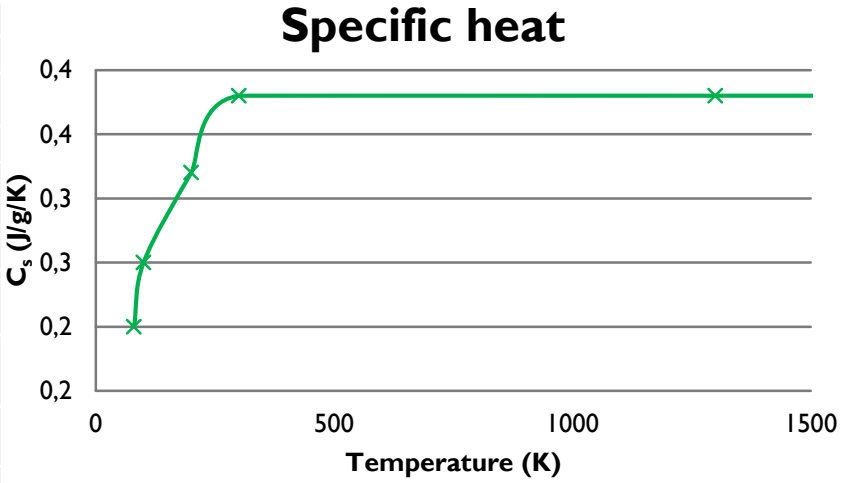
THERMAL SPIKE MODEL

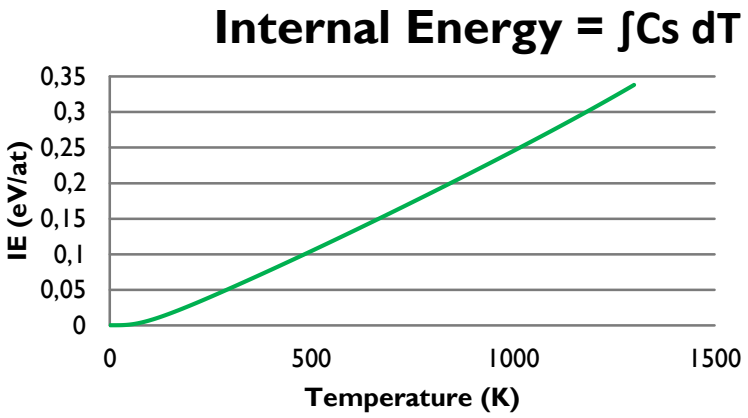
- Energy deposited :
  - on the electrons of the target
  - Transfer of the electrons energy to atoms
- Such phenomena is mathematically described by 2 coupled equations of energy diffusion on electrons and atoms
- Inputs of the model:
  - Beam energy and dE/dx
  - physical parameters of the target
  - electron-phonon coupling strength g (**free parameter**)

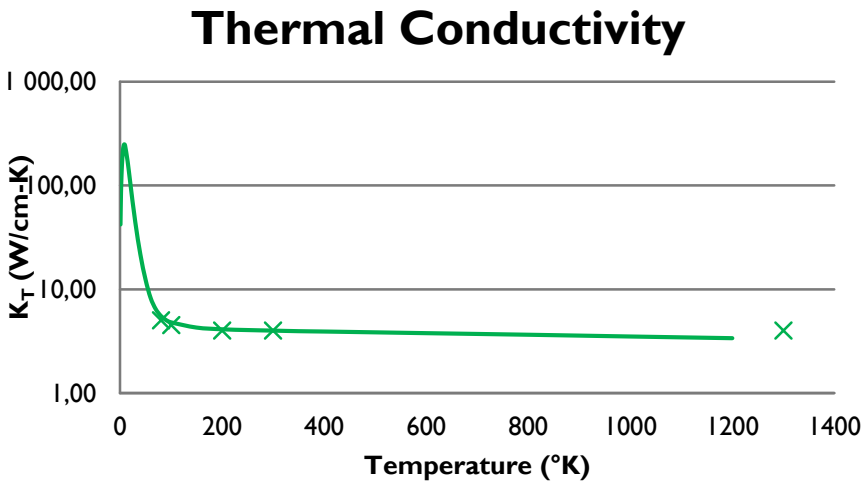


INPUTS OF THERMAL SPIKE MODEL

Projectile	Incident ion energy	*MeV/A*
	dE/dx (initial, final, steps)	*keV/A°*
Target	**initial temperature**	*K*
	Initial value of IE	*eV/at*
	type (Metal/insulator)	
	electron thermal diffusity at 300 K	*cm²/s*
	Minimal electron thermal diffusity at 300 K	*cm²/s*
	electron density	10^{22} *cm*$^{-3}$
	coupling g (initial, final, step)	10^{10} *W/cm³/K*
	evaporation energy	*eV*
	Latent heat of melting	*J/g*
	Latent heat of boiling	*J/g*
	Melting temperature	*K*
	Boiling temperature	*K*
	mean ionization potential	*eV*
	mean mass of one atom	*g*
	solid density	*g/cm³*
	Liquid density	*g/cm³*





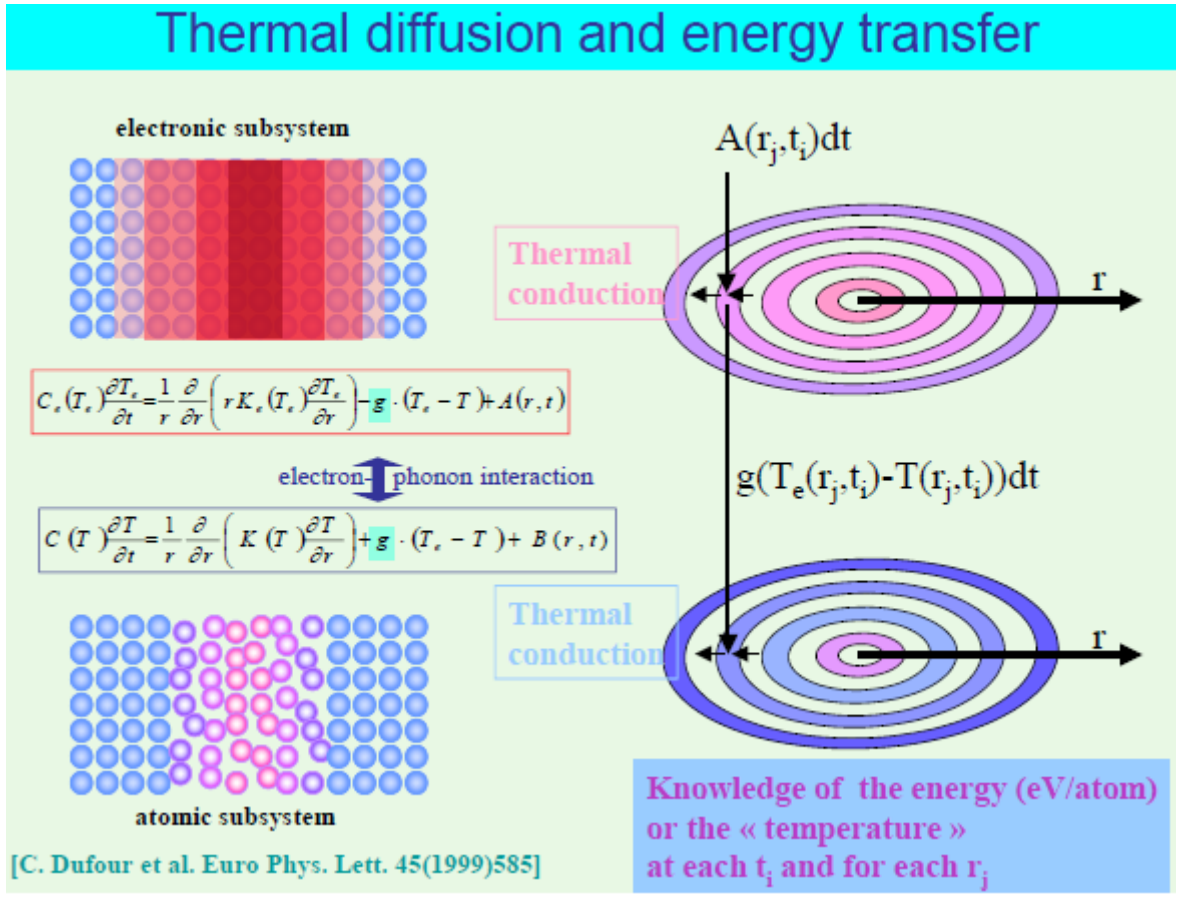


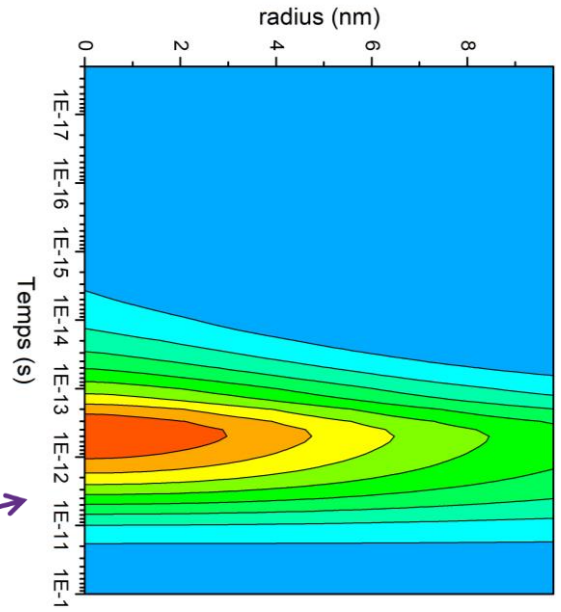
g, n_e: Z. G. Wang et al, J. Phys. Condens. Matter 6 (1994) 6733

g: M. Toulemonde et al NIM B277 (2012) 28

$$g \sim 1/K_{e-}$$

THERMAL SPIKE MODEL - OUTPUT

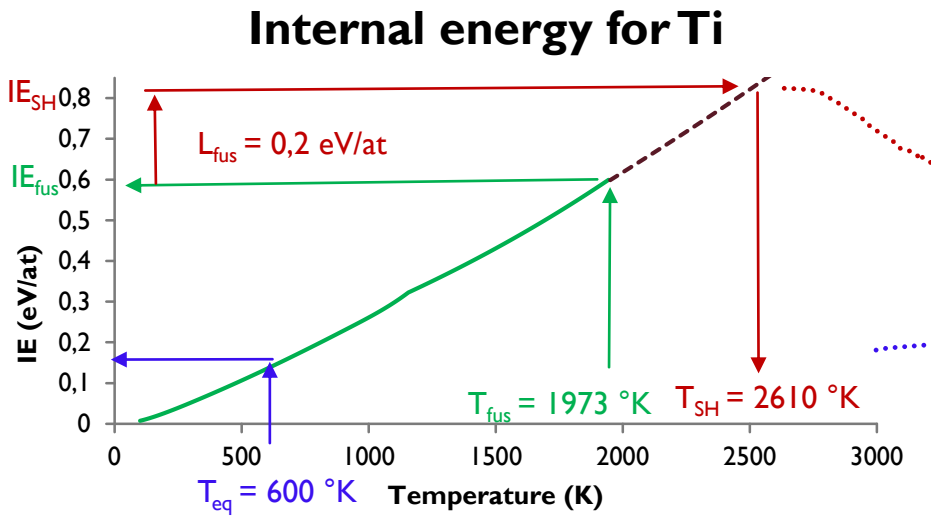


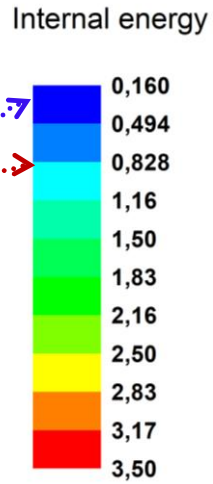


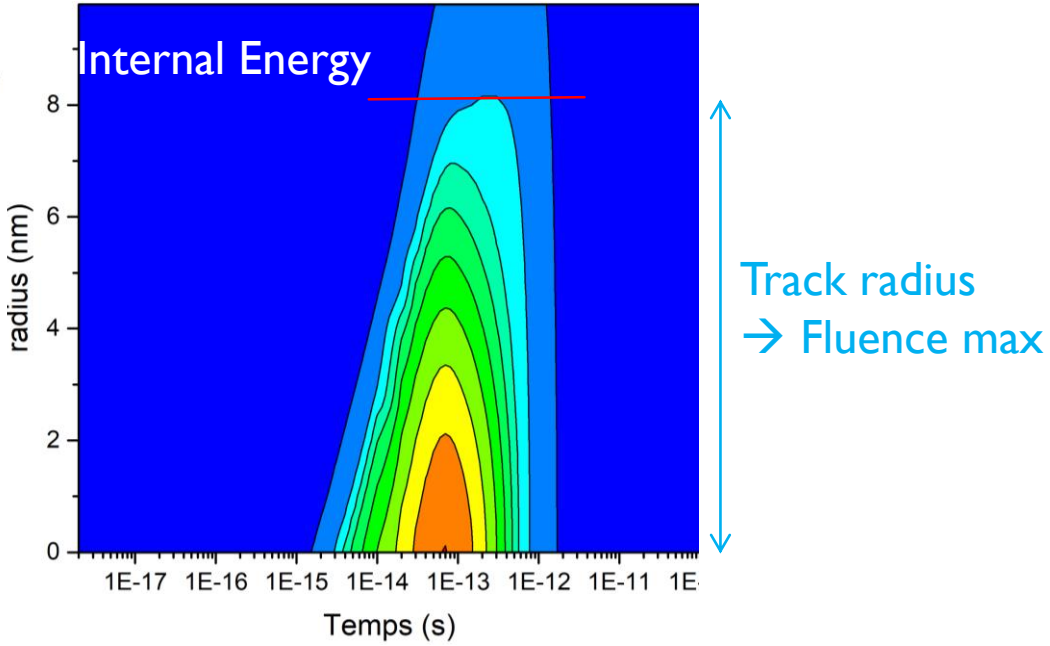
OUTPUTS OF THERMAL SPIKE MODEL

« Super-Heating » : Fast heating (~ 10^{-13} s) → material is not at equilibrium and its temperature increases above T_{fus} without melting;

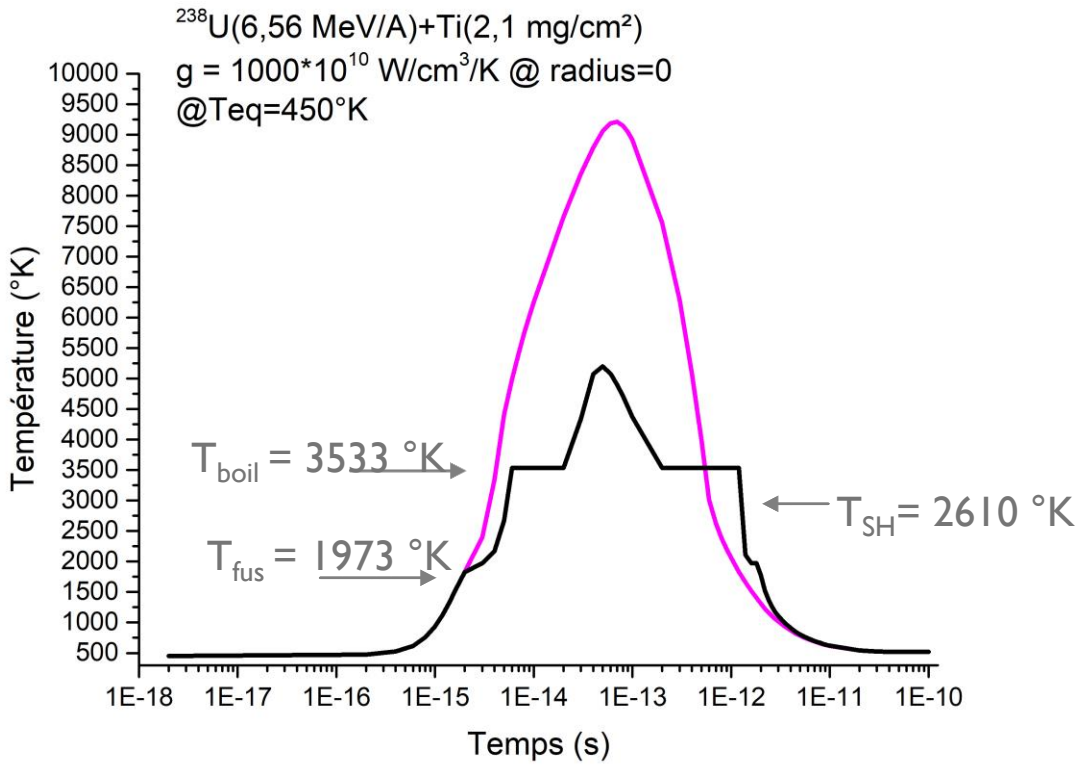
Melting occurs above a temperature limit, T_{SH}







OUTPUTS OF THERMAL SPIKE MODEL- PROJECTION @ RADIUS = 0



Inputs

$T_{fus} = T_{boil} = \infty$

T_{fus} = 1973°K & T_{boil} = 3533°K

APPLICATION TO PLUNGER EXPERIMENTS

Case 1 (E604): ^{238}U(6,2 MeV/u; 30 nA) + ^{64}Ni (2,6 mg/cm²) + Mg (5,2 mg/cm²)

No problem of target, degrader slightly deformed

Case 2 (E696): ^{238}U(6,76 MeV/u; 3 nA) + Cu (0,6 mg/cm²) + Ti (2,1 mg/cm²) + Mg (4,5 mg/cm²)

Target seriously deformed quickly I_{max}= 3 nA

Case 3 (E696): ^{238}U(6,76 MeV/u; 3 nA) + Ti (2,1 mg/cm²) + Mg (4,5 mg/cm²)

Target seriously deformed quickly I_{max}= 2 nA

Case 4 (E703): ^{50}Cr(200 MeV; 10 pnA) + Au(2,4 mg/cm²) +^{58}Ni (7-10 mg/cm²)

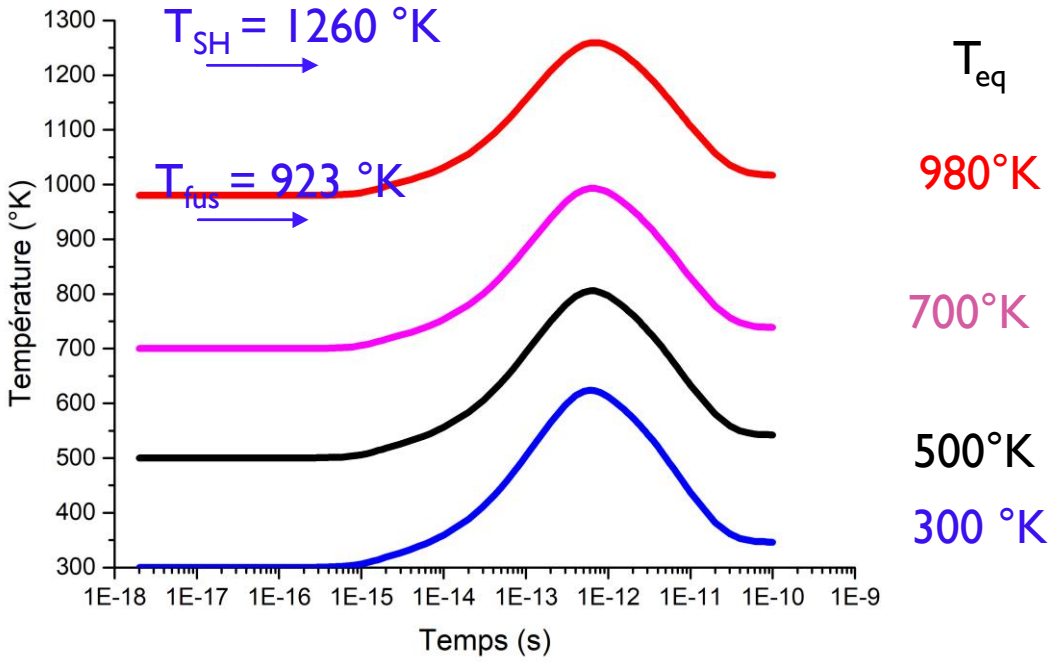
No problem

Case 5 (E667): ^{124}Xe(4 MeV/u; 1 pnA) + C (28 µg/cm²) +^{54}Fe (0,2 mg/cm²)

Some problem

APPLICATION TO PLUNGER EXPERIMENTS - *Mg*

Case 1-2-3: ^{238}U(5,2-5,75-5,95 MeV/u) + Mg (5,2-4,5 mg/cm²) → dE/dx = 1,93 keV/Å



Case 1: 540 mW → T_{eq} = 800±100 °K ≈ T_{fus}
but T_{calcTS} < T_{SH} degrader slightly deformed

Case 2/3: 48 mW → T_{eq} = 400±100 °K << T_{fus}
&& T_{calcTS} < T_{SH}

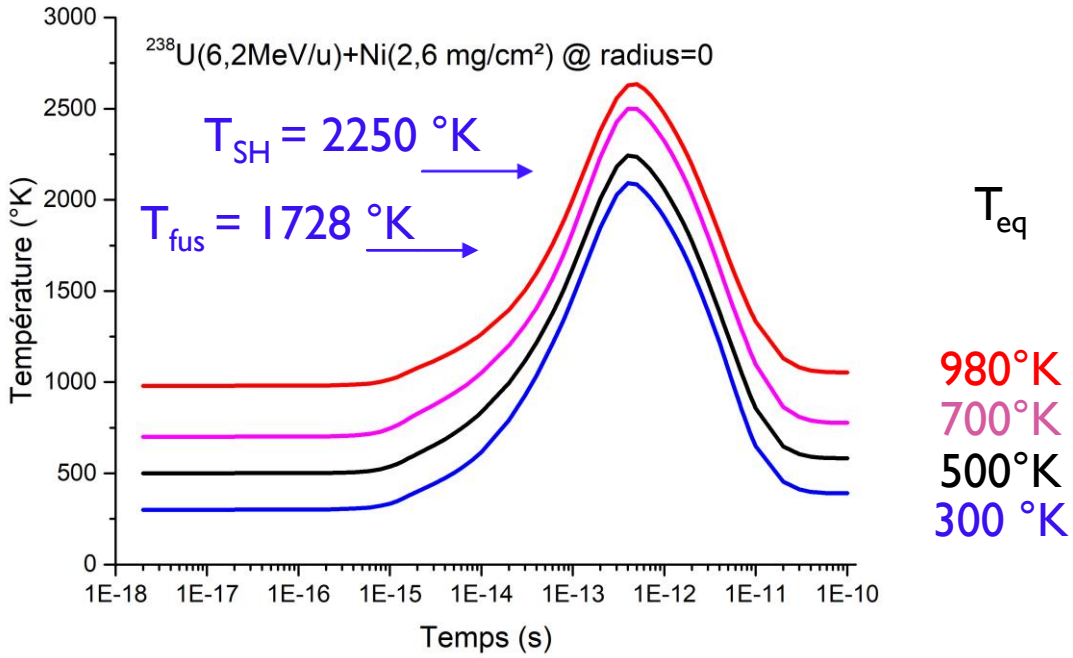
APPLICATION TO PLUNGER EXPERIMENTS - Ni

Case 1: ^{238}U(6,2 MeV/u; 30enA) + ^{64}Ni (2,6 mg/cm²)

dE/dx = 7,8 keV/Å

dP = 0,2 W → T_{eq} = 850±100 °K << T_{fus}

&& T_{calcTS} ≈ T_{SH} no problem

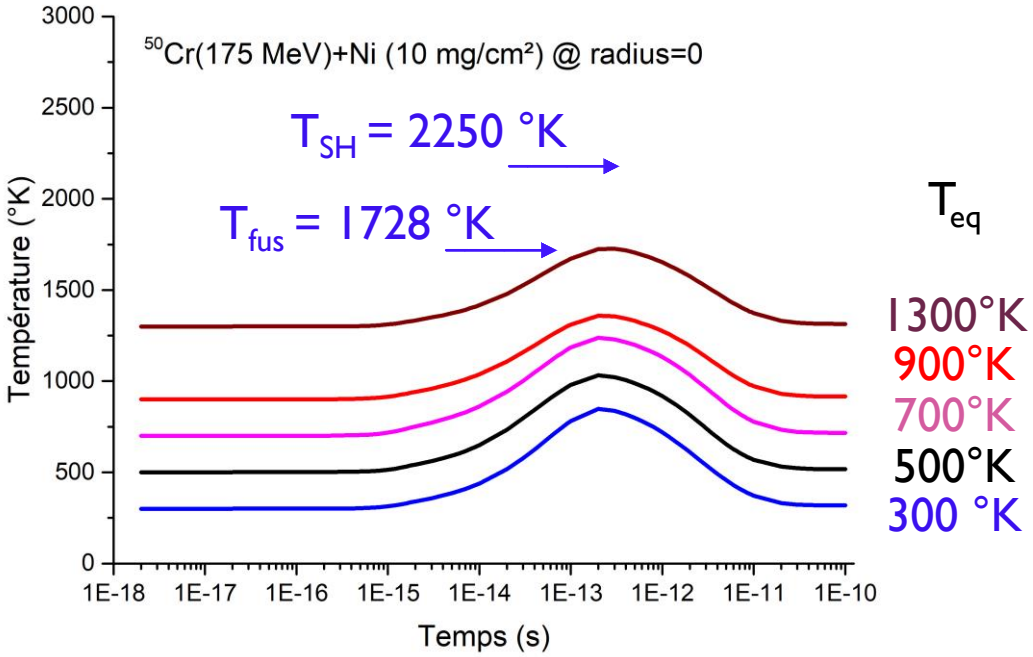


Case 4: ^{50}Cr(3,5 MeV/u; 10 pnA) + ^{58}Ni (7-10 mg/cm²)

dE/dx = 1,5 keV/Å

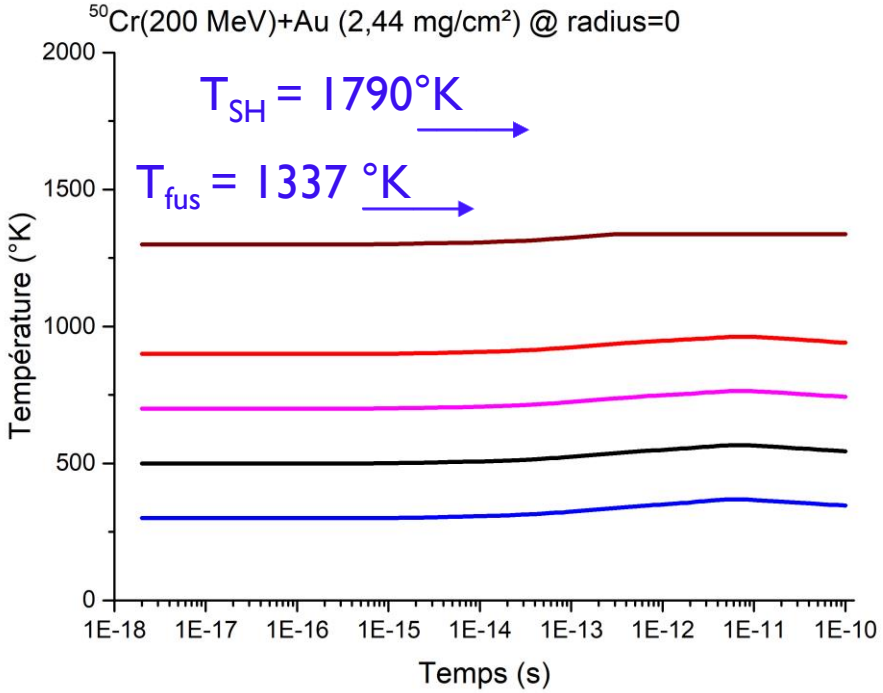
dP = 1,7 W → T_{eq} = 1000±100 °K < T_{fus}

&& T_{calcTS} << T_{SH} no problem



APPLICATION TO PLUNGER EXPERIMENTS - Au

Case 4: ^{50}Cr(4 MeV/u; 10 pnA) + Au(2,4 mg/cm²) → dE/dx = 2 keV/Å



T_{eq}

1300°K

900°K

700°K

500°K

300 °K

250 mW → T_{eq} = 750±100 °K < T_{fus}
&& T_{calcTS} << T_{SH}

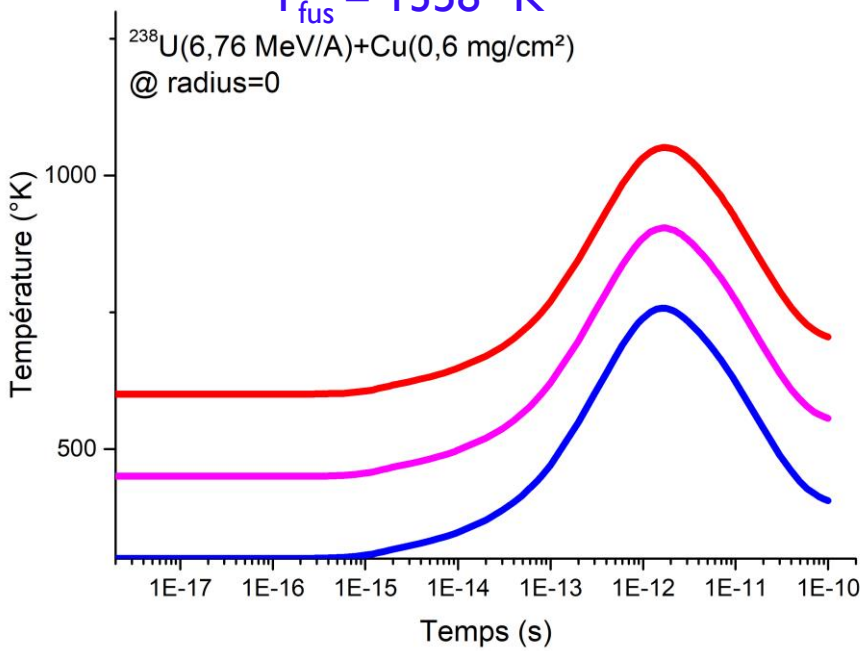
no problem

APPLICATION TO PLUNGER EXPERIMENTS - Cu

Case 2: ^{238}U(6,76 MeV/u) + Cu (0,6 mg/cm²) (+ Ti) → dE/dx = 7,2 keV/Å

T_{fus} = 1358 °K

T_{SH} = 1900 °K



T_{eq}

600°K

450°K

300 °K

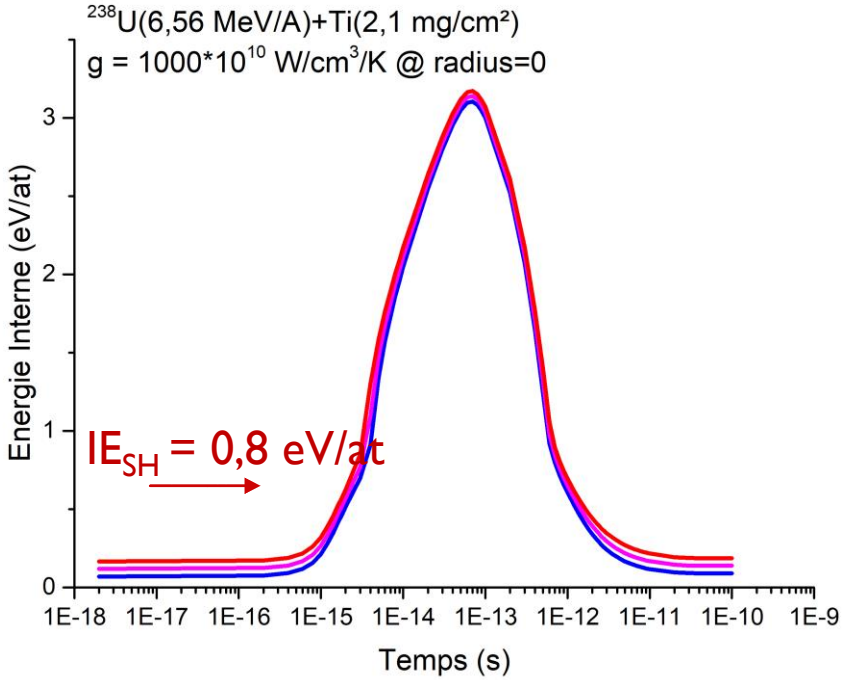
4mW → T_{eq}= 400±50 °K << T_{fus}
&& T_{calcTS} < T_{SH}

APPLICATION TO PLUNGER EXPERIMENTS - Ti

Case 2-3: ^{238}U(6,56-6,76 MeV/u) + Ti (2,1 mg/cm²) → dE/dx = 4,0 keV/Å

18mW → T_{eq}= 400-500±50 °K << T_{fus} but T_{calcTS} >>>T_{SH}

Target seriously deformed quickly

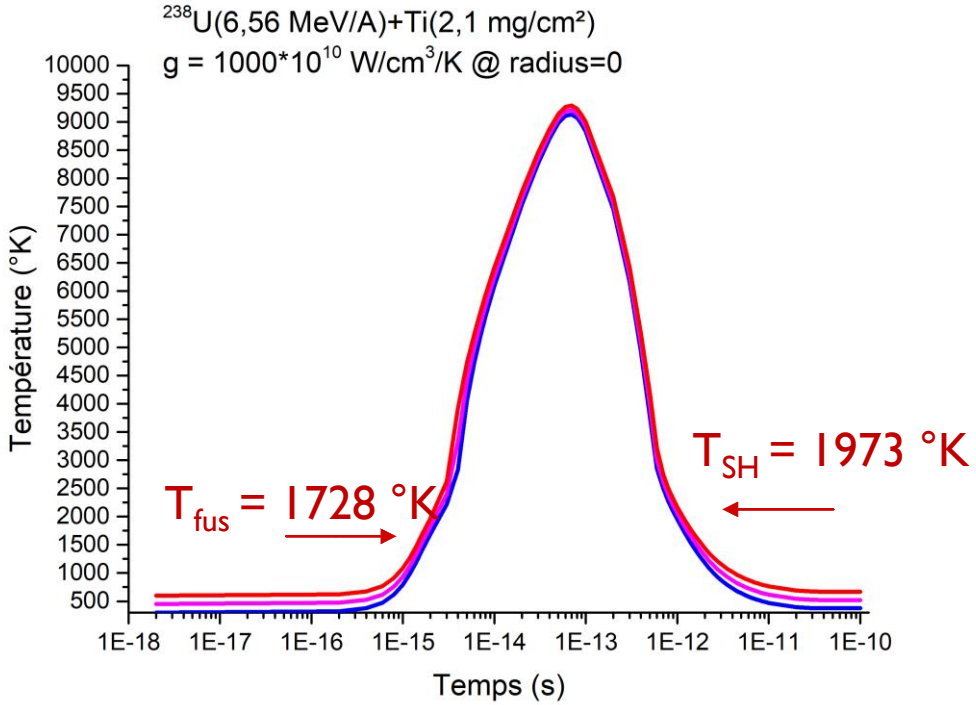


T_{eq}

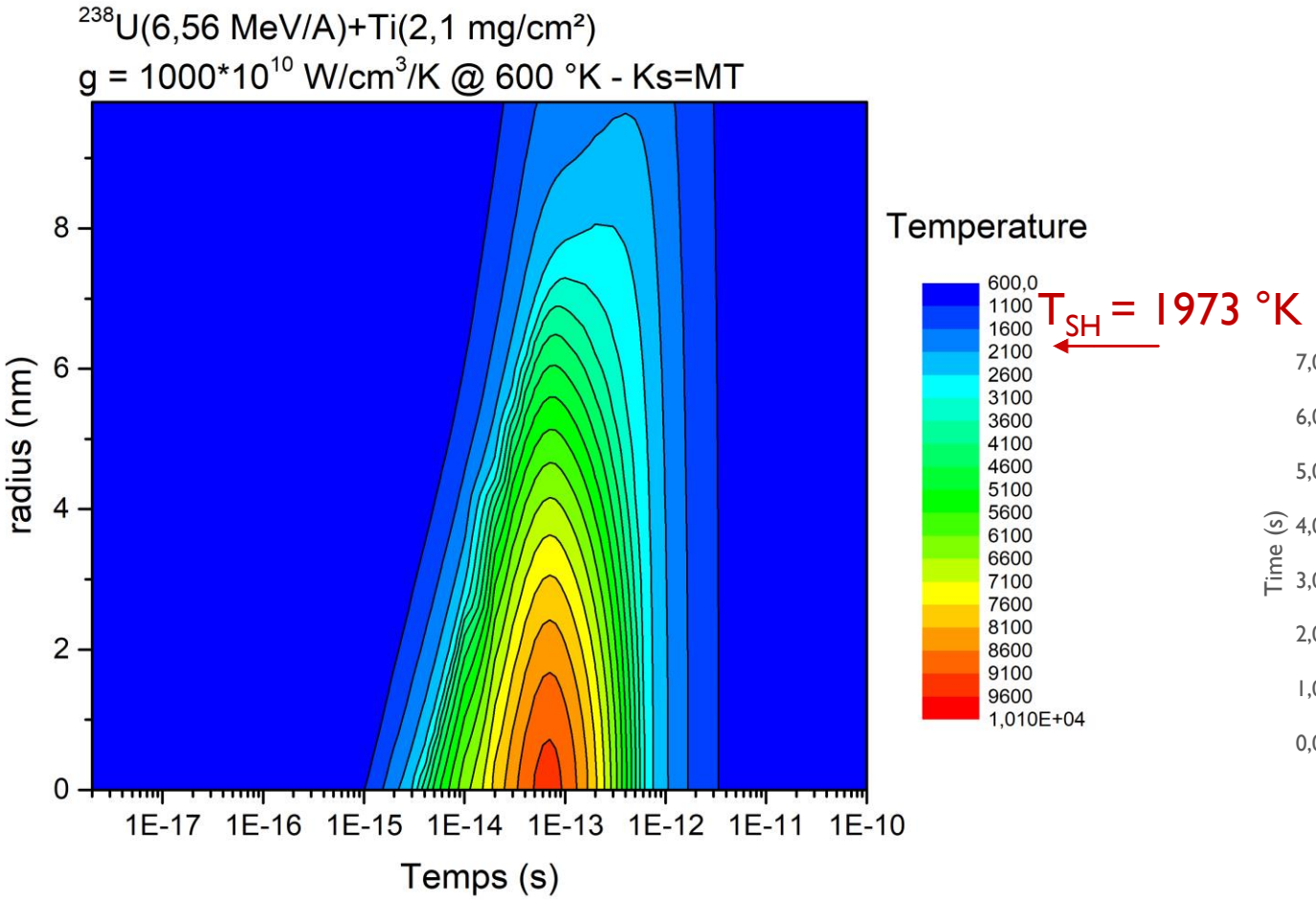
600°K

450°K

300 °K

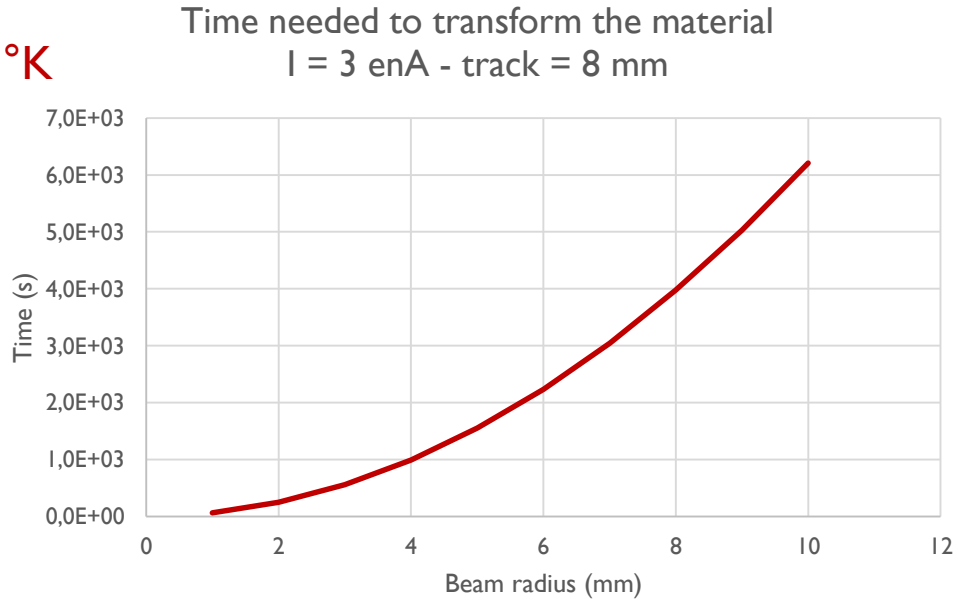


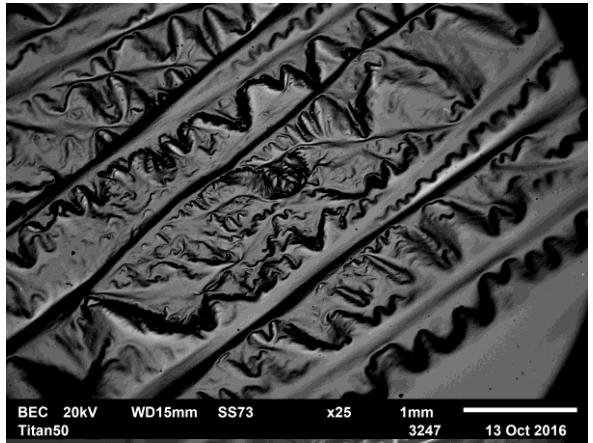
APPLICATION TO PLUNGER EXPERIMENTS - Ti

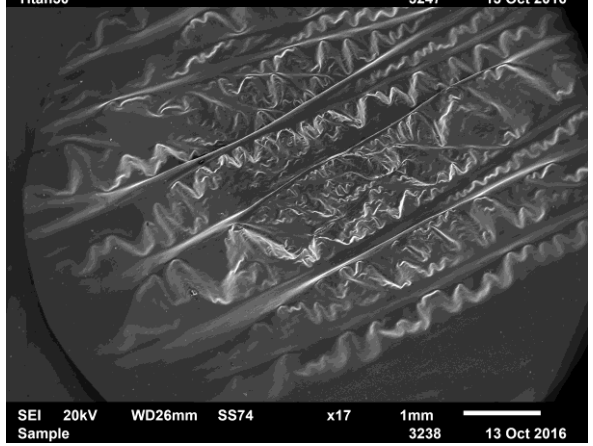


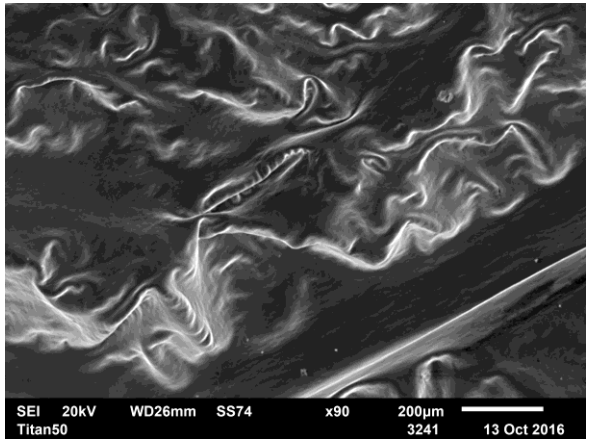
Target broken quickly

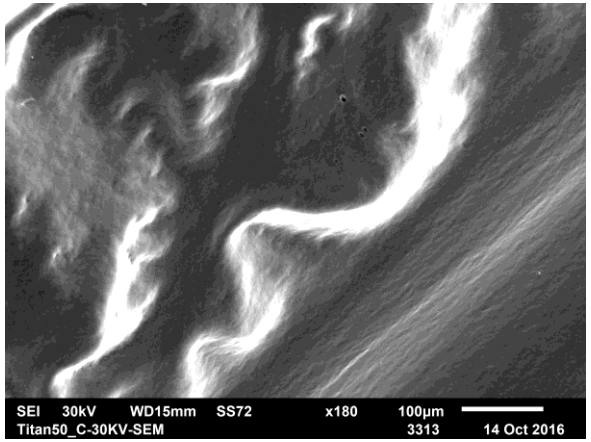
Track: 8mm → Fluence= $1,2*10^{12}$ part/cm²

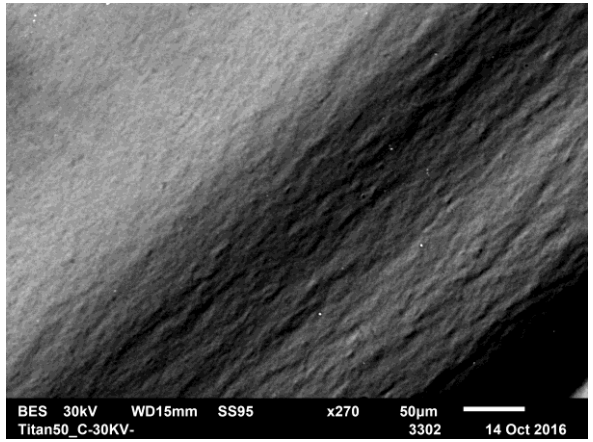


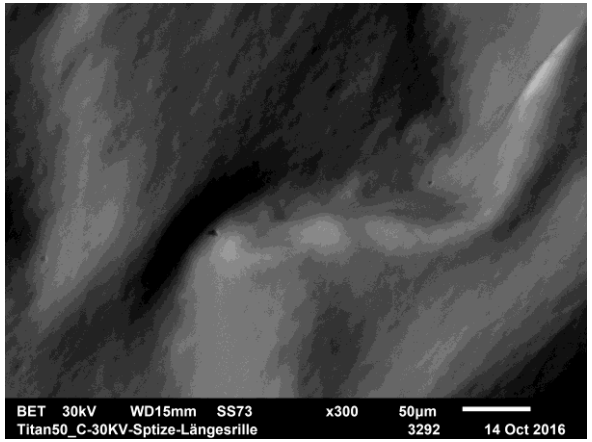












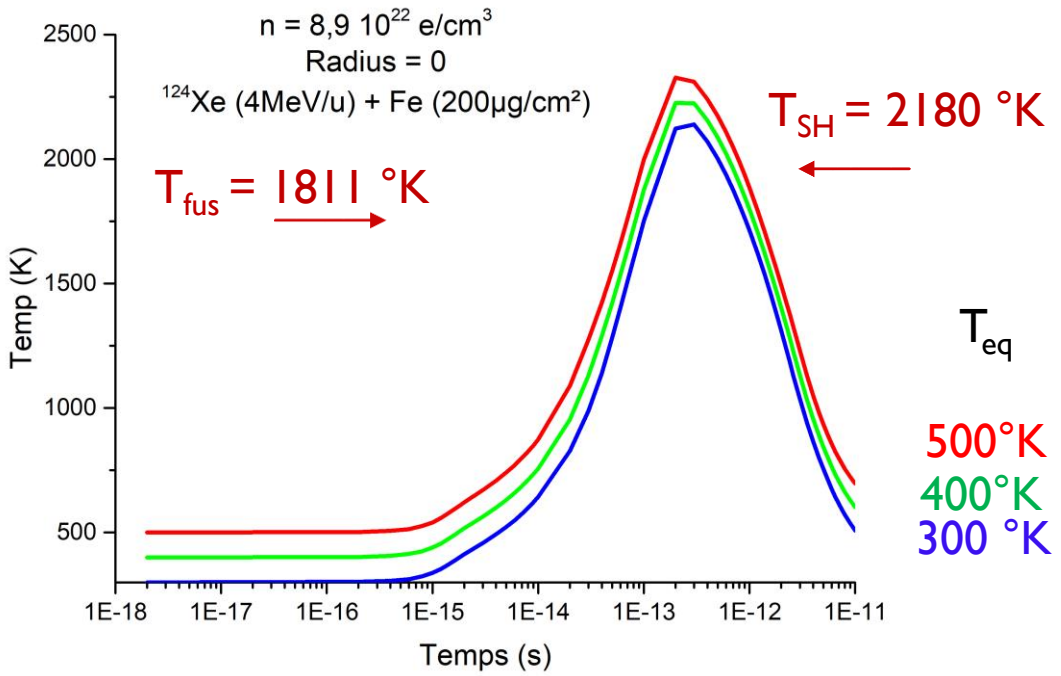
SCANNING ELECTRON MICROSCOPE PHOTOGRAPHS

- Back scattered (*25) and Secondary electrons (*25→ *300);
- With M>*300: « flat »;
- Height of wrinkles ~ 100 µm

- Target rolling might have induced a preferential direction
- Super-Heating overcome

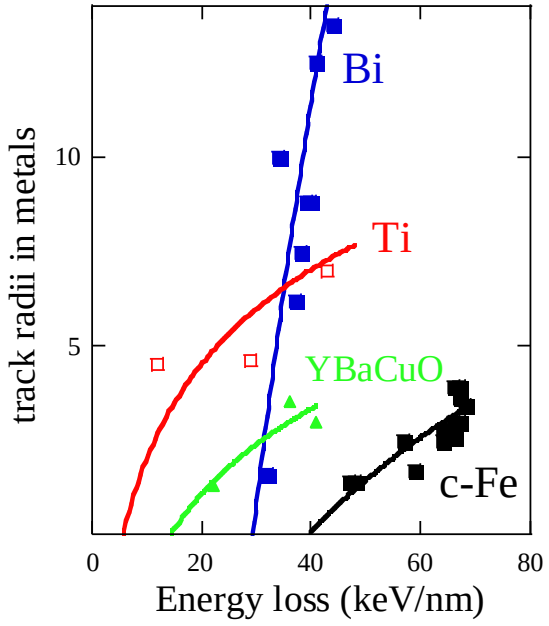
APPLICATION TO PLUNGER EXPERIMENTS – Fe

Case 5 (E667): ^{124}Xe(4 MeV/u) + C (28 µg/cm²) +^{54}Fe (0,2 mg/cm²) → dE/dx = 4 keV/Å



10 mW → T_{eq}= 450±50 °K > T_{fus}
&& T_{calcTS} > T_{SH}

- Problem : with 3 targets & 1 OK
- C+ Fe : phase change ??

CONCLUSIONS

- A set of experimental conditions analyzed with thermal spike model
- The local overheating could explain the degradation of some target such as iron and titanium (T_{calcTS} >>>T_{SH})
- Lesson learned:
  - take the necessary time to perform the calculations in realistic conditions taking into account a range of temperature at equilibrium and of the beam energy (→ dE/dx)
  - Choice of materials (pure or alloys…)
- Why not some systematic targets imaging after irradiation ?