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Damage Parameters and Cross Sections for Li_4SiO_4

As there are some inconsistencies in the displacement cross sections for Li_4SiO_4 the following report provides some additional information and concise data to be used in further damage assessments. In particular, the lattice temperature used in the BCA computer simulations of displacement cascades is 1180 K as opposed to the previous used static lattice (0 K).

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_4SiO_4

In order to perform realistic simulations of displacement cascades in Lithiumorthosilicate Li_4SiO_4, it is mandatory to provide some microscopic data, which is summarised in the following:

Crystalline structure: monocline, spacegroup $P2_1/m$

Lattice constants:

@293K: a=5.15 Å, b=6.11 Å, c=5.30 Å, γ=90.27°

@1180K: a=5.22 Å, b=6.31 Å, c=5.41 Å, γ=90.27°

Bonding: ionic, heat of formation $\Delta H_f = -536\ kcal/mole$

Crystallite models: static crystal @0K, thermal vibrations @1180K (rms of thermal displacements about 0.1 Å for each species)

Li^6-enrichment: 30 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_4SiO_4 the following reactions have been considered (data from ENDF/B-VI):

Li^6: elast., (n,n'), (n,t); Li^7: elast., (n,n'); O^{16}: elast., (n,n'); Si: elast., (n,n'), (n,p)Al^{28}, (n,α)Mg^{25}

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, Si 1.9 MeV, Al 1.6 MeV, Mg 3.5 MeV

RESULTS

Damage cross sections

In FIG. 1 the resulting displacement cross sections for Li_4SiO_4 with various Li^6-enrichments are shown (tabular data in TAB. 2, energy group structure: 100 groups of SPECTER). In the BCA-simulations thermal vibrations at 1180K have been taken into account which is around the maximum temperature expected in the HCPB Demo blanket. As in the other breeder materials (Li_2O, Li_2TiO_3) the temperature effect is sizeable (see below), but there are only minor changes at different temperatures.

Some details

Partial displacement cross sections in Li_4SiO_4 with a Li^6-enrichment of 30 at% are given in FIG. 2 (tabular data, not normalised, in TAB. 1). Similar to the other breeder materials, one can distinguish between the low energy α,t-contribution and shares of the heavier PKA's at higher neutron energies. Defect production is shared among the species Li, O, Si as 34%, 59%, 7% 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 the results obtained with a static lattice model (at T = 0 K) and data employed in the damage code SPECTER/SPECOMP. Both MARLOWE-results differ only slightly, whereas the discrepancy to the SPECOMP-values is obvious. This can be contributed to the lattice with partially occupied Li-sites (increasing the effective threshold energy due to an increased probability for recombination on Li-sites) and the strong covalent bonding of the central Si-ion within the silicate-tetrahedron (increasing the threshold for Si-displacements).

Because the damage efficiency at 1180 K differs from that at 0 K in a very distinct way (depending on type and energy of the PKA), the difference of the total displacement cross sections at both temperatures is strongly dependant on energy (cf. XXX, for the case of 30at% Li^6). In the low energy region the light mass PKA's are dominating the total cross section, so that their damage increase at higher temperatures can clearly be seen (+11.6%). In contrast to that the heavier PKA's do not show such a significant effect, even a slight decrease can be observed. At higher neutron energies (and hence at higher PKA energies) the difference curve climbs slightly up to around +6 %.

As a consequence, it can be stated that *dpa*-values obtained with the cross section at 1180 K differ at most by around 11% compared to those obtained at 0 K, but only in the case of a thermal neutron spectrum. In a mixed spectrum the effect is diminished, e.g. in a DEMO fusion reactor first wall spectrum the difference is typically around 3 %.

TABLES

TAB. 1: Displacement cross section [barn] in Li_4SiO_4: contributions of PKA's, not normalised

Energy [eV]	Li6	He4	T	Li7	O16	Si(nat)
1.00E-04	0.00E+00	8.82E+05	4.86E+05	0.00E+00	0.00E+00	0.00E+00
1.00E-03	0.00E+00	2.83E+05	1.56E+05	0.00E+00	0.00E+00	0.00E+00
1.00E-02	0.00E+00	1.69E+05	9.31E+04	0.00E+00	0.00E+00	0.00E+00
2.30E-02	0.00E+00	1.14E+05	6.28E+04	0.00E+00	0.00E+00	0.00E+00
5.00E-02	0.00E+00	8.67E+04	4.77E+04	0.00E+00	0.00E+00	0.00E+00
7.60E-02	0.00E+00	7.07E+04	3.89E+04	0.00E+00	0.00E+00	0.00E+00
1.15E-01	0.00E+00	5.79E+04	3.19E+04	0.00E+00	0.00E+00	0.00E+00
1.70E-01	0.00E+00	4.74E+04	2.61E+04	0.00E+00	0.00E+00	0.00E+00
2.55E-01	0.00E+00	3.88E+04	2.14E+04	0.00E+00	0.00E+00	0.00E+00
3.80E-01	0.00E+00	3.20E+04	1.76E+04	0.00E+00	0.00E+00	0.00E+00
5.50E-01	0.00E+00	2.63E+04	1.45E+04	0.00E+00	0.00E+00	0.00E+00
8.40E-01	0.00E+00	2.13E+04	1.17E+04	0.00E+00	0.00E+00	0.00E+00
1.28E+00	0.00E+00	1.74E+04	9.56E+03	0.00E+00	0.00E+00	0.00E+00
1.90E+00	0.00E+00	1.43E+04	7.84E+03	0.00E+00	0.00E+00	0.00E+00
2.80E+00	0.00E+00	1.17E+04	6.42E+03	0.00E+00	0.00E+00	0.00E+00
4.25E+00	0.00E+00	9.51E+03	5.24E+03	0.00E+00	0.00E+00	0.00E+00
6.30E+00	0.00E+00	7.84E+03	4.32E+03	0.00E+00	0.00E+00	0.00E+00
9.20E+00	0.00E+00	6.48E+03	3.57E+03	0.00E+00	0.00E+00	0.00E+00
1.35E+01	0.00E+00	5.28E+03	2.91E+03	0.00E+00	0.00E+00	0.00E+00
2.10E+01	1.45E-03	4.32E+03	2.38E+03	0.00E+00	0.00E+00	0.00E+00
3.00E+01	3.38E-02	3.57E+03	1.97E+03	3.22E-02	0.00E+00	0.00E+00
4.50E+01	9.87E-02	2.89E+03	1.59E+03	1.18E-01	2.43E-02	0.00E+00
6.90E+01	1.87E-01	2.34E+03	1.29E+03	2.49E-01	3.17E-01	0.00E+00
1.00E+02	2.64E-01	1.99E+03	1.10E+03	3.66E-01	7.40E-01	3.85E-02
1.35E+02	3.27E-01	1.75E+03	9.61E+02	4.58E-01	1.20E+00	9.68E-02
1.70E+02	3.94E-01	1.54E+03	8.50E+02	5.60E-01	1.68E+00	1.98E-01
2.20E+02	4.78E-01	1.36E+03	7.51E+02	6.77E-01	2.23E+00	3.47E-01
2.80E+02	5.85E-01	1.21E+03	6.64E+02	8.24E-01	2.76E+00	5.36E-01
3.60E+02	7.21E-01	1.07E+03	5.90E+02	1.01E+00	3.35E+00	8.42E-01
4.50E+02	8.94E-01	9.52E+02	5.24E+02	1.26E+00	4.01E+00	1.18E+00
5.75E+02	1.15E+00	8.34E+02	4.59E+02	1.62E+00	4.86E+00	1.78E+00
7.60E+02	1.46E+00	7.34E+02	4.04E+02	2.07E+00	5.86E+00	2.47E+00
9.60E+02	1.88E+00	6.45E+02	3.55E+02	2.68E+00	7.12E+00	3.29E+00
1.28E+03	2.39E+00	5.68E+02	3.13E+02	3.42E+00	8.67E+00	4.27E+00
1.60E+03	2.96E+00	5.08E+02	2.80E+02	4.22E+00	1.04E+01	5.25E+00
2.00E+03	3.81E+00	4.46E+02	2.46E+02	5.45E+00	1.29E+01	6.61E+00
2.70E+03	4.86E+00	3.91E+02	2.15E+02	6.97E+00	1.64E+01	8.17E+00
3.40E+03	6.14E+00	3.44E+02	1.89E+02	8.82E+00	2.06E+01	9.87E+00
4.50E+03	7.58E+00	3.05E+02	1.68E+02	1.10E+01	2.56E+01	1.21E+01
5.50E+03	9.23E+00	2.71E+02	1.49E+02	1.34E+01	3.16E+01	1.38E+01
7.20E+03	1.15E+01	2.38E+02	1.32E+02	1.67E+01	4.00E+01	1.63E+01
9.20E+03	1.41E+01	2.10E+02	1.16E+02	2.05E+01	5.11E+01	1.90E+01
1.20E+04	1.71E+01	1.87E+02	1.03E+02	2.50E+01	6.37E+01	2.26E+01
1.50E+04	2.04E+01	1.67E+02	9.25E+01	2.99E+01	7.90E+01	2.69E+01
1.90E+04	2.48E+01	1.47E+02	8.17E+01	3.64E+01	9.98E+01	3.20E+01

Energy [eV]	Li6	He4	T	Li7	O16	Si(nat)
2.55E+04	2.97E+01	1.31E+02	7.25E+01	4.35E+01	1.27E+02	3.81E+01
3.20E+04	3.46E+01	1.19E+02	6.59E+01	5.04E+01	1.53E+02	4.57E+01
4.00E+04	4.09E+01	1.08E+02	6.01E+01	5.87E+01	1.89E+02	3.95E+01
5.25E+04	4.84E+01	9.89E+01	5.55E+01	6.61E+01	2.32E+02	2.14E+02
6.60E+04	5.86E+01	9.35E+01	5.28E+01	7.25E+01	2.87E+02	9.29E+01
8.80E+04	7.42E+01	9.33E+01	5.29E+01	7.83E+01	3.55E+02	7.62E+01
1.10E+05	9.91E+01	1.02E+02	5.78E+01	8.33E+01	4.19E+02	4.93E+01
1.35E+05	1.49E+02	1.24E+02	7.07E+01	8.91E+01	4.83E+02	3.67E+01
1.60E+05	2.67E+02	1.80E+02	1.02E+02	1.01E+02	5.52E+02	8.73E+02
1.90E+05	5.77E+02	3.10E+02	1.76E+02	1.57E+02	6.29E+02	1.30E+03
2.20E+05	1.02E+03	4.48E+02	2.52E+02	6.56E+02	7.06E+02	8.65E+02
2.55E+05	9.17E+02	3.37E+02	1.89E+02	1.25E+03	8.02E+02	7.24E+02
2.90E+05	6.25E+02	2.02E+02	1.13E+02	5.02E+02	9.08E+02	6.80E+02
3.20E+05	4.52E+02	1.32E+02	7.39E+01	2.98E+02	1.09E+03	6.71E+02
3.60E+05	3.50E+02	9.33E+01	5.25E+01	2.38E+02	1.54E+03	6.81E+02
4.00E+05	2.92E+02	7.23E+01	4.08E+01	2.12E+02	3.06E+03	6.99E+02
4.50E+05	2.57E+02	5.96E+01	3.37E+01	1.98E+02	1.37E+03	7.23E+02
5.00E+05	2.37E+02	5.21E+01	2.96E+01	1.92E+02	8.98E+02	8.99E+02
5.50E+05	2.24E+02	4.73E+01	2.69E+01	1.93E+02	8.92E+02	1.24E+03
6.00E+05	2.15E+02	4.36E+01	2.49E+01	1.97E+02	9.24E+02	7.18E+02
6.60E+05	2.09E+02	4.08E+01	2.34E+01	2.05E+02	9.65E+02	7.69E+02
7.20E+05	2.05E+02	3.87E+01	2.23E+01	2.18E+02	1.01E+03	8.99E+02
7.80E+05	2.02E+02	3.71E+01	2.15E+01	2.36E+02	1.08E+03	1.65E+03
8.40E+05	2.00E+02	3.57E+01	2.07E+01	2.62E+02	1.30E+03	1.10E+03
9.20E+05	2.00E+02	3.45E+01	2.01E+01	2.94E+02	2.47E+03	1.48E+03
1.00E+06	2.02E+02	3.33E+01	1.96E+01	3.34E+02	1.94E+03	9.25E+02
1.20E+06	2.08E+02	3.23E+01	1.91E+01	3.54E+02	1.55E+03	1.18E+03
1.40E+06	2.19E+02	3.21E+01	1.92E+01	3.59E+02	1.03E+03	1.35E+03
1.60E+06	2.35E+02	3.26E+01	1.96E+01	3.60E+02	1.09E+03	1.63E+03
1.80E+06	2.57E+02	3.33E+01	2.02E+01	3.71E+02	1.16E+03	1.76E+03
2.00E+06	2.87E+02	3.26E+01	2.00E+01	3.96E+02	7.75E+02	1.36E+03
2.30E+06	3.26E+02	3.07E+01	1.90E+01	4.30E+02	4.67E+02	1.55E+03
2.60E+06	3.64E+02	2.83E+01	1.77E+01	4.55E+02	7.19E+02	1.57E+03
2.90E+06	4.12E+02	2.53E+01	1.60E+01	4.73E+02	1.08E+03	1.53E+03
3.30E+06	4.58E+02	2.14E+01	1.36E+01	4.94E+02	1.87E+03	1.38E+03
3.70E+06	4.75E+02	1.85E+01	1.19E+01	5.41E+02	1.47E+03	1.60E+03
4.10E+06	4.78E+02	1.69E+01	1.10E+01	5.93E+02	1.13E+03	1.79E+03
4.50E+06	4.77E+02	1.51E+01	9.95E+00	5.93E+02	8.18E+02	2.05E+03
5.00E+06	4.74E+02	1.37E+01	9.08E+00	5.32E+02	9.29E+02	1.85E+03
5.50E+06	4.69E+02	1.24E+01	8.35E+00	5.10E+02	9.89E+02	2.03E+03
6.00E+06	4.62E+02	1.13E+01	7.71E+00	4.96E+02	6.67E+02	1.90E+03
6.70E+06	4.51E+02	1.03E+01	7.06E+00	4.66E+02	8.17E+02	2.04E+03
7.40E+06	4.40E+02	9.35E+00	6.52E+00	4.47E+02	8.81E+02	2.25E+03
8.20E+06	4.28E+02	8.57E+00	6.04E+00	4.36E+02	9.12E+02	2.16E+03
9.00E+06	4.15E+02	7.77E+00	5.54E+00	4.22E+02	8.38E+02	2.19E+03
1.00E+07	3.99E+02	7.13E+00	5.15E+00	4.04E+02	9.50E+02	2.25E+03
1.10E+07	3.84E+02	6.61E+00	4.84E+00	3.87E+02	1.14E+03	2.30E+03
1.20E+07	3.70E+02	6.01E+00	4.45E+00	3.74E+02	1.11E+03	2.37E+03
1.30E+07	3.54E+02	5.55E+00	4.18E+00	3.54E+02	1.11E+03	2.28E+03
1.40E+07	3.47E+02	5.33E+00	4.05E+00	3.45E+02	1.14E+03	2.16E+03

Energy [eV]	Li6	He4	T	Li7	O16	Si(nat)
1.50E+07	3.36E+02	5.02E+00	3.73E+00	3.31E+02	1.18E+03	1.96E+03
1.60E+07	3.20E+02	4.59E+00	3.14E+00	3.09E+02	1.05E+03	1.71E+03
1.70E+07	3.06E+02	3.96E+00	2.67E+00	2.93E+02	1.03E+03	1.50E+03
1.80E+07	2.94E+02	3.39E+00	2.27E+00	2.79E+02	9.46E+02	1.37E+03
1.90E+07	2.83E+02	2.91E+00	1.94E+00	2.68E+02	8.97E+02	1.25E+03

TAB. 2: Total displacement cross sections [barn] for Li_4SiO_4: with different Li^6-enrichments

Energy [eV]	90at%	60at%	30at%	7.5at%	0.75at%
1.000E-04	5.47E+05	3.65E+05	1.82E+05	4.56E+04	4.56E+03
1.000E-03	1.75E+05	1.17E+05	5.84E+04	1.46E+04	1.46E+03
1.000E-02	1.05E+05	6.99E+04	3.49E+04	8.74E+03	8.74E+02
2.300E-02	7.08E+04	4.72E+04	2.36E+04	5.90E+03	5.90E+02
5.000E-02	5.38E+04	3.58E+04	1.79E+04	4.48E+03	4.48E+02
7.600E-02	4.39E+04	2.92E+04	1.46E+04	3.65E+03	3.65E+02
1.150E-01	3.59E+04	2.39E+04	1.20E+04	2.99E+03	2.99E+02
1.700E-01	2.94E+04	1.96E+04	9.81E+03	2.45E+03	2.45E+02
2.550E-01	2.41E+04	1.61E+04	8.03E+03	2.01E+03	2.01E+02
3.800E-01	1.98E+04	1.32E+04	6.62E+03	1.65E+03	1.65E+02
5.500E-01	1.63E+04	1.09E+04	5.43E+03	1.36E+03	1.36E+02
8.400E-01	1.32E+04	8.79E+03	4.40E+03	1.10E+03	1.10E+02
1.275E+00	1.08E+04	7.18E+03	3.59E+03	8.97E+02	8.97E+01
1.900E+00	8.84E+03	5.89E+03	2.95E+03	7.36E+02	7.36E+01
2.800E+00	7.23E+03	4.82E+03	2.41E+03	6.03E+02	6.03E+01
4.250E+00	5.90E+03	3.93E+03	1.97E+03	4.92E+02	4.92E+01
6.300E+00	4.86E+03	3.24E+03	1.62E+03	4.05E+02	4.05E+01
9.200E+00	4.02E+03	2.68E+03	1.34E+03	3.35E+02	3.35E+01
1.350E+01	3.27E+03	2.18E+03	1.09E+03	2.73E+02	2.73E+01
2.100E+01	2.68E+03	1.78E+03	8.92E+02	2.23E+02	2.23E+01
3.000E+01	2.21E+03	1.48E+03	7.38E+02	1.84E+02	1.85E+01
4.500E+01	1.79E+03	1.19E+03	5.97E+02	1.49E+02	1.50E+01
6.900E+01	1.45E+03	9.67E+02	4.84E+02	1.21E+02	1.23E+01
1.000E+02	1.23E+03	8.23E+02	4.12E+02	1.03E+02	1.08E+01
1.350E+02	1.08E+03	7.23E+02	3.62E+02	9.10E+01	9.77E+00
1.700E+02	9.58E+02	6.39E+02	3.20E+02	8.08E+01	8.99E+00
2.200E+02	8.47E+02	5.65E+02	2.83E+02	7.18E+01	8.38E+00
2.800E+02	7.49E+02	5.00E+02	2.51E+02	6.39E+01	7.88E+00
3.600E+02	6.66E+02	4.45E+02	2.23E+02	5.74E+01	7.57E+00
4.500E+02	5.93E+02	3.96E+02	1.99E+02	5.17E+01	7.39E+00
5.750E+02	5.20E+02	3.48E+02	1.75E+02	4.62E+01	7.39E+00
7.600E+02	4.59E+02	3.07E+02	1.56E+02	4.17E+01	7.59E+00
9.600E+02	4.05E+02	2.71E+02	1.38E+02	3.80E+01	8.05E+00
1.275E+03	3.58E+02	2.40E+02	1.23E+02	3.52E+01	8.78E+00
1.600E+03	3.22E+02	2.17E+02	1.12E+02	3.33E+01	9.68E+00
2.000E+03	2.85E+02	1.93E+02	1.01E+02	3.19E+01	1.12E+01
2.700E+03	2.53E+02	1.72E+02	9.18E+01	3.14E+01	1.33E+01
3.400E+03	2.26E+02	1.56E+02	8.48E+01	3.18E+01	1.59E+01
4.500E+03	2.05E+02	1.43E+02	8.02E+01	3.33E+01	1.92E+01
5.500E+03	1.88E+02	1.32E+02	7.70E+01	3.54E+01	2.29E+01
7.200E+03	1.73E+02	1.24E+02	7.56E+01	3.91E+01	2.82E+01
9.200E+03	1.62E+02	1.19E+02	7.67E+01	4.46E+01	3.50E+01
1.200E+04	1.55E+02	1.17E+02	7.96E+01	5.13E+01	4.29E+01
1.500E+04	1.51E+02	1.18E+02	8.47E+01	5.97E+01	5.22E+01
1.900E+04	1.51E+02	1.22E+02	9.31E+01	7.14E+01	6.48E+01
2.550E+04	1.56E+02	1.30E+02	1.05E+02	8.61E+01	8.04E+01
3.220E+04	1.63E+02	1.41E+02	1.18E+02	1.01E+02	9.62E+01

Energy [eV]	90at%	60at%	30at%	7.5at%	0.75at%
4.000E+04	1.74E+02	1.54E+02	1.34E+02	1.19E+02	1.15E+02
5.250E+04	2.11E+02	1.93E+02	1.74E+02	1.61E+02	1.57E+02
6.600E+04	2.23E+02	2.06E+02	1.88E+02	1.75E+02	1.71E+02
8.800E+04	2.58E+02	2.39E+02	2.20E+02	2.06E+02	2.02E+02
1.100E+05	2.99E+02	2.75E+02	2.52E+02	2.34E+02	2.29E+02
1.350E+05	3.60E+02	3.26E+02	2.92E+02	2.67E+02	2.59E+02
1.600E+05	5.67E+02	5.07E+02	4.47E+02	4.02E+02	3.89E+02
1.900E+05	8.56E+02	7.35E+02	6.15E+02	5.24E+02	4.97E+02
2.200E+05	1.13E+03	9.85E+02	8.43E+02	7.37E+02	7.05E+02
2.550E+05	1.07E+03	1.04E+03	1.02E+03	9.97E+02	9.91E+02
2.900E+05	8.77E+02	8.19E+02	7.61E+02	7.17E+02	7.04E+02
3.200E+05	8.34E+02	7.86E+02	7.38E+02	7.02E+02	6.91E+02
3.600E+05	9.68E+02	9.34E+02	8.99E+02	8.74E+02	8.66E+02
4.000E+05	1.61E+03	1.58E+03	1.56E+03	1.54E+03	1.53E+03
4.500E+05	8.37E+02	8.17E+02	7.97E+02	7.81E+02	7.77E+02
5.000E+05	6.35E+02	6.18E+02	6.01E+02	5.89E+02	5.85E+02
5.500E+05	6.62E+02	6.48E+02	6.34E+02	6.23E+02	6.20E+02
6.000E+05	6.13E+02	6.01E+02	5.89E+02	5.81E+02	5.78E+02
6.600E+05	6.32E+02	6.23E+02	6.14E+02	6.07E+02	6.05E+02
7.200E+05	6.65E+02	6.59E+02	6.52E+02	6.48E+02	6.46E+02
7.800E+05	7.78E+02	7.75E+02	7.72E+02	7.69E+02	7.69E+02
8.400E+05	8.13E+02	8.14E+02	8.14E+02	8.15E+02	8.15E+02
9.200E+05	1.38E+03	1.38E+03	1.39E+03	1.39E+03	1.39E+03
1.000E+06	1.08E+03	1.09E+03	1.10E+03	1.11E+03	1.11E+03
1.200E+06	9.40E+02	9.53E+02	9.66E+02	9.75E+02	9.78E+02
1.400E+06	7.34E+02	7.45E+02	7.57E+02	7.66E+02	7.69E+02
1.600E+06	7.97E+02	8.06E+02	8.16E+02	8.23E+02	8.25E+02
1.800E+06	8.53E+02	8.62E+02	8.70E+02	8.76E+02	8.77E+02
2.000E+06	6.49E+02	6.56E+02	6.64E+02	6.69E+02	6.71E+02
2.300E+06	5.49E+02	5.57E+02	5.64E+02	5.69E+02	5.71E+02
2.600E+06	6.78E+02	6.84E+02	6.90E+02	6.94E+02	6.96E+02
2.900E+06	8.55E+02	8.57E+02	8.60E+02	8.62E+02	8.62E+02
3.300E+06	1.20E+03	1.20E+03	1.20E+03	1.20E+03	1.20E+03
3.700E+06	1.06E+03	1.06E+03	1.06E+03	1.07E+03	1.07E+03
4.100E+06	9.27E+02	9.39E+02	9.51E+02	9.59E+02	9.62E+02
4.500E+06	8.18E+02	8.31E+02	8.43E+02	8.52E+02	8.54E+02
5.000E+06	8.40E+02	8.45E+02	8.50E+02	8.53E+02	8.54E+02
5.500E+06	8.84E+02	8.86E+02	8.89E+02	8.91E+02	8.92E+02
6.000E+06	7.22E+02	7.24E+02	7.26E+02	7.27E+02	7.28E+02
6.700E+06	7.98E+02	7.98E+02	7.97E+02	7.97E+02	7.97E+02
7.400E+06	8.44E+02	8.43E+02	8.41E+02	8.40E+02	8.40E+02
8.200E+06	8.41E+02	8.40E+02	8.40E+02	8.39E+02	8.39E+02
9.000E+06	8.06E+02	8.05E+02	8.04E+02	8.03E+02	8.03E+02
1.000E+07	8.54E+02	8.53E+02	8.52E+02	8.52E+02	8.51E+02
1.100E+07	9.36E+02	9.35E+02	9.34E+02	9.33E+02	9.33E+02
1.200E+07	9.25E+02	9.24E+02	9.23E+02	9.22E+02	9.22E+02
1.300E+07	9.06E+02	9.05E+02	9.04E+02	9.03E+02	9.02E+02
1.400E+07	9.04E+02	9.02E+02	9.01E+02	9.00E+02	8.99E+02
1.500E+07	8.95E+02	8.93E+02	8.92E+02	8.90E+02	8.90E+02
1.600E+07	8.04E+02	8.01E+02	7.99E+02	7.97E+02	7.96E+02

Energy [eV]	90at%	60at%	30at%	7.5at%	0.75at%
1.700E+07	7.64E+02	7.61E+02	7.59E+02	7.57E+02	7.56E+02
1.800E+07	7.05E+02	7.02E+02	6.99E+02	6.97E+02	6.97E+02
1.900E+07	6.65E+02	6.62E+02	6.59E+02	6.57E+02	6.57E+02

TAB. 3: Threshold values for defect species in Li_4SiO_4

Ed [eV]	Li	O	Si
Marlowe, @1180K	34	18	118
Marlowe, @0K	33	19	112
Specter/Specomp	10	30	25

FIGURES

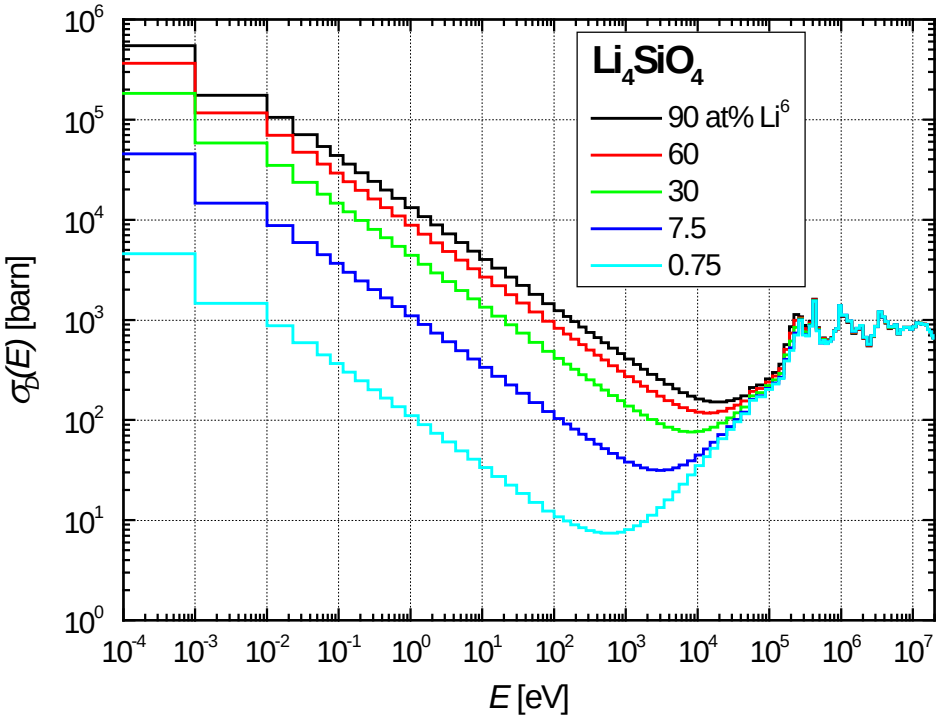

FIG. 1: Total displacement cross sections in Li_4SiO_4: with different Li^6-enrichments

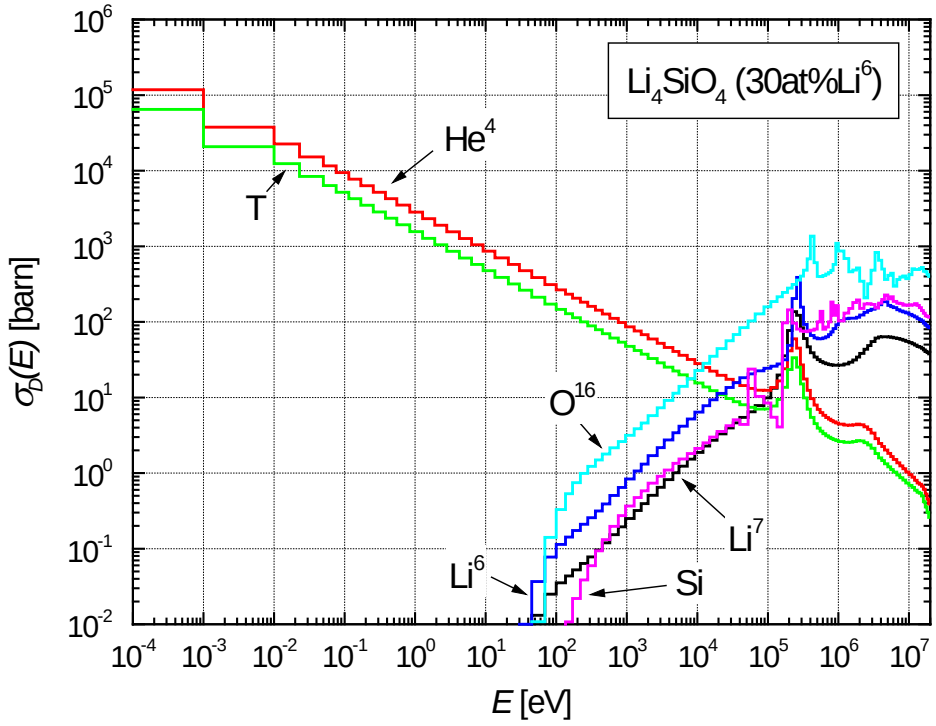

FIG. 2: Contributions to displacement cross section for Li_4SiO_4 (30at% Li^6)

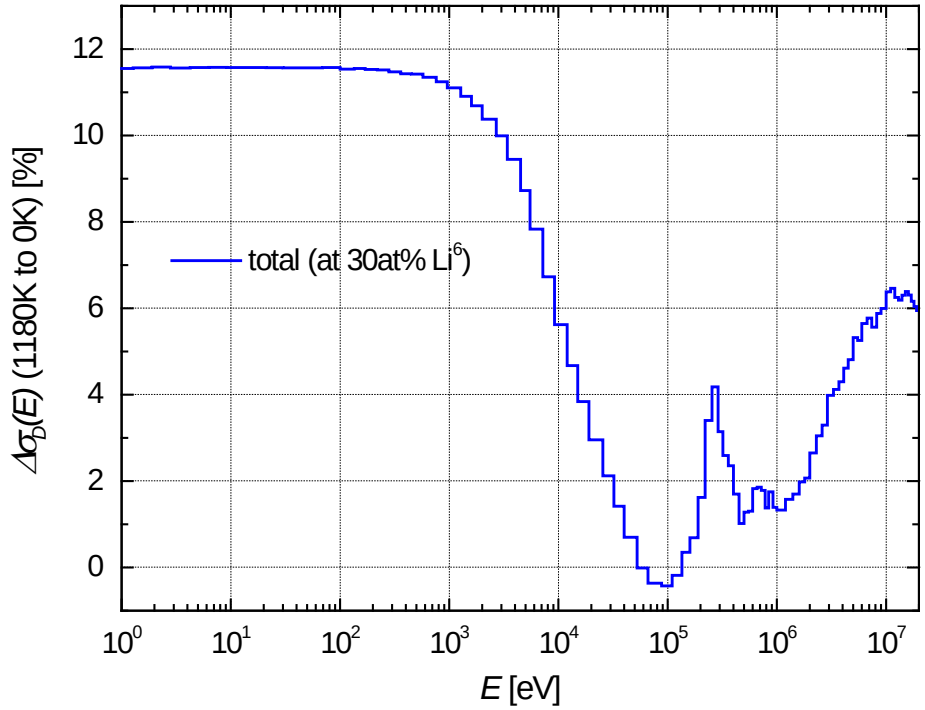

FIG. 3: Difference of total displacement cross sections of Li_4SiO_4 (30at%) at 1180 K and 0 K.