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Damage Parameters and Cross Sections for Li_2TiO_3

According to the actions agreed at the nculear expert group meeting on "International comparative irradiation of breeder materials" (Karlsruhe, March 17, 1999) the following report provides displacement cross sections for Li_2TiO_3, the last dataset needed for the candidate breeder materials under consideration.

Please refer to the report "Damage Parameters and Cross Sections for Li_2O" (16/04/99) for the nomenclature, codes and references used.

Simulation model for Li_2TiO_3

In order to perform realistic simulations of displacement cascades in Lithiummetatitanate Li_2TiO_3, it is mandatory to provide some microscopic data, which is summarised in the following:

Crystalline structure: monocline, spacegroup C2/c

Lattice constants:

@293K: a=5.041 Å, b=8.806 Å, c=9.726 Å, β=100.008°

@800K: a=5.086 Å, b=8.885 Å, c=9.814 Å, β=100.008°

Bonding: ionic, heat of formation $\Delta H_f = -399{,}3\ kcal/mole$

Crystallite models: static crystal @0K, thermal vibrations @800K (rms of thermal displacements about 0.1 ... 0.2 Å)

Li^6-enrichment: 90 at%, 60 at%, 30 at%, 7.5 at%, 0.75 at%

Nuclear reactions involved

In addition to damage functions (i.e. number of lattice/disorder defects, damage energy vs. PKA-energy) as obtained by MARLOWE simulations, PKA-spectra of all relevant neutron induced reactions are needed for the calculation of σ_D (displacement cross section) and *dpa*. For Li_2TiO_3 the following reactions have been considered (data from ENDF/B-VI, JENDL/FF 3.2):

Li^6: elast., (n,n'), (n,t); Li^7: elast., (n,n'); O^{16}: elast., (n,n'); Ti: elast., (n,n'), (n,2n)

In the case of 14 MeV-neutrons the maximum recoil energies are:

Li^6 6.9 MeV, α 14.1 MeV, t 16.2 MeV, Li^7 6.1 MeV, O^{16} 3.1 MeV, Ti 1.4 MeV

RESULTS

Damage cross sections

In FIG. 1 the resulting displacement cross sections for Li_2TiO_3 with various Li^6-enrichments are shown (tabular data in TAB. 1, energy group structure: 100 groups of SPECTER). In the BCA-simulations thermal vibrations at 800K have been taken into account which should be representative for operational temperatures. As in Li_2O the temperature effect is sizeable, but there are only minor changes at different temperatures.

It is worthwhile to compare the cross section as obtained by MARLOWE with the one by L. Greenwood, supplied for tentative nuclear calculations within the framework of the present activity (Dec. 1998). As can be readily seen from FIG. 3, the MARLOWE-cross section is 60 to 90 % higher in the α,t-region whereas the higher energy part is lower by some 30 to 50 %. Both effects can be contributed to the improved damage efficiency of the light mass PKA's and the higher effective displacement threshold energies of Li and Ti (compared to those used by Greenwood in the SPECOMP code).

Some details

Partial displacement cross sections in Li_2TiO_3 with a Li^6-enrichment of 90 at% are given in FIG. 2. Similar to other lithium ceramics, one can distinguish between the low energy α,t-contribution and shares of the heavier PKA's at higher neutron energies. Titanium is responsible for a local maximum of the cross section within the depression around some keV, which can be contributed to resonances in its elastic neutron cross section. Because the damage efficiency of Titanium (M=47.88 amu) does not saturate, its contribution to the total displacement cross section increases with neutron energy and, finally, is commeasurable to Oxygen (in spite of its low abundance of only 16 at%). Defect production is shared among the species Li, O, Ti as 30%, 60%, 10% nearly independent on type and energy of PKA's. From the respective damage cross sections one can deduce effective threshold energies Q by calculating $Q(E) = \sigma_{dam}(E) / \sigma_D(E)$. Its relation to the threshold energy E_d as defined in the NRT-model is given by $Q = 2.5E_d$.

From the results of this work, values for E_d averaged over neutron energy can be obtained and are listed in TAB. 3 together with data employed in the damage code SPECTER/SPECOMP.

TABLES

TAB. 1: Displacement cross section [barn] in Li_2TiO_3: contributions of PKA's, not normalised

Energy [eV]	Li6	He4	T	Li7	O16	Ti(nat)
1.00E-04	0.00E+00	9.87E+05	5.70E+05	0.00E+00	0.00E+00	0.00E+00
1.00E-03	0.00E+00	3.16E+05	1.82E+05	0.00E+00	0.00E+00	0.00E+00
1.00E-02	0.00E+00	1.89E+05	1.09E+05	0.00E+00	0.00E+00	0.00E+00
2.30E-02	0.00E+00	1.28E+05	7.37E+04	0.00E+00	0.00E+00	0.00E+00
5.00E-02	0.00E+00	9.70E+04	5.60E+04	0.00E+00	0.00E+00	0.00E+00
7.60E-02	0.00E+00	7.93E+04	4.57E+04	0.00E+00	0.00E+00	0.00E+00
1.15E-01	0.00E+00	6.50E+04	3.73E+04	0.00E+00	0.00E+00	0.00E+00
1.70E-01	0.00E+00	5.30E+04	3.06E+04	0.00E+00	0.00E+00	0.00E+00
2.55E-01	0.00E+00	4.33E+04	2.51E+04	0.00E+00	0.00E+00	0.00E+00
3.80E-01	0.00E+00	3.57E+04	2.07E+04	0.00E+00	0.00E+00	0.00E+00
5.50E-01	0.00E+00	2.94E+04	1.70E+04	0.00E+00	0.00E+00	0.00E+00
8.40E-01	0.00E+00	2.38E+04	1.37E+04	0.00E+00	0.00E+00	0.00E+00
1.28E+00	0.00E+00	1.94E+04	1.12E+04	0.00E+00	0.00E+00	0.00E+00
1.90E+00	0.00E+00	1.60E+04	9.20E+03	0.00E+00	0.00E+00	0.00E+00
2.80E+00	0.00E+00	1.31E+04	7.53E+03	0.00E+00	0.00E+00	0.00E+00
4.25E+00	0.00E+00	1.07E+04	6.13E+03	0.00E+00	0.00E+00	0.00E+00
6.30E+00	0.00E+00	8.77E+03	5.07E+03	0.00E+00	0.00E+00	0.00E+00
9.20E+00	0.00E+00	7.27E+03	4.20E+03	0.00E+00	0.00E+00	0.00E+00
1.35E+01	0.00E+00	5.90E+03	3.40E+03	0.00E+00	0.00E+00	0.00E+00
2.10E+01	2.29E-03	4.83E+03	2.79E+03	0.00E+00	0.00E+00	0.00E+00
3.00E+01	5.32E-02	4.00E+03	2.30E+03	5.28E-02	0.00E+00	0.00E+00
4.50E+01	1.54E-01	3.23E+03	1.86E+03	1.91E-01	1.98E-02	0.00E+00
6.90E+01	2.85E-01	2.62E+03	1.51E+03	3.92E-01	2.58E-01	0.00E+00
1.00E+02	3.89E-01	2.23E+03	1.28E+03	5.56E-01	6.12E-01	0.00E+00
1.35E+02	4.67E-01	1.95E+03	1.13E+03	6.76E-01	9.93E-01	0.00E+00
1.70E+02	5.44E-01	1.73E+03	9.97E+02	7.94E-01	1.38E+00	0.00E+00
2.20E+02	6.33E-01	1.53E+03	8.80E+02	9.20E-01	1.80E+00	1.67E-03
2.80E+02	7.36E-01	1.35E+03	7.80E+02	1.07E+00	2.20E+00	2.27E-02
3.60E+02	8.61E-01	1.20E+03	6.93E+02	1.25E+00	2.63E+00	9.28E-02
4.50E+02	1.01E+00	1.07E+03	6.13E+02	1.48E+00	3.12E+00	2.30E-01
5.75E+02	1.23E+00	9.33E+02	5.40E+02	1.81E+00	3.76E+00	6.70E-01
7.60E+02	1.50E+00	8.23E+02	4.73E+02	2.21E+00	4.55E+00	1.27E+00
9.60E+02	1.85E+00	7.23E+02	4.17E+02	2.74E+00	5.55E+00	2.42E+00
1.28E+03	2.28E+00	6.37E+02	3.67E+02	3.39E+00	6.81E+00	3.99E+00
1.60E+03	2.75E+00	5.70E+02	3.28E+02	4.08E+00	8.19E+00	5.92E+00
2.00E+03	3.47E+00	5.00E+02	2.88E+02	5.16E+00	1.04E+01	9.67E+00
2.70E+03	4.35E+00	4.37E+02	2.52E+02	6.49E+00	1.33E+01	3.58E+01
3.40E+03	5.43E+00	3.83E+02	2.22E+02	8.15E+00	1.69E+01	3.95E+01
4.50E+03	6.62E+00	3.40E+02	1.97E+02	1.01E+01	2.14E+01	3.52E+01
5.50E+03	7.97E+00	3.03E+02	1.75E+02	1.22E+01	2.66E+01	5.36E+01
7.20E+03	9.77E+00	2.67E+02	1.54E+02	1.51E+01	3.40E+01	1.12E+02
9.20E+03	1.18E+01	2.36E+02	1.36E+02	1.86E+01	4.37E+01	2.05E+02
1.20E+04	1.43E+01	2.09E+02	1.21E+02	2.26E+01	5.46E+01	4.89E+02
1.50E+04	1.69E+01	1.87E+02	1.08E+02	2.70E+01	6.79E+01	9.38E+02
1.90E+04	2.06E+01	1.65E+02	9.57E+01	3.30E+01	8.62E+01	8.22E+02
2.55E+04	2.47E+01	1.46E+02	8.50E+01	3.97E+01	1.10E+02	2.58E+02
3.20E+04	2.89E+01	1.33E+02	7.73E+01	4.62E+01	1.33E+02	4.14E+02
4.00E+04	3.42E+01	1.21E+02	7.03E+01	5.41E+01	1.64E+02	2.34E+02
5.25E+04	4.03E+01	1.11E+02	6.50E+01	6.10E+01	2.01E+02	4.11E+02
6.60E+04	4.83E+01	1.05E+02	6.17E+01	6.68E+01	2.48E+02	2.02E+02
8.80E+04	6.00E+01	1.05E+02	6.17E+01	7.19E+01	3.06E+02	1.32E+02

Energy [eV]	Li6	He4	T	Li7	O16	Ti(nat)
1.10E+05	7.87E+01	1.14E+02	6.73E+01	7.62E+01	3.60E+02	1.11E+02
1.35E+05	1.16E+02	1.39E+02	8.23E+01	8.12E+01	4.15E+02	9.82E+01
1.60E+05	2.06E+02	2.02E+02	1.19E+02	9.21E+01	4.73E+02	9.55E+01
1.90E+05	4.40E+02	3.47E+02	2.04E+02	1.42E+02	5.37E+02	1.68E+02
2.20E+05	7.79E+02	5.03E+02	2.94E+02	5.84E+02	6.00E+02	1.70E+02
2.55E+05	6.98E+02	3.77E+02	2.20E+02	1.10E+03	6.80E+02	2.90E+02
2.90E+05	4.76E+02	2.27E+02	1.32E+02	4.41E+02	7.67E+02	2.18E+02
3.20E+05	3.43E+02	1.48E+02	8.60E+01	2.60E+02	9.15E+02	2.93E+02
3.60E+05	2.66E+02	1.05E+02	6.10E+01	2.08E+02	1.29E+03	1.81E+02
4.00E+05	2.22E+02	8.13E+01	4.73E+01	1.84E+02	2.58E+03	2.48E+02
4.50E+05	1.95E+02	6.70E+01	3.90E+01	1.71E+02	1.16E+03	4.44E+02
5.00E+05	1.80E+02	5.87E+01	3.40E+01	1.66E+02	7.58E+02	3.11E+02
5.50E+05	1.71E+02	5.30E+01	3.10E+01	1.67E+02	7.50E+02	3.62E+02
6.00E+05	1.64E+02	4.90E+01	2.87E+01	1.70E+02	7.75E+02	3.64E+02
6.60E+05	1.59E+02	4.60E+01	2.68E+01	1.77E+02	8.07E+02	5.93E+02
7.20E+05	1.56E+02	4.37E+01	2.55E+01	1.88E+02	8.46E+02	6.79E+02
7.80E+05	1.54E+02	4.17E+01	2.45E+01	2.04E+02	9.04E+02	4.66E+02
8.40E+05	1.52E+02	4.03E+01	2.36E+01	2.26E+02	1.08E+03	5.78E+02
9.20E+05	1.52E+02	3.90E+01	2.29E+01	2.53E+02	2.06E+03	7.10E+02
1.00E+06	1.53E+02	3.77E+01	2.21E+01	2.87E+02	1.63E+03	6.59E+02
1.20E+06	1.58E+02	3.63E+01	2.15E+01	3.05E+02	1.30E+03	8.20E+02
1.40E+06	1.66E+02	3.63E+01	2.14E+01	3.10E+02	8.63E+02	1.01E+03
1.60E+06	1.77E+02	3.70E+01	2.17E+01	3.10E+02	9.11E+02	1.05E+03
1.80E+06	1.93E+02	3.77E+01	2.22E+01	3.20E+02	9.70E+02	1.25E+03
2.00E+06	2.15E+02	3.70E+01	2.17E+01	3.43E+02	6.44E+02	1.37E+03
2.30E+06	2.43E+02	3.47E+01	2.04E+01	3.72E+02	3.88E+02	1.52E+03
2.60E+06	2.71E+02	3.21E+01	1.88E+01	3.94E+02	5.96E+02	1.58E+03
2.90E+06	3.07E+02	2.88E+01	1.68E+01	4.08E+02	8.94E+02	1.65E+03
3.30E+06	3.41E+02	2.43E+01	1.41E+01	4.27E+02	1.54E+03	1.75E+03
3.70E+06	3.53E+02	2.09E+01	1.22E+01	4.67E+02	1.21E+03	1.77E+03
4.10E+06	3.55E+02	1.91E+01	1.11E+01	5.11E+02	9.25E+02	1.88E+03
4.50E+06	3.55E+02	1.71E+01	9.90E+00	5.10E+02	6.70E+02	1.93E+03
5.00E+06	3.52E+02	1.54E+01	8.90E+00	4.58E+02	7.57E+02	1.96E+03
5.50E+06	3.48E+02	1.40E+01	8.03E+00	4.39E+02	8.06E+02	2.00E+03
6.00E+06	3.43E+02	1.27E+01	7.30E+00	4.26E+02	5.40E+02	2.05E+03
6.70E+06	3.35E+02	1.14E+01	6.53E+00	4.00E+02	6.61E+02	2.11E+03
7.40E+06	3.26E+02	1.04E+01	5.90E+00	3.83E+02	7.15E+02	2.17E+03
8.20E+06	3.17E+02	9.43E+00	5.33E+00	3.73E+02	7.38E+02	2.20E+03
9.00E+06	3.07E+02	8.50E+00	4.77E+00	3.61E+02	6.78E+02	2.26E+03
1.00E+07	2.95E+02	7.70E+00	4.33E+00	3.45E+02	7.67E+02	2.29E+03
1.10E+07	2.84E+02	7.10E+00	3.93E+00	3.30E+02	9.18E+02	2.30E+03
1.20E+07	2.73E+02	6.40E+00	3.53E+00	3.18E+02	8.97E+02	2.33E+03
1.30E+07	2.61E+02	5.87E+00	3.21E+00	3.01E+02	8.97E+02	2.35E+03
1.40E+07	2.55E+02	5.63E+00	3.06E+00	2.93E+02	9.22E+02	2.37E+03
1.50E+07	2.47E+02	5.27E+00	2.86E+00	2.82E+02	9.57E+02	2.37E+03
1.60E+07	2.35E+02	4.87E+00	2.61E+00	2.63E+02	8.56E+02	2.36E+03
1.70E+07	2.25E+02	4.43E+00	2.36E+00	2.49E+02	8.42E+02	2.33E+03
1.80E+07	2.15E+02	4.03E+00	2.09E+00	2.37E+02	7.71E+02	2.32E+03
1.90E+07	2.07E+02	3.67E+00	1.78E+00	2.28E+02	7.32E+02	2.30E+03

TAB. 2: Total displacement cross sections [barn] for Li_2TiO_3: with different Li6-enrichments

Energy [eV]	90at%	60at%	30at%	7.5at%	0.75at%
1.000E-04	4.67E+05	3.11E+05	1.56E+05	3.89E+04	3.89E+03
1.000E-03	1.50E+05	9.97E+04	4.99E+04	1.25E+04	1.25E+03
1.000E-02	8.95E+04	5.97E+04	2.98E+04	7.46E+03	7.46E+02
2.300E-02	6.04E+04	4.03E+04	2.01E+04	5.03E+03	5.03E+02
5.000E-02	4.59E+04	3.06E+04	1.53E+04	3.82E+03	3.82E+02
7.600E-02	3.75E+04	2.50E+04	1.25E+04	3.12E+03	3.12E+02
1.150E-01	3.07E+04	2.05E+04	1.02E+04	2.56E+03	2.56E+02
1.700E-01	2.51E+04	1.67E+04	8.36E+03	2.09E+03	2.09E+02
2.550E-01	2.05E+04	1.37E+04	6.84E+03	1.71E+03	1.71E+02
3.800E-01	1.69E+04	1.13E+04	5.63E+03	1.41E+03	1.41E+02
5.500E-01	1.39E+04	9.28E+03	4.64E+03	1.16E+03	1.16E+02
8.400E-01	1.13E+04	7.51E+03	3.76E+03	9.39E+02	9.39E+01
1.275E+00	9.19E+03	6.13E+03	3.06E+03	7.66E+02	7.66E+01
1.900E+00	7.55E+03	5.03E+03	2.52E+03	6.29E+02	6.29E+01
2.800E+00	6.18E+03	4.12E+03	2.06E+03	5.15E+02	5.15E+01
4.250E+00	5.04E+03	3.36E+03	1.68E+03	4.20E+02	4.20E+01
6.300E+00	4.15E+03	2.77E+03	1.38E+03	3.46E+02	3.46E+01
9.200E+00	3.44E+03	2.29E+03	1.15E+03	2.87E+02	2.87E+01
1.350E+01	2.79E+03	1.86E+03	9.30E+02	2.32E+02	2.32E+01
2.100E+01	2.29E+03	1.52E+03	7.62E+02	1.90E+02	1.90E+01
3.000E+01	1.89E+03	1.26E+03	6.30E+02	1.58E+02	1.58E+01
4.500E+01	1.53E+03	1.02E+03	5.09E+02	1.27E+02	1.28E+01
6.900E+01	1.24E+03	8.26E+02	4.13E+02	1.04E+02	1.06E+01
1.000E+02	1.05E+03	7.02E+02	3.51E+02	8.82E+01	9.27E+00
1.350E+02	9.25E+02	6.17E+02	3.09E+02	7.77E+01	8.42E+00
1.700E+02	8.18E+02	5.46E+02	2.73E+02	6.90E+01	7.76E+00
2.200E+02	7.23E+02	4.83E+02	2.42E+02	6.14E+01	7.23E+00
2.800E+02	6.40E+02	4.27E+02	2.14E+02	5.47E+01	6.78E+00
3.600E+02	5.70E+02	3.80E+02	1.91E+02	4.91E+01	6.48E+00
4.500E+02	5.06E+02	3.38E+02	1.70E+02	4.41E+01	6.29E+00
5.750E+02	4.44E+02	2.97E+02	1.50E+02	3.94E+01	6.27E+00
7.600E+02	3.92E+02	2.62E+02	1.33E+02	3.56E+01	6.46E+00
9.600E+02	3.46E+02	2.32E+02	1.18E+02	3.26E+01	6.94E+00
1.275E+03	3.06E+02	2.06E+02	1.05E+02	3.03E+01	7.70E+00
1.600E+03	2.75E+02	1.86E+02	9.61E+01	2.89E+01	8.68E+00
2.000E+03	2.44E+02	1.66E+02	8.71E+01	2.82E+01	1.05E+01
2.700E+03	2.21E+02	1.52E+02	8.34E+01	3.19E+01	1.65E+01
3.400E+03	1.99E+02	1.38E+02	7.80E+01	3.28E+01	1.92E+01
4.500E+03	1.80E+02	1.27E+02	7.33E+01	3.32E+01	2.12E+01
5.500E+03	1.69E+02	1.21E+02	7.38E+01	3.82E+01	2.75E+01
7.200E+03	1.66E+02	1.24E+02	8.23E+01	5.11E+01	4.18E+01
9.200E+03	1.72E+02	1.35E+02	9.87E+01	7.13E+01	6.31E+01
1.200E+04	2.13E+02	1.81E+02	1.49E+02	1.24E+02	1.17E+02
1.500E+04	2.85E+02	2.56E+02	2.28E+02	2.06E+02	2.00E+02
1.900E+04	2.65E+02	2.41E+02	2.16E+02	1.97E+02	1.92E+02
2.550E+04	1.76E+02	1.54E+02	1.33E+02	1.16E+02	1.12E+02
3.220E+04	2.09E+02	1.89E+02	1.70E+02	1.56E+02	1.51E+02
4.000E+04	1.90E+02	1.73E+02	1.56E+02	1.43E+02	1.39E+02
5.250E+04	2.36E+02	2.20E+02	2.05E+02	1.93E+02	1.90E+02
6.600E+04	2.24E+02	2.10E+02	1.95E+02	1.84E+02	1.80E+02
8.800E+04	2.45E+02	2.30E+02	2.14E+02	2.03E+02	1.99E+02
1.100E+05	2.79E+02	2.61E+02	2.42E+02	2.29E+02	2.24E+02
1.350E+05	3.28E+02	3.02E+02	2.77E+02	2.57E+02	2.52E+02
1.600E+05	4.13E+02	3.70E+02	3.27E+02	2.94E+02	2.84E+02

Energy [eV]	90at%	60at%	30at%	7.5at%	0.75at%
1.900E+05	5.99E+02	5.14E+02	4.29E+02	3.65E+02	3.46E+02
2.200E+05	8.21E+02	7.21E+02	6.22E+02	5.48E+02	5.26E+02
2.550E+05	8.13E+02	7.94E+02	7.75E+02	7.60E+02	7.56E+02
2.900E+05	6.85E+02	6.45E+02	6.06E+02	5.76E+02	5.68E+02
3.200E+05	6.88E+02	6.57E+02	6.25E+02	6.01E+02	5.94E+02
3.600E+05	8.13E+02	7.90E+02	7.68E+02	7.51E+02	7.46E+02
4.000E+05	1.44E+03	1.42E+03	1.41E+03	1.40E+03	1.39E+03
4.500E+05	7.50E+02	7.37E+02	7.24E+02	7.14E+02	7.11E+02
5.000E+05	5.18E+02	5.08E+02	4.97E+02	4.89E+02	4.86E+02
5.500E+05	5.17E+02	5.08E+02	5.00E+02	4.93E+02	4.91E+02
6.000E+05	5.26E+02	5.19E+02	5.12E+02	5.07E+02	5.05E+02
6.600E+05	5.78E+02	5.72E+02	5.67E+02	5.63E+02	5.62E+02
7.200E+05	6.10E+02	6.06E+02	6.02E+02	6.00E+02	5.99E+02
7.800E+05	6.02E+02	6.01E+02	5.99E+02	5.98E+02	5.97E+02
8.400E+05	7.10E+02	7.11E+02	7.12E+02	7.13E+02	7.13E+02
9.200E+05	1.22E+03	1.23E+03	1.23E+03	1.23E+03	1.23E+03
1.000E+06	9.97E+02	1.00E+03	1.01E+03	1.02E+03	1.02E+03
1.200E+06	8.61E+02	8.70E+02	8.79E+02	8.86E+02	8.88E+02
1.400E+06	6.77E+02	6.86E+02	6.95E+02	7.01E+02	7.03E+02
1.600E+06	7.10E+02	7.18E+02	7.25E+02	7.31E+02	7.33E+02
1.800E+06	7.79E+02	7.86E+02	7.93E+02	7.98E+02	7.99E+02
2.000E+06	6.44E+02	6.50E+02	6.57E+02	6.63E+02	6.64E+02
2.300E+06	5.50E+02	5.57E+02	5.65E+02	5.70E+02	5.72E+02
2.600E+06	6.72E+02	6.79E+02	6.86E+02	6.91E+02	6.93E+02
2.900E+06	8.41E+02	8.47E+02	8.52E+02	8.57E+02	8.58E+02
3.300E+06	1.19E+03	1.19E+03	1.20E+03	1.20E+03	1.20E+03
3.700E+06	1.03E+03	1.04E+03	1.05E+03	1.05E+03	1.05E+03
4.100E+06	9.07E+02	9.20E+02	9.33E+02	9.42E+02	9.45E+02
4.500E+06	7.89E+02	8.01E+02	8.14E+02	8.24E+02	8.27E+02
5.000E+06	8.34E+02	8.42E+02	8.50E+02	8.56E+02	8.58E+02
5.500E+06	8.62E+02	8.69E+02	8.76E+02	8.81E+02	8.82E+02
6.000E+06	7.35E+02	7.41E+02	7.48E+02	7.52E+02	7.54E+02
6.700E+06	8.02E+02	8.07E+02	8.11E+02	8.15E+02	8.16E+02
7.400E+06	8.35E+02	8.39E+02	8.43E+02	8.46E+02	8.47E+02
8.200E+06	8.48E+02	8.52E+02	8.56E+02	8.59E+02	8.60E+02
9.000E+06	8.23E+02	8.27E+02	8.31E+02	8.34E+02	8.35E+02
1.000E+07	8.68E+02	8.72E+02	8.76E+02	8.79E+02	8.80E+02
1.100E+07	9.41E+02	9.45E+02	9.48E+02	9.51E+02	9.52E+02
1.200E+07	9.32E+02	9.36E+02	9.39E+02	9.42E+02	9.42E+02
1.300E+07	9.32E+02	9.35E+02	9.38E+02	9.40E+02	9.41E+02
1.400E+07	9.45E+02	9.48E+02	9.51E+02	9.53E+02	9.54E+02
1.500E+07	9.60E+02	9.63E+02	9.65E+02	9.67E+02	9.68E+02
1.600E+07	9.03E+02	9.05E+02	9.07E+02	9.08E+02	9.09E+02
1.700E+07	8.88E+02	8.89E+02	8.91E+02	8.92E+02	8.93E+02
1.800E+07	8.47E+02	8.48E+02	8.50E+02	8.51E+02	8.51E+02
1.900E+07	8.21E+02	8.23E+02	8.24E+02	8.25E+02	8.26E+02

TAB. 3: Threshold values for defect species in Li_2TiO_3

Ed [eV]	Li	O	Ti
Marlowe, @800K	45	23	76
Specter/Specomp	10	30	40

FIGURES

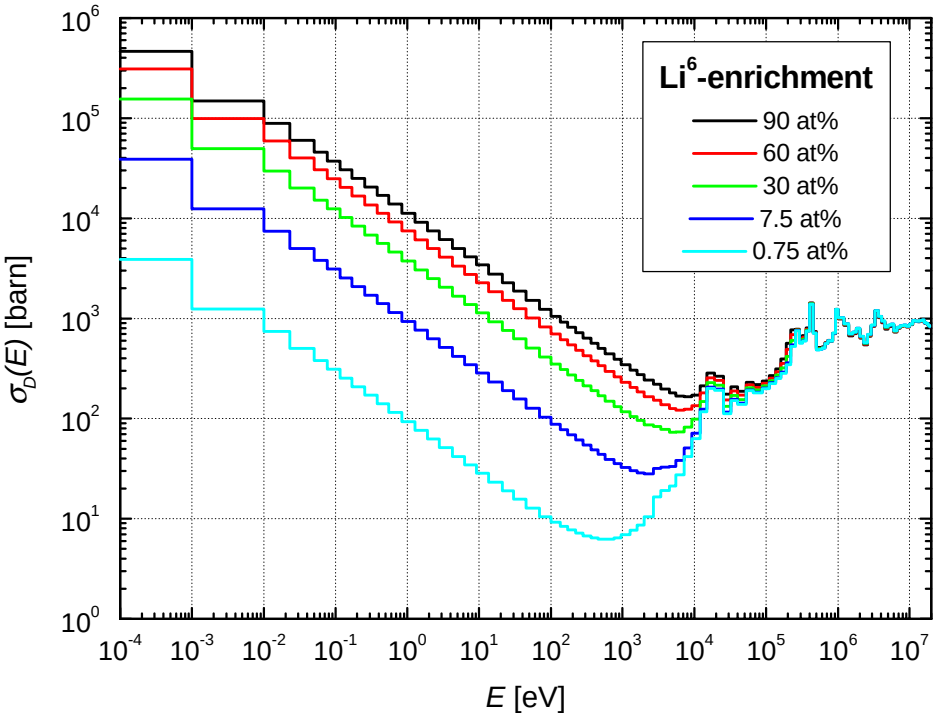

FIG. 1: Total displacement cross sections in Li_2TiO_3: with different Li^6-enrichments

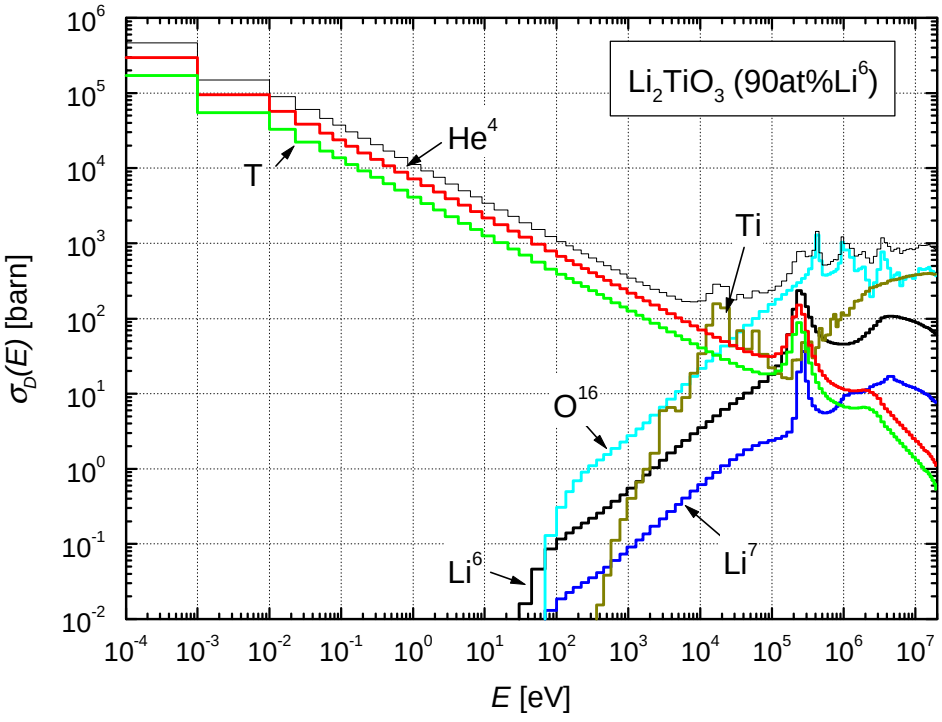

FIG. 2: Contributions to displacement cross section for Li_2TiO_3 (90at% Li^6)

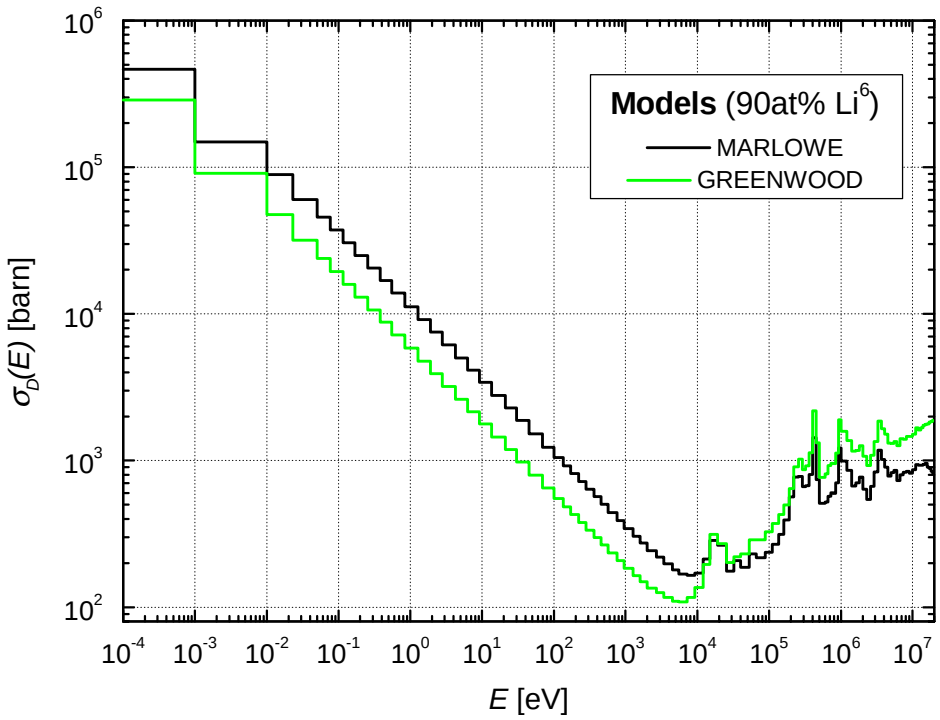

FIG. 3: Comparison of displacement cross sections (at 90at%-enrichment): „MARLOWE“ is the present result, „GREENWOOD“ is a SPECOMP-result with an improved treatment of the α,t-contribution.