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Damage Parameters and Cross Sections for Li_2O

INTRODUCTION

International comparative irradiation of breeder materials

Ceramic breeder materials in future fusion power reactor blankets will be exposed to high levels of neutron irradiation doses. This will cause primary damage effects which may significantly deteriorate material properties like mechanical stiffness, chemical integrity, and thermal conductivity and thereby limit the blanket lifetime. In order to assess the expected damage for such conditions, irradiation experiments in available fission reactors are being performed. The comparability between fission and fusion irradiation effects (fusion-fission correlation) generally is evaluated on the basis of calculations of damage correlation parameters like Lithium burn-up, displacements per atom (*dpa*) and gas production.

A program was initiated at the meeting on "International comparative irradiation of breeder materials" held at Petten, September 16, 1998 which in the first step should select methods and provide data for damage correlation parameters to compare candidate fission reactors with respect to their potential for simulating, as much as possible, fusion reactor conditions. A nuclear expert group was established which met together at Karlsruhe, March 17, 1999. During this meeting it was agreed that a novel approach to calculate *dpa* in breeder materials should be used for all candidate materials. This present report will summarise the calculational procedure and results for Lithiumoxide Li_2O and provide displacement cross section (σ_D) data to be used in *dpa*-analyses.

Computer simulation of displacement damage

For light mass and polyatomic solids displacement damage calculations based on standard NRT [1] are not appropriate. Furthermore, analytical formulations like NRT are not capable to include specific atomistic or microscopic material properties. Therefore a simulational approach has been pursued to establish proper damage parameters in these materials.

A extensively modified and adapted version of the binary collision code MARLOWE [2] was used to simulate displacement cascades in candidate breeder materials.

BCA-SIMULATIONS

Methodology

Displacement cascades, initiated by a primary knock-on atom (PKA), are simulated within the framework of the binary collision approximation (BCA). It is based essentially on the assumption that all collisions of projectiles and target atoms can be regarded as a sequence of solely binary encounters with an asymptotic description of the real atomic trajectories. This picture as implemented in the code MARLOWE provides a fast and rather well founded description of the "primary defect state" in the evolution of PKA-induced atomic cascades. However, due to the requirements of the materials under concern especially in fast neutron irradiations some additional issues have to be included in the simulation like ionic binding and long range interactions. The details of this sophisticated model and the development work can be found in Ref. [3].

Simulational model for Li_2O

In order to perform realistic simulations of displacement cascades in Lithiumoxide Li_2O, it is mandatory to provide some microscopic data, which is summarised in the following:

Crystalline structure: antifluorite, spacegroup Fm3m
Lattice constant: a=4.6114 Å (at 293 K), 4.676 (at 800K)
Bonding: ionic, heat of formation $\Delta H_f = -142{,}4 kcal / mole$
Crystallite models: static crystal @0K, thermal vibrations @800K (rms about 0.1 ... 0.2 Å)
Li^6-enrichment: 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 and *dpa*. For Li_2O the following reactions have been considered:

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

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

RESULTS

Damage cross sections

In FIG. 1 the resulting displacement cross sections for Li_2O 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 is representative for temperatures expected in irradiation experiments. Moreover, the effect of changes in temperature in the crystalline model is negligibly compared to the difference to a static crystal. As an example, FIG. 2 shows total displacement cross sections of Li_2O (enriched to 30 at% Li^6) at 800K and 0K (cf. TAB. 2). The cross section at 800K increases by about 55 % below 1 keV and around 20 % above 0.1 MeV.

Some details

Partial displacement cross sections (Li_2O, 800K, 30 at% Li^6) are given in FIG. 3. They clearly indicate two irradiation regimes: neutrons below 10 keV will produce damage via t and He^4, above this energy mainly O^{16} and Li^7 are responsible for the rise up to around 700 barn.

Defect production is mainly due to Li-defects with a share of about 80 %, 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 [4].

Besides lattice defects of interstitial and vacancy type, disorder defects (substitutional type) are created in Li_2O which amount to roughly 14 % of the number of lattice defects at 800 K. In static crystal conditions the efficiency increases up to more than 17 %. Compared to results for Li_4SiO_4 and Li_2SiO_3 (Ref. [5]) the disorder defect fraction is quite low because of the simple fcc structure of Li_2O.

Comparison with NRT-dpa

The damage code SPECTER/SPECOMP has been selected as a reference system which calculates displacement damage parameters based on Lindhard-NRT.

Compound cross sections for Li_2O have been calculated by Specomp with Li^6-enrichments of 30 at%, 7.5 at%, and 0.75 at% with E_d(Li) = 10 eV, E_d(O) = 30 eV. Except for the low energy regime where the displacement cross sections of Marlowe and of Specomp nearly coincide, Specomp overestimates the Marlowe-result by roughly 30 %, most pronounced for the contribution of O^{16}.

The latter behaviour can be attributed, at least partly, to the different values of E_d. Accordingly, the contribution of α and t in Specomp is significantly to low which is once more a indication that a simple NRT-treatment is not appropriate in the case of light mass particles.

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TABLES

TAB. 1: Displacement cross section [barn] in Li_20: contributions of PKA's, not normalised

Energy [eV]	Li6	He4	T	Li7	O16
1.000E-04	0.000E+00	1.386E+06	4.358E+05	0.000E+00	0.000E+00
1.000E-03	0.000E+00	4.441E+05	1.396E+05	0.000E+00	0.000E+00
1.000E-02	0.000E+00	2.656E+05	8.352E+04	0.000E+00	0.000E+00
2.300E-02	0.000E+00	1.793E+05	5.637E+04	0.000E+00	0.000E+00
5.000E-02	0.000E+00	1.362E+05	4.283E+04	0.000E+00	0.000E+00
7.600E-02	0.000E+00	1.111E+05	3.493E+04	0.000E+00	0.000E+00
1.150E-01	0.000E+00	9.103E+04	2.862E+04	0.000E+00	0.000E+00
1.700E-01	0.000E+00	7.456E+04	2.344E+04	0.000E+00	0.000E+00
2.550E-01	0.000E+00	6.101E+04	1.918E+04	0.000E+00	0.000E+00
3.800E-01	0.000E+00	5.028E+04	1.581E+04	0.000E+00	0.000E+00
5.500E-01	0.000E+00	4.129E+04	1.298E+04	0.000E+00	0.000E+00
8.400E-01	0.000E+00	3.343E+04	1.051E+04	0.000E+00	0.000E+00
1.275E+00	0.000E+00	2.728E+04	8.578E+03	0.000E+00	0.000E+00
1.900E+00	0.000E+00	2.239E+04	7.039E+03	0.000E+00	0.000E+00
2.800E+00	0.000E+00	1.833E+04	5.762E+03	0.000E+00	0.000E+00
4.250E+00	0.000E+00	1.495E+04	4.701E+03	0.000E+00	0.000E+00
6.300E+00	0.000E+00	1.232E+04	3.874E+03	0.000E+00	0.000E+00
9.200E+00	0.000E+00	1.018E+04	3.201E+03	0.000E+00	0.000E+00
1.350E+01	0.000E+00	8.294E+03	2.608E+03	0.000E+00	0.000E+00
2.100E+01	3.738E-03	6.782E+03	2.132E+03	0.000E+00	0.000E+00
3.000E+01	8.628E-02	5.608E+03	1.763E+03	6.674E-02	0.000E+00
4.500E+01	2.143E-01	4.535E+03	1.426E+03	2.297E-01	2.221E-02
6.900E+01	3.587E-01	3.676E+03	1.156E+03	4.494E-01	2.894E-01
1.000E+02	4.803E-01	3.126E+03	9.829E+02	6.369E-01	6.888E-01
1.350E+02	5.800E-01	2.744E+03	8.626E+02	7.824E-01	1.151E+00
1.700E+02	6.873E-01	2.425E+03	7.624E+02	9.397E-01	1.653E+00
2.200E+02	8.174E-01	2.143E+03	6.739E+02	1.113E+00	2.318E+00
2.800E+02	9.730E-01	1.894E+03	5.956E+02	1.325E+00	2.990E+00
3.600E+02	1.165E+00	1.684E+03	5.294E+02	1.588E+00	3.788E+00
4.500E+02	1.402E+00	1.496E+03	4.704E+02	1.922E+00	4.661E+00
5.750E+02	1.744E+00	1.311E+03	4.121E+02	2.410E+00	5.748E+00
7.600E+02	2.152E+00	1.154E+03	3.628E+02	3.009E+00	6.989E+00
9.600E+02	2.686E+00	1.014E+03	3.188E+02	3.809E+00	8.482E+00
1.275E+03	3.318E+00	8.928E+02	2.807E+02	4.778E+00	1.027E+01
1.600E+03	4.003E+00	7.983E+02	2.510E+02	5.812E+00	1.220E+01
2.000E+03	5.038E+00	7.010E+02	2.204E+02	7.375E+00	1.522E+01
2.700E+03	6.293E+00	6.142E+02	1.931E+02	9.265E+00	1.931E+01
3.400E+03	7.833E+00	5.400E+02	1.698E+02	1.157E+01	2.430E+01
4.500E+03	9.563E+00	4.790E+02	1.507E+02	1.423E+01	3.043E+01
5.500E+03	1.153E+01	4.260E+02	1.341E+02	1.726E+01	3.762E+01
7.200E+03	1.419E+01	3.749E+02	1.181E+02	2.130E+01	4.777E+01
9.200E+03	1.722E+01	3.312E+02	1.044E+02	2.607E+01	6.121E+01
1.200E+04	2.072E+01	2.940E+02	9.272E+01	3.159E+01	7.635E+01
1.500E+04	2.443E+01	2.630E+02	8.297E+01	3.760E+01	9.472E+01
1.900E+04	2.935E+01	2.321E+02	7.327E+01	4.571E+01	1.196E+02
2.550E+04	3.478E+01	2.060E+02	6.506E+01	5.452E+01	1.515E+02
3.220E+04	4.020E+01	1.869E+02	5.907E+01	6.291E+01	1.838E+02
4.000E+04	4.725E+01	1.697E+02	5.376E+01	7.303E+01	2.267E+02
5.250E+04	5.555E+01	1.560E+02	4.953E+01	8.186E+01	2.788E+02
6.600E+04	6.647E+01	1.475E+02	4.691E+01	8.932E+01	3.458E+02
8.800E+04	8.249E+01	1.472E+02	4.689E+01	9.572E+01	4.272E+02
1.100E+05	1.081E+02	1.603E+02	5.110E+01	1.012E+02	5.030E+02
1.350E+05	1.589E+02	1.958E+02	6.245E+01	1.077E+02	5.788E+02
1.600E+05	2.814E+02	2.839E+02	9.050E+01	1.220E+02	6.582E+02
1.900E+05	6.002E+02	4.886E+02	1.555E+02	1.875E+02	7.452E+02
2.200E+05	1.059E+03	7.042E+02	2.235E+02	7.691E+02	8.305E+02
2.550E+05	9.457E+02	5.295E+02	1.677E+02	1.445E+03	9.380E+02
2.900E+05	6.424E+02	3.168E+02	1.003E+02	5.786E+02	1.055E+03
3.200E+05	4.625E+02	2.062E+02	6.532E+01	3.420E+02	1.255E+03
3.600E+05	3.568E+02	1.460E+02	4.627E+01	2.732E+02	1.767E+03
4.000E+05	2.966E+02	1.131E+02	3.587E+01	2.428E+02	3.532E+03

Energy [eV]	Li6	He4	T	Li7	O16
4.500E+05	2.597E+02	9.313E+01	2.958E+01	2.260E+02	1.599E+03
5.000E+05	2.385E+02	8.135E+01	2.587E+01	2.195E+02	1.042E+03
5.500E+05	2.248E+02	7.370E+01	2.345E+01	2.204E+02	1.027E+03
6.000E+05	2.150E+02	6.795E+01	2.167E+01	2.252E+02	1.060E+03
6.600E+05	2.078E+02	6.342E+01	2.026E+01	2.335E+02	1.103E+03
7.200E+05	2.031E+02	6.012E+01	1.924E+01	2.480E+02	1.155E+03
7.800E+05	2.000E+02	5.761E+01	1.847E+01	2.692E+02	1.234E+03
8.400E+05	1.979E+02	5.541E+01	1.779E+01	2.979E+02	1.480E+03
9.200E+05	1.969E+02	5.352E+01	1.721E+01	3.341E+02	2.833E+03
1.000E+06	1.979E+02	5.147E+01	1.660E+01	3.776E+02	2.241E+03
1.200E+06	2.035E+02	4.974E+01	1.610E+01	3.987E+02	1.786E+03
1.400E+06	2.134E+02	4.926E+01	1.601E+01	4.018E+02	1.187E+03
1.600E+06	2.277E+02	4.978E+01	1.623E+01	4.001E+02	1.253E+03
1.800E+06	2.487E+02	5.062E+01	1.656E+01	4.109E+02	1.331E+03
2.000E+06	2.773E+02	4.935E+01	1.623E+01	4.367E+02	8.825E+02
2.300E+06	3.140E+02	4.615E+01	1.524E+01	4.717E+02	5.315E+02
2.600E+06	3.502E+02	4.233E+01	1.406E+01	4.980E+02	8.143E+02
2.900E+06	3.962E+02	3.763E+01	1.257E+01	5.158E+02	1.213E+03
3.300E+06	4.395E+02	3.149E+01	1.058E+01	5.384E+02	2.084E+03
3.700E+06	4.559E+02	2.702E+01	9.141E+00	5.892E+02	1.634E+03
4.100E+06	4.581E+02	2.454E+01	8.346E+00	6.458E+02	1.249E+03
4.500E+06	4.571E+02	2.178E+01	7.459E+00	6.470E+02	9.017E+02
5.000E+06	4.536E+02	1.952E+01	6.726E+00	5.815E+02	1.012E+03
5.500E+06	4.487E+02	1.761E+01	6.111E+00	5.582E+02	1.077E+03
6.000E+06	4.411E+02	1.592E+01	5.566E+00	5.427E+02	7.160E+02
6.700E+06	4.306E+02	1.423E+01	5.017E+00	5.097E+02	8.761E+02
7.400E+06	4.195E+02	1.281E+01	4.555E+00	4.887E+02	9.493E+02
8.200E+06	4.072E+02	1.160E+01	4.157E+00	4.756E+02	9.765E+02
9.000E+06	3.934E+02	1.037E+01	3.746E+00	4.597E+02	8.948E+02
1.000E+07	3.780E+02	9.374E+00	3.413E+00	4.400E+02	1.007E+03
1.100E+07	3.628E+02	8.572E+00	3.141E+00	4.209E+02	1.207E+03
1.200E+07	3.487E+02	7.692E+00	2.832E+00	4.062E+02	1.181E+03
1.300E+07	3.321E+02	7.010E+00	2.588E+00	3.843E+02	1.183E+03
1.400E+07	3.249E+02	6.701E+00	2.476E+00	3.741E+02	1.216E+03
1.500E+07	3.143E+02	6.265E+00	2.251E+00	3.594E+02	1.262E+03
1.600E+07	2.983E+02	5.748E+00	1.889E+00	3.355E+02	1.130E+03
1.700E+07	2.846E+02	5.208E+00	1.604E+00	3.176E+02	1.114E+03
1.800E+07	2.723E+02	4.512E+00	1.362E+00	3.026E+02	1.023E+03
1.900E+07	2.615E+02	3.864E+00	1.159E+00	2.903E+02	9.720E+02

TAB. 2: Total displacement cross sections [barn] for Li_2O: with different Li6-enrichments

Energy [eV]	30at%	7.5at%	0.75at%
1.000E-04	3.644E+05	9.110E+04	9.110E+03
1.000E-03	1.167E+05	2.918E+04	2.918E+03
1.000E-02	6.983E+04	1.746E+04	1.746E+03
2.300E-02	4.713E+04	1.178E+04	1.178E+03
5.000E-02	3.581E+04	8.953E+03	8.953E+02
7.600E-02	2.921E+04	7.302E+03	7.302E+02
1.150E-01	2.393E+04	5.982E+03	5.982E+02
1.700E-01	1.960E+04	4.900E+03	4.900E+02
2.550E-01	1.604E+04	4.009E+03	4.009E+02
3.800E-01	1.322E+04	3.304E+03	3.304E+02
5.500E-01	1.085E+04	2.713E+03	2.713E+02
8.400E-01	8.788E+03	2.197E+03	2.197E+02
1.275E+00	7.172E+03	1.793E+03	1.793E+02
1.900E+00	5.886E+03	1.471E+03	1.471E+02
2.800E+00	4.817E+03	1.204E+03	1.204E+02
4.250E+00	3.930E+03	9.826E+02	9.826E+01
6.300E+00	3.240E+03	8.099E+02	8.099E+01
9.200E+00	2.676E+03	6.691E+02	6.691E+01
1.350E+01	2.180E+03	5.451E+02	5.451E+01
2.100E+01	1.783E+03	4.457E+02	4.457E+01
3.000E+01	1.474E+03	3.686E+02	3.690E+01
4.500E+01	1.192E+03	2.982E+02	2.997E+01
6.900E+01	9.666E+02	2.419E+02	2.455E+01
1.000E+02	8.224E+02	2.061E+02	2.120E+01
1.350E+02	7.221E+02	1.812E+02	1.893E+01
1.700E+02	6.386E+02	1.605E+02	1.711E+01
2.200E+02	5.649E+02	1.424E+02	1.560E+01
2.800E+02	4.998E+02	1.264E+02	1.433E+01
3.600E+02	4.449E+02	1.130E+02	1.338E+01
4.500E+02	3.960E+02	1.011E+02	1.266E+01
5.750E+02	3.479E+02	8.962E+01	1.213E+01
7.600E+02	3.075E+02	8.013E+01	1.192E+01
9.600E+02	2.717E+02	7.195E+01	1.202E+01
1.275E+03	2.410E+02	6.521E+01	1.247E+01
1.600E+03	2.174E+02	6.032E+01	1.318E+01
2.000E+03	1.938E+02	5.594E+01	1.459E+01
2.700E+03	1.735E+02	5.283E+01	1.664E+01
3.400E+03	1.570E+02	5.111E+01	1.934E+01
4.500E+03	1.446E+02	5.088E+01	2.276E+01
5.500E+03	1.349E+02	5.177E+01	2.682E+01
7.200E+03	1.273E+02	5.442E+01	3.255E+01
9.200E+03	1.231E+02	5.912E+01	3.992E+01
1.200E+04	1.217E+02	6.530E+01	4.839E+01
1.500E+04	1.232E+02	7.328E+01	5.830E+01
1.900E+04	1.281E+02	8.479E+01	7.179E+01
2.550E+04	1.371E+02	9.942E+01	8.811E+01
3.220E+04	1.479E+02	1.144E+02	1.043E+02
4.000E+04	1.638E+02	1.341E+02	1.252E+02
5.250E+04	1.834E+02	1.565E+02	1.484E+02
6.600E+04	2.091E+02	1.834E+02	1.757E+02
8.800E+04	2.424E+02	2.153E+02	2.071E+02
1.100E+05	2.788E+02	2.460E+02	2.362E+02
1.350E+05	3.267E+02	2.802E+02	2.663E+02
1.600E+05	4.075E+02	3.274E+02	3.034E+02
1.900E+05	5.847E+02	4.262E+02	3.787E+02
2.200E+05	1.033E+03	8.504E+02	7.956E+02
2.550E+05	1.316E+03	1.286E+03	1.277E+03
2.900E+05	8.334E+02	7.613E+02	7.396E+02
3.200E+05	7.246E+02	6.658E+02	6.482E+02
3.600E+05	8.262E+02	7.848E+02	7.724E+02
4.000E+05	1.380E+03	1.349E+03	1.340E+03
4.500E+05	7.149E+02	6.914E+02	6.844E+02
5.000E+05	5.188E+02	4.999E+02	4.942E+02
5.500E+05	5.096E+02	4.943E+02	4.898E+02

Energy [eV]	30at%	7.5at%	0.75at%
6.000E+05	5.192E+02	5.073E+02	5.037E+02
6.600E+05	5.349E+02	5.262E+02	5.236E+02
7.200E+05	5.573E+02	5.521E+02	5.505E+02
7.800E+05	5.922E+02	5.912E+02	5.909E+02
8.400E+05	6.867E+02	6.908E+02	6.920E+02
9.200E+05	1.154E+03	1.164E+03	1.167E+03
1.000E+06	9.765E+02	9.933E+02	9.983E+02
1.200E+06	8.352E+02	8.546E+02	8.605E+02
1.400E+06	6.389E+02	6.574E+02	6.630E+02
1.600E+06	6.631E+02	6.791E+02	6.838E+02
1.800E+06	6.987E+02	7.130E+02	7.172E+02
2.000E+06	5.665E+02	5.806E+02	5.848E+02
2.300E+06	4.724E+02	4.868E+02	4.911E+02
2.600E+06	5.851E+02	5.988E+02	6.030E+02
2.900E+06	7.343E+02	7.447E+02	7.478E+02
3.300E+06	1.042E+03	1.051E+03	1.053E+03
3.700E+06	9.181E+02	9.326E+02	9.370E+02
4.100E+06	8.158E+02	8.390E+02	8.459E+02
4.500E+06	6.998E+02	7.239E+02	7.311E+02
5.000E+06	7.047E+02	7.199E+02	7.245E+02
5.500E+06	7.140E+02	7.269E+02	7.307E+02
6.000E+06	5.845E+02	5.965E+02	6.001E+02
6.700E+06	6.199E+02	6.289E+02	6.316E+02
7.400E+06	6.318E+02	6.396E+02	6.420E+02
8.200E+06	6.320E+02	6.399E+02	6.423E+02
9.000E+06	5.943E+02	6.021E+02	6.045E+02
1.000E+07	6.191E+02	6.264E+02	6.287E+02
1.100E+07	6.736E+02	6.806E+02	6.826E+02
1.200E+07	6.552E+02	6.622E+02	6.644E+02
1.300E+07	6.419E+02	6.483E+02	6.502E+02
1.400E+07	6.468E+02	6.528E+02	6.546E+02
1.500E+07	6.529E+02	6.584E+02	6.601E+02
1.600E+07	5.944E+02	5.989E+02	6.002E+02
1.700E+07	5.779E+02	5.818E+02	5.830E+02
1.800E+07	5.378E+02	5.415E+02	5.426E+02
1.900E+07	5.128E+02	5.163E+02	5.174E+02

TAB. 3: Threshold values for defect species in Li2O

Ed [eV]	Li	O
MARLOWE, @800K	19	57
MARLOWE, @0K	23	61
SPECTER/SPECOMP	10	30

FIGURES

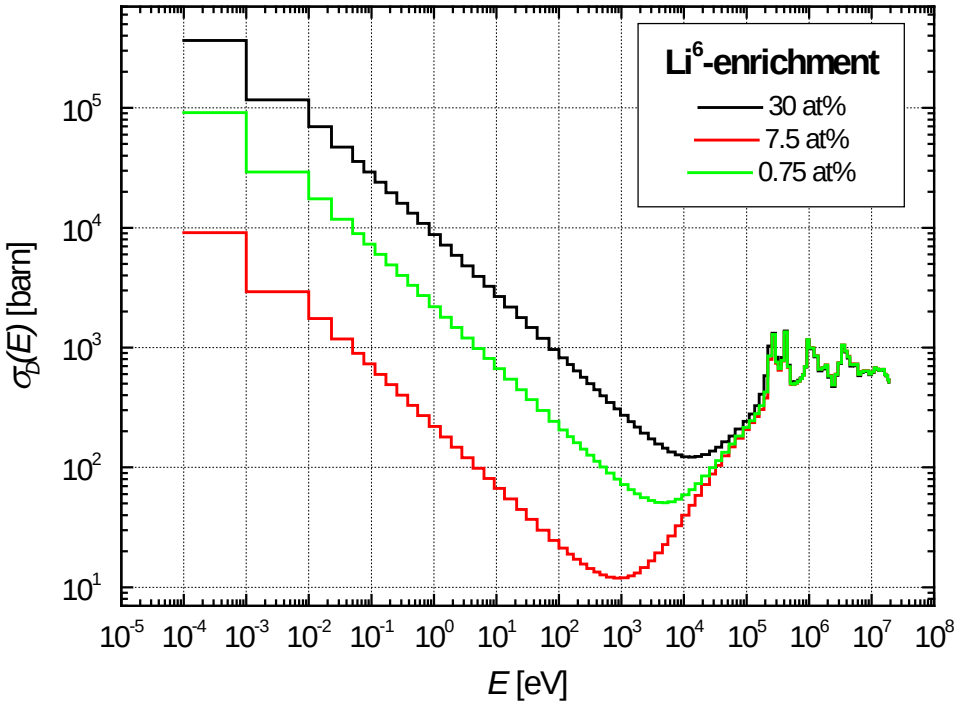

FIG. 1: Total displacement cross sections in Li_2O: with different Li^6-enrichments

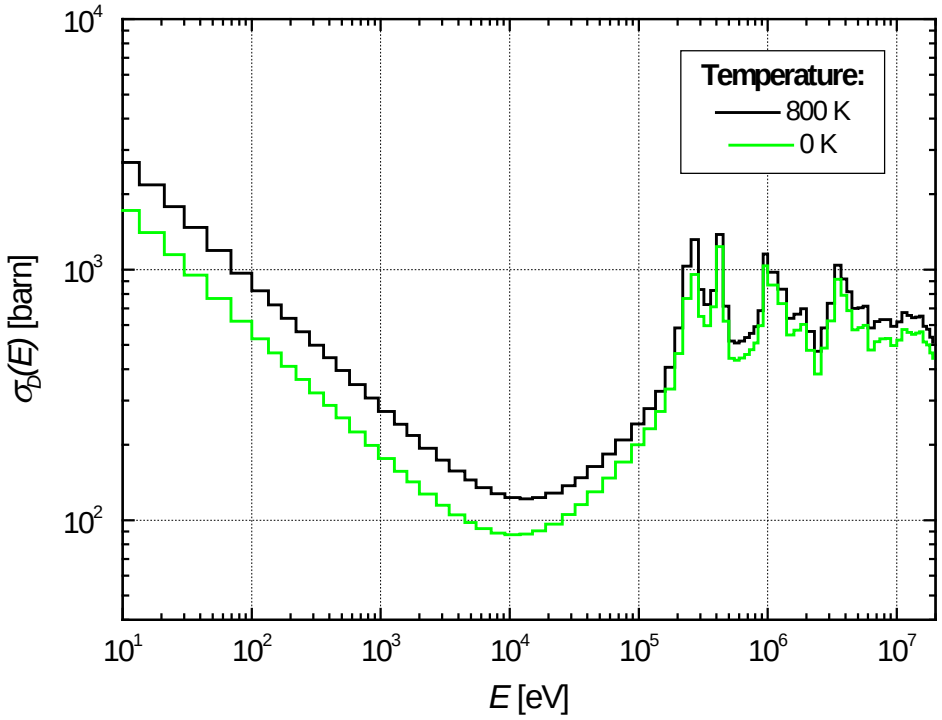

FIG. 2: Total displacement cross sections for Li_2O at 800K and 0K

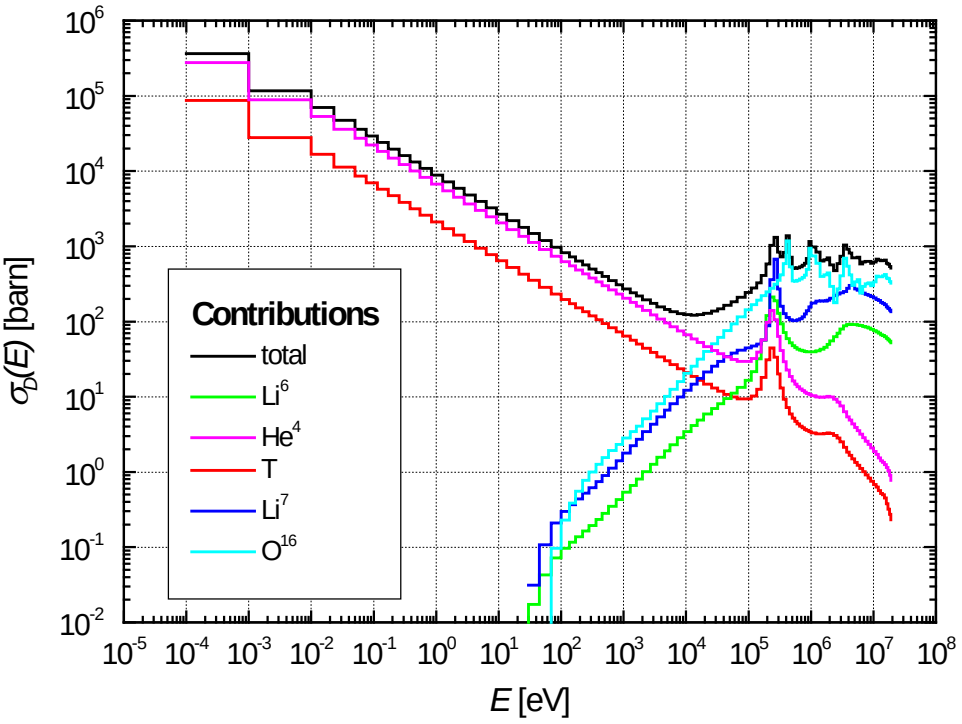

FIG. 3: Contributions to displacement cross section for Li_2O (30at% Li^6)