



MODELIZATION OF RADIATION-INDUCED DAMAGE IN FLUKA AND MATERIAL DAMAGE ESTIMATES FOR CERN INJECTORS AND FUTURE FACILITIES

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FLUKA is a Monte Carlo code for calculations of particle transport and interactions with matter.

- Wide range of applications:
 - Proton and electron accelerator shielding, target design, calorimetry, activation, dosimetry, detector design, Accelerator Driven Systems, cosmic rays, neutrino physics, Radiotherapy, etc.

• Extensively used at CERN for:

- o Beam-machine interactions
- Radio-Protection calculations
- Facility design of future projects









Interaction and Transport Monte Carlo Code



- Hadron-nucleus interactions
- Nucleus-Nucleus interactions
- Electron interactions
- Photon interactions
- Muon interactions (inc. photonuclear)
- Neutrino interactions
- Decay

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• Low energy neutrons

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Info: http://www.fluka.org

- Ionization
- Multiple scattering
- Combinatorial geometry
- Voxel geometry
- Magnetic field
- Analogue or biased
- On-line buildup and evolution of induced radioactivity and dose
- User-friendly GUI thanks to *Flair*

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Different kinds of damage

from Radiation-Matter interaction

Precious materials (healthy/tragic damage)

energy (dose) deposition, radioisotope production and decay & positron annihilation and photon pair detection
 Oxidation by generation of chemically active radicals (e.g. PVC de-hydrochlorination by X and g-rays, radiolysis,...)

Accidents energy (power) deposition

Gas production

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Degradation energy (dose) deposition, particle fluence, DPA

residual nuclei production

Electronics high energy hadron fluence, neutron fluence, energy (dose) deposition

Activation residual activity and dose rate

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DPA as Radiation Damage Estimator

The **dpa** quantity is a measure of the amount of radiation damage in irradiated materials. It means the **average number of displacements that every atom in the crystal structure has suffered**.

$$dpa = \frac{A}{N_A \rho} N_F$$

A is the mass number N_A is the Avogadro number ρ is the density N_F is the number of defects or *Frenkel pairs*.

Experimentally: no direct determination. Indirect through study of macroscopic effects (electric and thermal conductivities, radiation hardening, swelling...)

Amount of dpa \iff Macroscopic effects







Frenkel pairs

 Frenkel pair N_F (defect or disorder), is a compound crystallographic defect formed when an atom or ion leaves its place in the lattice (leaving a vacancy), and lodges nearby in the crystal (becoming an interstitial)

$$N_{_{NRT}} \equiv N_{_{F}} = \kappa \frac{\xi(T)T}{2E_{_{th}}}$$

N_{NRT} Defects by Norgert, Robinson and Torrens

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- $\kappa=0.8$ is the displacement efficiency
- *T* kinetic energy of the primary knock-on atom (PKA)
- $\xi(T)$ partition function (LSS theory)
- $\xi(T)$ T directly related to the NIEL(non ionizing energy loss)
- *E_{th}* damage threshold energy

S T







Damage Threshold

 $N_{NRT} \equiv N_F = \kappa \frac{\xi(T)T}{\xi(E_{th})}$

From: NEA/NSC/DOC(2015)9

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- Damage threshold depends on the direction of the recoil in the crystal lattice.
- Also depends on the compound combination: e.g. NaCl: E_{th}(Na-Na), E_{th}(Na-Cl), E_{th}(Cl-Na), E_{th}(Cl-Cl)
- FLUKA use the "average" threshold over all crystallographic directions (user defined)
- Sensitivity studies using different E_{th} values can provide upper and lower limits on dpa





Displacement efficiency κ Stoller vs Nordlund

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 $N_{_{NRT}} \equiv N_{_{F}} =$







Lindhard partition function ξ









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The total (S), nuclear (S_n) and electronic (S_e) stopping power. The partition

function $S_n/(S_n+S_e)$ is also plotted. The abscissa is the ion total kinetic energy

Partition function decreases with energy And increases with charge

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NIEL/DPA are dominated by Low energy (heavy) recoils

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Restricted Nuclear Stopping Power



- Lindhard approximation uses the unrestricted NIEL. Including all the energy losses also those below the threshold $E_{th} \rightarrow Overestimation of DPAs$
- FLUKA is using a more accurate way by employing the restricted nuclear losses

$$S(E, E_{th}) = N \int_{E_{th}}^{\gamma E} T\left(\frac{d\sigma}{dT}\right) dT$$

where:

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 $S(E,E_{th}) = \frac{S(E,E_{th})}{N}$ is the restricted energy loss atomic density T = energy transfer during ion-solid interaction $d\sigma/dT$ differential scattering cross section $\gamma = \frac{2E(2m+E)}{M + \frac{m^2}{M} + 2(m+E)}$ maximum fraction of energy transfer during collision



Comparison with other simulation codes

 ^{76}Ge ion pencil beam of 130 MeV/A uniform in W target a disc of R=0.3568 mm, 1.2 mm thickness









FLUKA Implementation

Charged particles and heavy ions

- **During transport** Calculate the restricted non ionizing energy loss
- Below threshold Calculate the integrated nuclear stopping power with the Lindhard partition function
- At (elastic and inelastic) interactions
 Calculate the recoil, to be transported or treated as below threshold

Neutrons:

- High energy E_n>20 MeV
 - Calculate the recoils after interaction Treat recoil as a "normal" charged particle/ion
- Low energy E_n≤20 MeV (group-wise)
 - Calculate the NIEL from NJOY
- Low energy E_n≤20 MeV (point-wise)
 - Calculate the recoil if possible Treat recoil as a "normal" charged particle/ion

Implementation in FLUKA: A. Fasso et al. Prog. In Nucl. Science and Technology, Vol. 2, p769-775 (2011)







Example of fission/evaporation

1 A GeV ²⁰⁸Pb + p reactions Nucl. Phys. A 686 (2001) 481-524





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Isotope production for natFe(p,x):





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Estimates for CERN injectors and future facilities

- Beam Dump Facility
- BLIP capsule
- PS Internal Beam Dumps







Beam Dump Facility (BDF)

Beam:

- Protons: 400 GeV/c
- Sweep pattern:
 - radius 3 cm
 - 1σ 0.6 cm

Geometry:

 1.4 m long cylinder discs of TZM enclosed in Ta W enclosed in Ta
 1.5 mm Ta cladding and 5 mm water gaps

Materials:

- Tungsten $E_d = 90 \text{ eV}$
- SS 316N E_d=40 eV
- Tantalum $E_d = 53 \text{ eV}$

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• TZM (Mo,Zr,Ti...) E_d=60 eV









BDF Results: H/He[appm] vs DPA





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BLIP capsule

- Beam
 - Proton E=181 MeV
 - $\sigma_{x,y} = 5.1 \text{ mm}$
- Geometry: Layers of

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DPA High-Z BLIP [FLUKA vs MARS]



Courtesy: J. Canhoto-Espadanal

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Note: NRT model of MARS





H appm/DPA High-Z BLIP





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He appm/DPA High-Z BLIP Probably due to "Old" MARS event generator used



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PS Internal Beam Dumps

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Challenging Energy density

Superficial energy deposition

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PS Internal Beam Dumps: Damage

Beam properties:

- 26 GeV/c proton beam
- 2.4e17 POT per year
- $\sigma_{\rm h}$ =1.74 mm $\sigma_{\rm v}$ =0.87 mm
- Beam is shaved in a thin top most layer

Graphite:

Experience at CERN with **CNGS** air cooled graphite target (SPS beam). About 1200°C reached for each pulse. At the end of operation: 1.5 DPA

 \rightarrow No problem observed on graphite

Damage threshold energies considered: $E_{th}(Graphite) = 30 \text{ eV} - \text{ typical value 30-35 eV}$ $E_{th}(CuCrZr \text{ and }SS304L) = 40 \text{ eV}$

CuCrZr:

Literature on neutron irratiation indicated for **similar dpa damage some** possible radiation hardening and thermal conductivity **degradation but not dramatic** effects

Summary

- FLUKA dpa model uses a **restricted NIEL** computed during initialization and run time.
- Not based on Lindhard but reworked all formulas
- The **only free parameter** for the user is the **damage threshold.** It depends on the direction of the recoil. Simple averaging is not correct
- Uniform treatment from the transport threshold up to the highest energies
- Use of Stoller displacement efficiency instead of a fixed 0.8 as NRT suggests
- Not considered thermal recombination of defects -> overestimation of dpa.
 Improving the estimate would require Molecular Dynamics simulations

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Summary

- FLUKA is employed to evaluate radiation-induced damage on new dumps facilities (BDF, BLIP) and elements of the CERN injector chain (PS internal dumps)
- Simulations provided a way of quantifying the damage through estimation of dpa and gas production (H, He)
- Comparison of estimations of dpa (simulations) and modifications of macroscopic quantities (experimental: thermal, electric, etc..., properties) helps to extract conclusions on radiation-induced damage

Possible Future improvements:

- Implementation of the Nordlund arc-dpa
- More accurate recoil momentum cross section for pair production and Bremsstrahlung
- Point wise treatment of low energy neutrons will provide correct recoil
 information
- Multiple damage thresholds for compounds

Thank you for your attention!

Any question?

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Extra slides

E_{th} Damage Threshold Energy

• *E_{th}* is the value of the threshold displacement energy averaged over all crystallographic directions or a minimum energy to produce a defect

Element	Eth(eV)	Element	Eth(eV)
Lithium	10	Со	40
C in SiC	20	Ni	40
Graphite	3035	Cu	40
AI	27	Nb	40
Si	25	Мо	60
Mn	40	W	90
Fe	40	Pb	25

Typical values used in NJOY99 code

• The only variable requested for FLUKA MAT-PROP $WHAT(1) = E_{th} (eV)$ WHAT(4,5,6) = Material rangeSDUM = DPA-ENER

Damage Threshold in Compounds

> NJOY (MT=444) sums up the cross section multiplied by the damage energies, which is the damage production cross section representing the effective kinetic energy of recoiled atom for reaction types *i* at neutron energy E_n

$$(E\sigma)_{DPA} = \sum_{i} E_{th,i}\sigma_i(E_n)$$

Problematic:

- Damage threshold depends on the lattice structure
- Damage threshold can be quite different for each combination for the specific compound

e.g. NaCl: E_{th} (Na-Na), E_{th} (Na-Cl), E_{th} (Cl-Na), E_{th} (Cl-Cl)

- Simple weighting with the atom/mass fraction doesn't work
- FLUKA's approximation is using a unique average damage threshold E_{th} for the compounds as well → A sensitivity study can be performed

Only free parameter for the FLUKA user is E_{th}

к displacement efficiency

- κ=0.8 value deviates from the hard sphere model (K&P), and compensates for the forward scattering in the displacement cascade
- The displacement efficiency κ can be considered as independent of T only in the range of $T \le 1-2 \text{ keV}$. At higher energies, the development of collision cascades results in defect migration and recombination of Frenkel pairs due to overlapping of different branches of a cascade which translates into decay of $\kappa(T)$.
- From molecular dynamics (MD^{*}) simulations of the primary cascade the number of surviving displacements, N_{MD} , normalized to the number of those from NRT model, N_{NRT} , decreases down to the values about 0.2–0.3 at $T \approx 20-100 \text{ keV}$. The efficiency in question only slightly depends on atomic number Z and the temperature. $N_{MD}/N_{NRT} = 0.3-1.3$

$$N_{MD} / N_{NRT} = 0.3 - 1.3 \left(-\frac{9.57}{X} + \frac{17.1}{X^{4/3}} - \frac{8.81}{X^{5/3}} \right)$$

where $X \equiv 20 T$ (in keV).

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sequence of two-body elastic

 In the collision process, the energy transferred to the lattice is zero

The cascade is created by a

- For all energies T < E_c electronic stopping is ignored and only atomic collisions take place. No additional displacement occur above the cut-off energy E_c
- The energy transfer cross section is given by the hard-sphere model.

Factor of 2 (Kinchin & Pease)

Schematic relation between the number of displaced atoms in the cascade and the kinetic energy T of the primary knock-on atom

Energy is equally shared between two atoms after the first collision Compensates for the energy lost to sub threshold reactions

Lindhard partition function ξ ^[1/2]

- The partition function gives the fraction of stopping power S that goes to NIEL
- Approximations used: Electrons do not produce recoil nuclei with appreciable energy, lattice binding energy is neglected, etc...

$$(S_n + S_e)E'_n(E) = \int E_n(T)\frac{d\sigma_n}{dT}dT$$

 $S_{n_{\ell}}(E) = \int T_{n_{\ell}} d\sigma_{n_{\ell}}$

where

approximated to

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$$\xi(T) = \frac{1}{1 + F_L \cdot (3.4008 \cdot \varepsilon(T)^{1/6} + 0.40244 \cdot \varepsilon(T)^{3/4} + \varepsilon(T))}$$

$$F_{L} = 30.724 \cdot Z_{1} \cdot Z_{2} \sqrt{Z_{1}^{2/3} + Z_{2}^{2/3}}$$

$$\varepsilon(T) = \frac{T}{0.0793 \frac{Z_{1}^{2/3} \cdot \sqrt{Z_{2}}}{(Z_{1}^{2/3} + Z_{2}^{2/3})^{3/4}} \cdot \frac{(A_{1} + A_{2})^{3/2}}{A_{1}^{3/2} \sqrt{A_{2}}}}$$

Z,A charge and mass
1 projectile
2 medium
T recoil energy (eV)

Nice feature: It can handle any projectile Z_1, A_1 whichever charged particle

Nuclear Stopping power

• Nuclear stopping power (unrestricted)

$$\frac{1}{\rho}S_n(E,E_{th}) = -2\pi N \int_0^{b \max} \frac{db}{d\theta} W(\theta,E) db$$

• Energy transferred to recoil atom

$$W(\theta,T) = \gamma T \sin^2(\theta/2)$$

• Deflection angle, by integrating over all impact parameters b

$$\theta = \pi - 2\int \frac{bdr}{r^2 \sqrt{1 - \frac{V(r)}{E_{cms}} - \frac{b^2}{r^2}}}$$

• Universal potential

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$$V(r) = \frac{Z_1 Z_2 e^2}{r} F_s \left(\frac{r}{r_s}\right)$$

where:

$$F_{s}(x) = \Sigma a_{i} \exp(-c_{i} x)$$

$$r_{s}=0.88534 r_{B} / (Z_{1}^{0.23} + Z_{2}^{0.23})$$

$$r_{s}=0.88534 r_{B} Z_{1}^{-1/3}$$

screening function screening length in case of particle

Ziegler approximation

• Reduced kinetic energy ε (*T* in keV)

$$\varepsilon = \frac{32.536 \ T}{\left(Z_1^{0.23} + Z_2^{0.23}\right) \left(1 + \frac{M_1}{M_2}\right) Z_1 Z_2}$$

Reduced stopping power

if
$$\varepsilon < 30$$
 $\hat{S}_n(\varepsilon) = \frac{0.5 \ln(1+1.1383 \varepsilon)}{\varepsilon + 0.01321 \varepsilon^{0.21226} + 0.19593 \sqrt{\varepsilon}}$
if $\varepsilon \ge 30$ $\hat{S}_n(\varepsilon) = \frac{\ln(\varepsilon)}{2\varepsilon}$

Important features of Reduced Stopping Power

- Independent from the projectile and target combination
- Accurate within 1% for ε <1 and to within 5% or better for ε >3
- Stopping power (MeV/g/cm²)

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$$\frac{1}{\rho}S_{n}(T) = \frac{5105.3 \ Z_{1}Z_{2} \ \hat{S}_{n}(\varepsilon)}{\left(Z_{1}^{0.23} + Z_{2}^{0.23}\right)\left(1 + \frac{M_{2}}{M_{1}}\right)A}$$

Restricted Stopping Power

• The restricted nuclear stopping power is calculated the same way only integrating from 0 impact parameter up to a maximum b_{max} which corresponds to a transfer of energy equal to the $E_{th} = W_{min}(\theta_{min}, T)$

$$\frac{1}{\rho}S_n(E,E_{th}) = -2\pi N \int_0^{b\max} \frac{db}{d\theta} W(\theta,E) db$$

• To find b_{max} we have to approximately solve the previous θ integral using an iterative approach for

$$\theta_{min} = 2 \arcsin\left(\sqrt{\frac{E_{th}}{\gamma T}}\right)$$

This can be done either by integrating numerically for θ or using the magic scattering formula from Biersack-Haggmark that gives a fitting to $sin^2(\theta/2)$

Implementation: Charged Particles

- During the transport of all charged particles and heavy ions the dpa estimation is based on the restricted nuclear stopping power while for NIEL on the unrestricted one.
- For every charged particle above the transport threshold and for every Monte Carlo step, the number of defects is calculated based on a modified multiple integral
- Taking into account also the second level of sub-cascades initiated by the projectile

$$N(E) = \int_{E_{th}}^{\gamma E} \left[\xi_r(T, E_{th}) \left(\frac{d\sigma}{dT} \right)_E \int_{E_{th}}^{\gamma T} \kappa(T') \xi(T') T' \left(\frac{d\sigma}{dT'} \right)_T dT' \right] dT$$
Induction function

• Below the transport threshold (1 keV) it employs the Lindhard approximation

Group Wise Neutron Artifacts

- Due to the group treatment of low-energy neutrons, there is no direct way to calculate properly the recoils.
- Therefore the evaluation is based on the KERMA factors calculated by NJOY, which in turn is based on the Unrestricted Nuclear losses from using the NRT model.

Implementation: others

For Bremsstrahlung and pair production the recoil is sampled randomly from an approximation of the recoil momentum cross section

Bremsstrahlung

$$\frac{d\sigma}{dp_{\perp}} = \frac{32a(Za)^2}{kp_{\perp}^3} \left[1 - \frac{k}{E} + \frac{1}{2} \left(\frac{k}{E}\right)^2 \right] \ln\left(\frac{p_{\perp}}{m_e}\right)$$

Pair production

$$\frac{d\sigma}{dp} = \frac{0.183 \cdot 10^{-2} Z^2}{p^3} (\ln(p) + 0.5)$$

both can be written in the same approximate way as

$$\frac{d\sigma}{dp} \propto \frac{\ln(p/c)}{p^3}$$

where the recoil momentum is sampled randomly by rejection from a similar function

Coalescence:

- > d, t, ³He, and alpha's generated during the (G)INC and preequilibrium stage
- All possible combinations of (unbound) nucleons and/or light fragments checked at each stage of system evolution
- FOM evaluation based on phase space "closeness" used to decide whether a light fragment is formed rather than not
 - FOM evaluated in the CMS of the candidate fragment at the time of minimum distance
 - Naively a momentum or position FOM should be used, but not both due to quantum non commutation
 - ... however the best results are obtained with a Wigner transform FOM (assuming gaussian wave packets) which should be the correct way of considering together positions and momenta
- Binding energy redistributed between the emitted fragment and residual excitation (exact conservation of 4-momenta)

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Coalescence

High energy light fragments are emitted through the coalescence mechanism: "put together" emitted nucleons that are near in phase space.

Example : double differential t production from 542 MeV neutrons on Copper Warning: coalescence is OFF by default Can be important, ex for . residual nuclei.

To activate it:

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COALESCE

If coalescence is on, switch on Heavy ion transport and interactions (see later)

Particle production in C(p,x) reaction

H,He production from p on C

Data: JNST36 313 1999, PRC7 2179 1973

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Energy Density Distribution from FLUKA

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Structural Damage on Dump Core

Lower general damage than current dump (~1 order of magnitude)

Lower peak DPA on copper region than current dump (~2 orders of magnitude)

Graphite protects the copper block from structural damage

Damage threshold energies considered: $E_{th}(Graphite) = 30 \text{ eV} - \text{ typical value 30-35 eV}$ $E_{th}(CuCrZr \text{ and } SS304L) = 40 \text{ eV}$

POT=2.4e17 (assumed same POT for current and future dumps)

PS Dump Review Meeting

Irradiation on Graphite

0.03 DPA/year estimated in Graphite block of PS dump

Experience at CERN: CNGS air cooled graphite target (SPS beam)

- \rightarrow About 1200°C reached for each pulse
- \rightarrow At the end of operation: **1.5 DPA**
- ightarrow No problem observed on graphite

Graphite rods 2020PT (Mersen)

[*Ref*]: Spallation materials R&D for CERN's fixed target program, M. Calviani et al. IWSMT, Oct. 2014, Austria

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→3.5 x 10¹³ protons per pulse,
 →10.5 µs pulse length < 1 mm spot size
 →2 extractions per cycle separated by 50 ms, occurring every 6 s
 → 2 000 000 extractions achieved by end of 2009
 → 4.5 x 10¹⁹ protons at 400 GeV/c on CNGS target per year

PS dump graphite irradiation shall not be a concern

04/10/2017

PS Dump Review Meeting

Irradiation on CuCrZr

- Peak value obtained of 0.002 DPA per year (0.04 DPA in 20 years) in CuCrZr block of PS Dump
- Localized peak DPA
- Information for neutron irradiation found in literature
- CuCrZr shows radiation hardening until saturation values around 0.1 - 0.5 DPA [1][3] \rightarrow Some hardening may occur
- CuCrZr is void swelling resistant [1][2] (below 2% density change for up to 150 DPA [1])
- Some thermal conductivity degradation may occur (5 - 10% reduction for doses > 0.1 DPA at < 150 °C [2])

[1] C. Bobeldijk (ed.). (1994). Atomic and Plasma-Material Interaction Data for Fusion. Vol. 5. Supplement to the Journal Nuclear Fusion

[2] S.A. Fabritsiev & S.J. Zinkle & B.N. Singh. (1996). Evaluation of copper alloys for fusion reactor divertor and first wall components. Journal of Nuclear Materials. Vol. 233-237. pp. 127-137.

[3] M. Li & M.A. Sokolov & S.J. Zinkle. (2009). Tensile and fracture toughness properties of neutron-irradiated CuCrZr, Journal of Nuclear Materials, Vol. 393, pp. 36-46.

10 Damage Level (dpa)

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FIG. 21. Effect of solid transmutations on the thermal conductivity of copper at a fusion reactor first wall. The calculations were performed for three different initial conductivities, expressed in terms of percent International Annealed Copper Standard (IACS).

1.5

1st Wall Fluence (MW-yr/m²)

2 2.5 3

1

[1]

85% IACS

55% IACS

0.5

400

300 tivity

250

200

100

0

ŝ 350

-m/m)

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> Fig. 3. Irradiation-induced swelling of neutron-irradiated copper and copper alloys. (a) Temperature dependence of void swelling in copper [20]. (b) Dose dependence of volumetric swelling in pure copper and copper alloys at ~ 400°C [17-19,21,23].

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