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Determination of the primary damage production in ionic-covalent complex oxides : the DART code

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Cooking elements for processing the damage energy with the DART code

Interest

Damage energy calculated taking into account all interactions for complex targets (multi components)

Post processing of the nuclear data : the damage energy is calculated for each isotope

- ENDF format libraries (ENDF-B, JEFF, TENDL...)
- Impact of the Fission Products on the energy partitioning

Determination of the energy partitioning

- BCA within the LSS theory : electronic (Se) and nuclear stopping power (Sn)

Lindhard formalism for Sn, Ziegler tabulation for Se

- averaging over isotopes and not species (different from SPECOMP)

Results

- determination of Primary Knocked-on Atoms spectra (PKA spectra)
- determination of energy partitioning : recoil spectra (ion, neutron, electron)
- DPA rate calculation

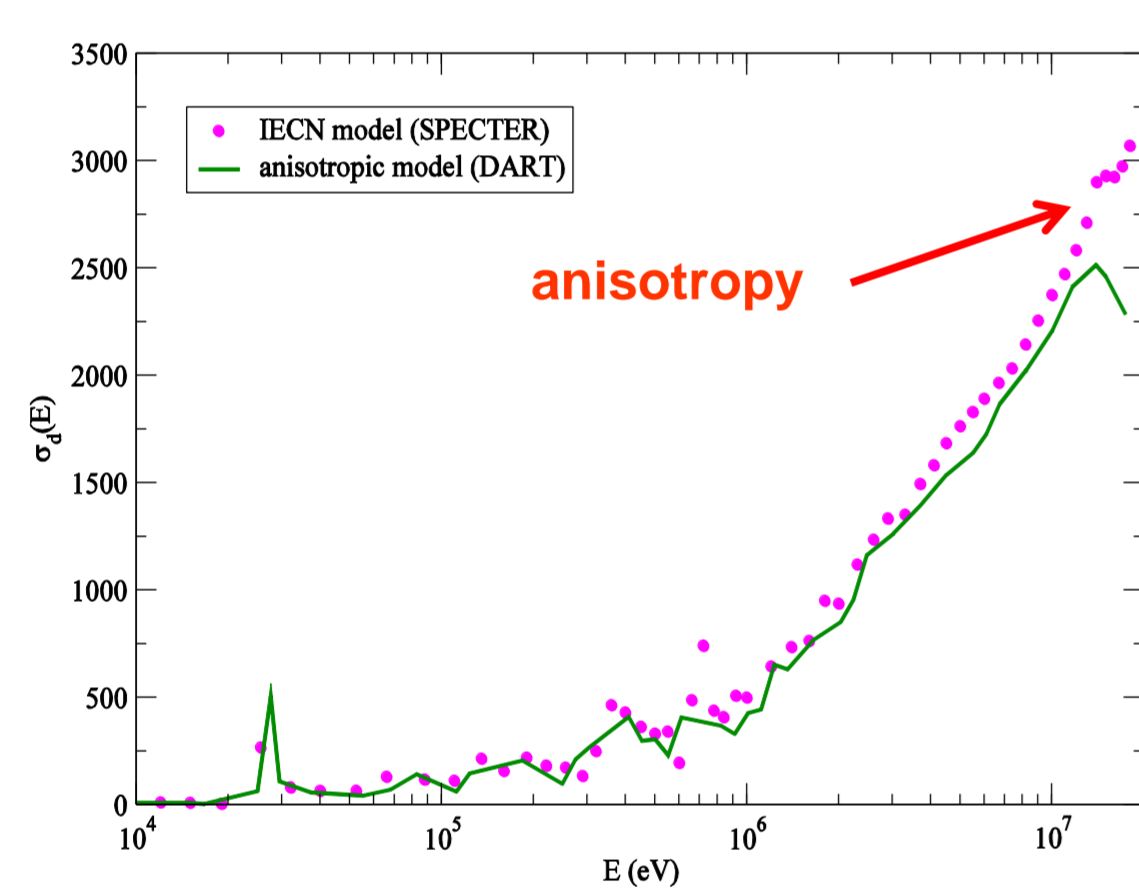
Limitations

- uncertainties on the neutron cross sections libraries not taken into account
- Se neglected in the formation of defects
- no link with MD simulations for calculating the real number of defects (loops, voids..)

Application to ceramics

Anisotropy

- Measured cross sections different from the isotropic intra cascade model (IECN) noticeable impact above 10 MeV...
- Discrepancies in the distribution of the displacement cross section at high energy



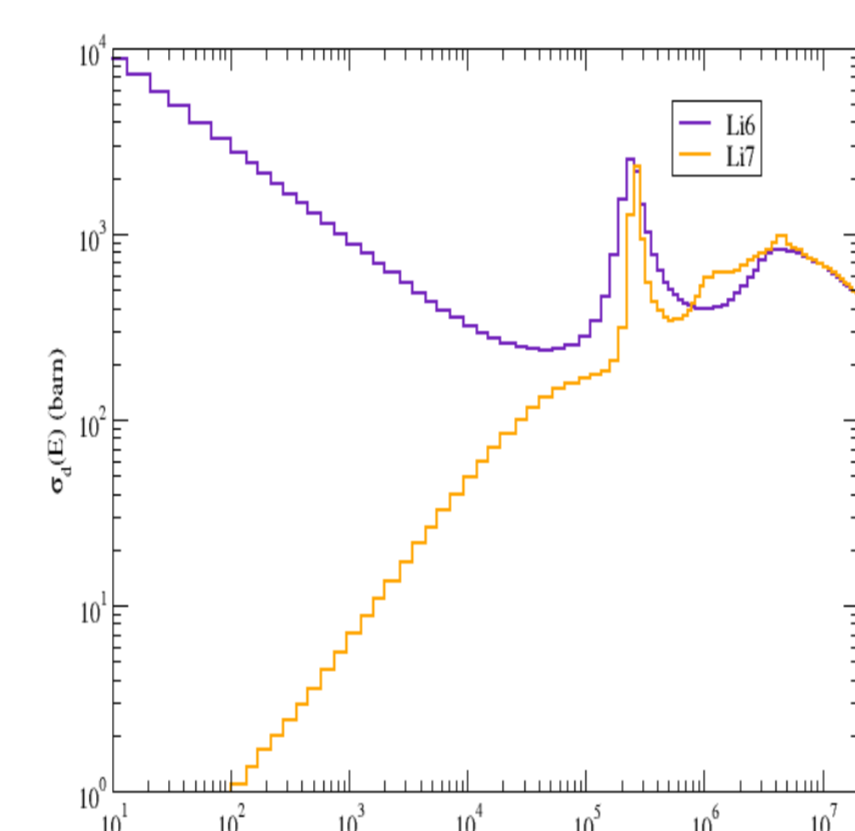
Displacement cross section in iron

Impact of cross section (xs) libraries

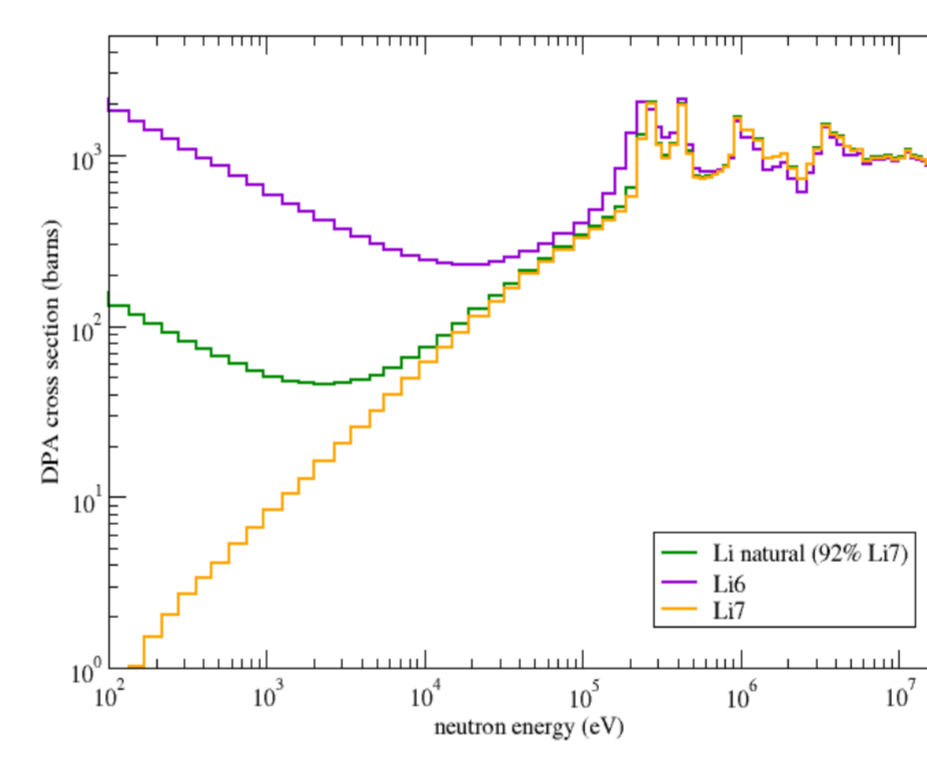
Xs for each isotope and all interactions

DART takes into account neutron cross sections for each isotope computing all known open channels

- Impact of fission products
- Example of dpa cross section in Lithium (⁶Li and ⁷Li)
- Increase of dpa xs in ⁶Li due to the reaction : ${}^6\text{Li} + {}^1_0\text{n} \rightarrow {}^4_2\text{He} + {}^3_1\text{H}$ $Q=4.8$ MeV



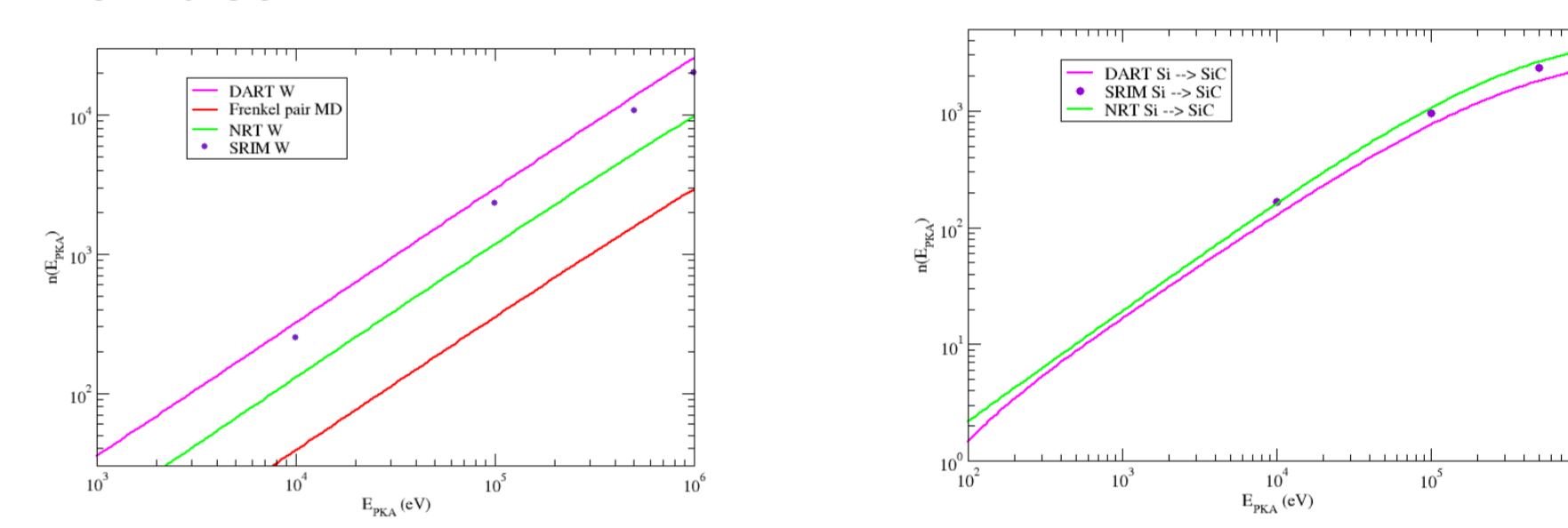
Dpa cross section in Li⁶ and Li⁷



Dpa cross section in Li₂O

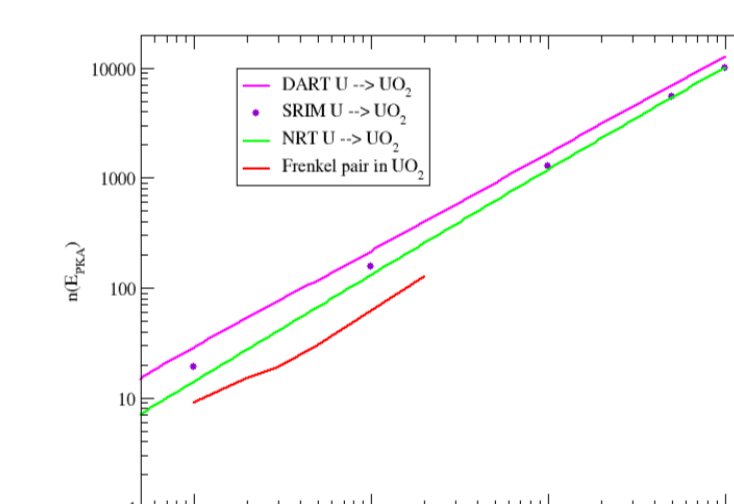
Calculation of the number of displaced atoms

Comparison of the number of displaced atoms (Nd) between DART (magenta), SRIM_2013 (purple), NRT (green) and Frenkel pairs from MD simulations (red) in Tungsten and polyatomic oxides



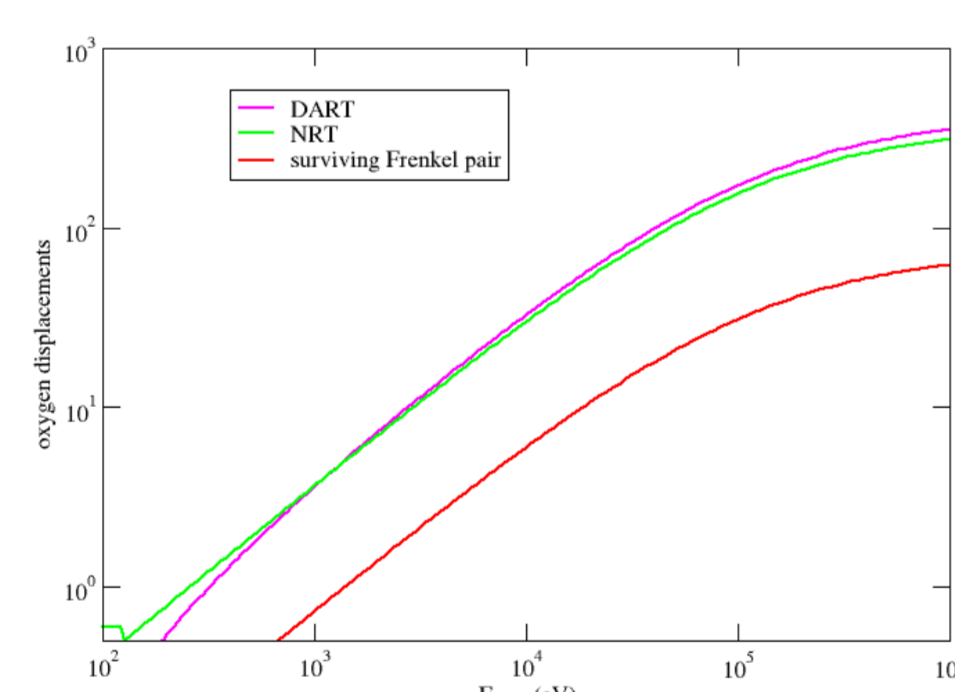
Nd in Tungsten (MD [Stoller])

Nd in SiC

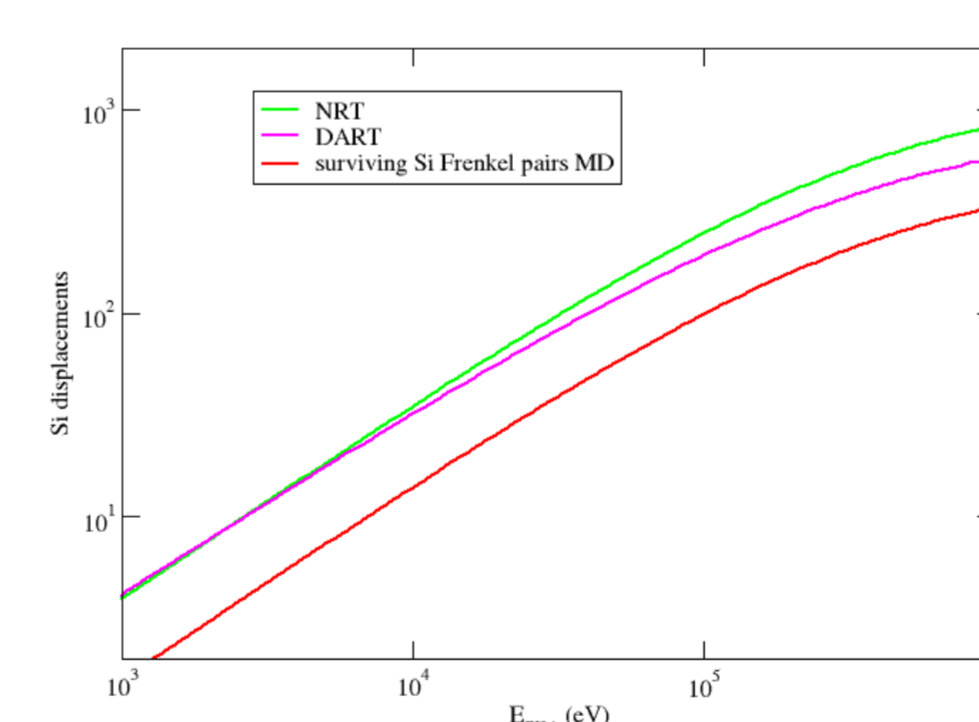


Nd in UO₂ (MD [Martin])

From DPA to number of defects



Number of oxygen atoms displaced in the O sublattice as a function of the O PKA in Al₂O₃
Measured O vacancies [Zinkle]



Number of Si atoms displaced in the Si sublattice as a function of the Si PKA in SiC
Surviving FP from [Gao]

Dpa is not the number of surviving defects

Summary and limitations

DART is a freeware available at OECD

- Important impact of nuclear reactions and xs libraries
- Determination of correct PKA spectra for experiments or MD simulations
- A theoretical LSS model used for the calculation of the displacement cross section (different from SPECTER, NJOY-HEATR)
- Determination of recoil spectra to mimic neutron irradiations with ion beam facilities
 - ❖ choice of the ion
 - ❖ sampling the PKA spectra for MD simulations in polyatomic materials

Limitations

- How to propagate uncertainties to PKA and displacement cross sections?
- What is the meaning of dpa in semi conductors and oxides?
- Impact of the electronic stopping power at high energy for recoils of few hundreds of MeV?
- Amorphisation nothing to do with dpa

Bibliography

[Gao] F. Gao, W. Weber, PRB 63, 54101 (2000)

[Zinkle] Zinkle, JNM 251,200 (1997)

[Stoller] Radiation damage: Mechanisms and Modelling, Stoller TN (2012)

[Martin] G. Martin, NIMB 269, 1727 (2011)

L. Luneville, D. Simeone C. Jouanne, Calculation of radiation damage induced by neutrons in compound materials, JNM 353, 89 (2006)

L. Luneville, D. Simeone, D. Gosset, A new tool to compare neutron and ion irradiation in materials, NIMB 250,71 (2006)