Appendix B

Scattering Length Tables and Sample Thickness Calculations

In this appendix we list commonly used information that is useful in planning and analyzing neutron scattering experiments.

The tables are for the scattering lengths for the atoms, and for some isotopes. All absorbtion cross-sections are listed for neutrons of 25.3 meV. At a glance, the tables will tell the experimenter whether a particular element absorbs so strongly that it can be a problem in neutron scattering experiments. But the tables will also help in calculating how much material one needs to obtain a sample that scatters neutrons by the desired amount. We give an example of the latter.

Suppose we wish to investigate a sample of $CeFe_2Ge_2$. The unit cell of this sample contains 2 formula units, and the tetragonal unit cell measures 4 x 4 x 10 $Å^3$. We wish to calculate what thickness we would need for about a 10 % scatterer. In other words, we are looking for the thickness L that yields a 90 % transmission as in $T = 0.9e^{-n\sigma L}$, or $n\sigma L \approx 0.1$. n is the number density, which in this case would be 2 formula units per 160 $Å^3$, or 1.25 x $10^{22}/\text{cm}^3$. We use units of cm, so that we get our thickness in cm.

Next we need to calculate the scattering cross section per formula unit, which is a combination of the coherent and incoherent scattering cross-sections. We use the table below to find

$$\sigma_{\text{scat,formula unit}} = \sigma_{\text{Ce,coh}} + \sigma_{\text{Ce,inc}} + 2\sigma_{\text{Fe,coh}} + 2\sigma_{\text{Fe,inc}} + 2\sigma_{\text{Ge,coh}} + 2\sigma_{\text{Ge,inc}}.$$

Putting in the numbers we find $\sigma_{\text{formula unit}}$= 43.78 barn = 43.78 x 10^{-24} cm ^{2}. With these numbers we find L= 0.18 cm, so not very thick at all.

Let us also check on the absorbtion cross-section, to see if this would be a problem. We evaluate this for neutrons that have an energy of 25.3 meV, thus,

$$\sigma_{\text{abs,formula unit}} = \sigma_{\text{Ce,abs}} + 2\sigma_{\text{Fe,abs}} + 2\sigma_{\text{Ge,abs}}.$$

Using the tables below we find $\sigma_{\text{abs,formula unit}}$= 10.15 barn. For a sample of 0.18 cm thickness, this would lead an absorbtion of about 2.2 % of the neutrons. This is a very manageable number, so we do not have to worry about the feasibility of the experiment, but we probably should correct for it during the analysis stages.

These tables have the incoherent cross-sections listed per element. This incoherent cross-section can come from different isotopes that make up the element as found in nature, and it can come from the incoherent cross-section of individual atoms. We can have another source of incoherent scattering in samples, namely when we have more than one atom that can sit on identical positions in the unit cell. For instance, going back to our example of $CeFe_2Ge_2$, we can decide to substitute some ruthenium in place of the iron atoms. This will give rise to incoherent scattering since now the scattered waves originating from nominally identical positions within the crystal lattice, will have a different scattering strength. We would have to recalculate the coherent and incoherent cross section in this case.

This calculation follows the following recipe. We define an average scattering length $\bar{b}$ and an average of the scattering length squared $(\bar{b^2})$. With these numbers we define the coherent and incoherent cross-sections by

$$\sigma_{\mathrm{coh}} = 4\pi\bar{b}^2$$

$$\sigma_{\mathrm{inc}} = 4\pi[(\bar{b^2}) - \bar{b}^2].$$

Looking at the total scattering, we see that we do not add or subtract from the total level of scattering which still is $4\pi(\bar{b^2})$, but rather some of the coherent scattering now becomes incoherent scattering.

Suppose we substitute 25 % Ru on the Fe sites in $CeFe_2Ge_2$. We then find that the average scattering length on the Fe/Ru site is 8.96 fm, and the average scattering length squared is 81.25 fm^2. This gives us $\sigma_{\mathrm{coh,\ Fe/Ru}}=$ 10.09 barn and $\sigma_{\mathrm{inc,\ Fe/Ru}}=$ 0.122 barn. To this latter number for the incoherent cross-section, we would still have to add the incoherent cross-section per atom, that is, 0.75 x $\sigma_{\mathrm{inc,\ Fe}}$ + 0.25 x $\sigma_{\mathrm{inc,\ Ru}}=$ 0.4 barn. The reason for this is that we still have the incoherent cross-section that each individual atom contributes, but we have added to the loss of coherence by randomly substituting Ru atoms on Fe sites. We would then use those numbers ($\sigma_{\mathrm{coh,\ Fe/Ru}}=$ 10.09 barn and $\sigma_{\mathrm{inc,\ Fe/Ru}}=$ 0.52 barn) in our further calculations to calculate the scattering cross-section per formula unit.

Table B.1 The element and isotope dependent scattering lengths and cross-sections. '*' refers to the naturally occurring isotope mixture for an element. 1 barn = 10^{-24} cm^2.

Z	Name	A	mass [au]	b_{coh} [fm]	σ_{coh} [barn]	σ_{inc} [barn]	σ_{abs} [barn]
1	H	*	1.008	-3.739	1.757	80.263	0.333
1	D	2	2.016	6.671	5.592	2.048	0.001
1	T	3	3.024	4.940	3.067	0.000	0.000
2	He	*	4.003	3.260	1.336	0.004	0.007
2	He	3	3.003	5.740	4.140	1.460	5333
2	He	4	4.003	3.260	1.336	0.004	0.000
3	Li	*	6.941	-1.900	0.454	0.916	70.500
3	Li	6	6.015	1.870	0.439	0.541	940
3	Li	7	7.016	-2.200	0.608	0.832	0.045
4	Be	*	9.012	7.790	7.626	0.004	0.008
5	B	*	10.810	5.300	3.530	1.710	767.000
5	B	10	10.013	0.000	0.000	0.980	3837
5	B	11	11.009	6.660	5.574	0.226	0.001
6	C	*	12.011	6.646	5.550	0.001	0.004
7	N	*	14.007	9.360	11.009	0.501	1.900
8	O	*	15.999	5.803	4.232	0.000	0.000
9	F	*	18.998	5.654	4.017	0.001	0.010
10	Ne	*	20.179	4.566	2.620	0.008	0.039
11	Na	*	22.990	3.580	1.611	1.674	0.530
12	Mg	*	24.305	5.375	3.631	0.079	0.063
13	Al	*	26.982	3.449	1.495	0.008	0.231
14	Si	*	28.086	4.153	2.168	0.003	0.171
15	P	*	30.974	5.130	3.307	0.005	0.172
16	S	*	32.060	2.847	1.019	0.007	0.530
17	Cl	*	35.453	9.577	11.526	5.274	33.500
18	Ar	*	39.948	1.909	0.458	0.225	0.675
19	K	*	39.098	3.670	1.693	0.267	2.100
20	Ca	*	40.080	4.760	2.847	0.043	0.430
21	Sc	*	44.956	12.290	18.981	4.519	27.500
22	Ti	*	47.900	-3.438	1.485	2.865	6.090
23	V	*	50.942	-0.382	0.018	5.082	5.080
24	Cr	*	51.996	3.635	1.660	1.830	3.050

Table B.2 The element and isotope dependent scattering lengths and cross-sections, continued

Z	Name	A	mass [au]	b_{coh} [fm]	σ_{coh} [barn]	σ_{inc} [barn]	σ_{abs} [barn]
25	Mn	*	54.938	-3.730	1.748	0.402	13.300
26	Fe	*	55.847	9.540	11.437	0.383	2.560
27	Co	*	58.933	2.780	0.971	4.829	37.180
28	Ni	*	58.700	10.300	13.332	5.168	4.490
29	Cu	*	63.546	7.718	7.485	0.545	3.780
30	Zn	*	65.380	5.680	4.054	0.077	1.110
31	Ga	*	69.720	7.288	6.675	0.155	2.750
32	Ge	*	72.590	8.185	8.419	0.181	2.200
33	As	*	74.922	6.580	5.441	0.059	4.500
34	Se	*	78.960	7.970	7.982	0.318	11.700
35	Br	*	79.904	6.795	5.802	0.098	6.900
36	Kr	*	83.800	7.810	7.665	0.015	25.000
37	Rb	*	85.468	7.090	6.317	0.483	0.380
38	Sr	*	87.620	7.020	6.193	0.057	1.280
39	Y	*	88.906	7.750	7.548	0.152	1.280
40	Zr	*	91.220	7.160	6.442	0.018	0.185
41	Nb	*	92.906	7.054	6.253	0.002	1.150
42	Mo	*	95.940	6.715	5.666	0.044	2.480
43	Tc	*	97.000	6.800	5.811	0.489	20.000
44	Ru	*	101.070	7.210	6.533	0.067	2.560
45	Rh	*	102.906	5.880	4.345	0.255	144.800
46	Pd	*	106.400	5.910	4.389	0.091	6.900
47	Ag	*	107.868	5.922	4.407	0.583	63.300
48	Cd	*	112.410	5.100	3.269	2.431	2520
49	In	*	114.820	4.065	2.076	0.544	193.800
50	Sn	*	118.690	6.225	4.870	0.022	0.626
51	Sb	*	121.750	5.570	3.899	0.001	4.910
52	Te	*	127.600	5.800	4.227	0.093	4.700
53	I	*	126.905	5.280	3.503	0.307	6.150
55	Cs	*	132.905	5.420	3.692	0.208	29.000
56	Ba	*	137.330	5.070	3.230	0.150	1.100
57	La	*	138.906	8.240	8.532	1.128	8.970

Table B.3 The element and isotope dependent scattering lengths and cross-sections, continued

Z	Name	A	mass [au]	b_{coh} [fm]	σ_{coh} [barn]	σ_{inc} [barn]	σ_{abs} [barn]
58	Ce	*	140.120	4.840	2.944	0.000	0.630
59	Pr	*	140.907	4.450	2.488	0.042	11.500
60	Nd	*	144.240	7.690	7.431	9.169	50.500
61	Pm	*	145.000	12.600	19.950	1.350	168.400
62	Sm	*	150.400	0.800	0.080	38.920	5922
63	Eu	*	151.960	7.220	6.551	2.649	4530
64	Gd	*	157.250	6.500	5.309	174.691	49700
65	Tb	*	158.925	7.380	6.844	0.000	23.400
66	Dy	*	162.500	16.900	35.891	54.409	994
67	Ho	*	164.930	8.010	8.063	0.357	64.700
68	Er	*	167.260	8.160	8.367	0.833	159
69	Tm	*	168.934	7.070	6.281	0.099	100
70	Yb	*	173.040	12.430	19.416	3.984	34.800
71	Lu	*	174.967	7.210	6.533	0.667	74.000
72	Hf	*	178.490	7.770	7.587	2.613	104.100
73	Ta	*	180.948	6.910	6.000	0.010	20.600
74	W	*	183.850	4.860	2.968	1.632	18.300
75	Re	*	186.200	9.200	10.636	0.864	89.700
76	Os	*	190.200	10.700	14.387	0.313	16.00
77	Ir	*	192.220	10.600	14.120	0.000	425
78	Pt	*	195.090	9.600	11.581	0.129	10.300
79	Au	*	196.967	7.630	7.316	0.434	98.650
80	Hg	*	200.590	12.692	20.243	6.557	372.300
81	Tl	*	204.370	8.776	9.678	0.212	3.430
82	Pb	*	207.200	9.405	11.115	0.003	0.171
83	Bi	*	208.980	8.532	9.148	0.008	0.034
88	Ra	*	226.025	10.000	12.566	0.434	12.800
90	Th	*	232.038	10.520	13.907	0.003	7.370
91	Pa	*	231.036	9.100	10.406	0.094	200.600
92	U	*	238.029	8.417	8.903	0.005	7.570
93	Np	*	237.048	10.550	13.987	0.513	175.900

Appendix A
Conversions

Depending on whether one is talking to chemists, physicists or biologists, and depending where they come from, different units are being used to quantify the amount of energy transferred from the neutron to the sample. For instance, one can encounter various units such as meV, THz and ps^{-1}, as well as some less common ones such as cm^{-1}. The table below lists the conversions between the various common units, and the not so common ones. For example, if one wants to evaluate the exponential e^{-E/k_BT} with E expressed in meV and T in Kelvin, then this exponential would become $e^{-E*11.605/T}$.

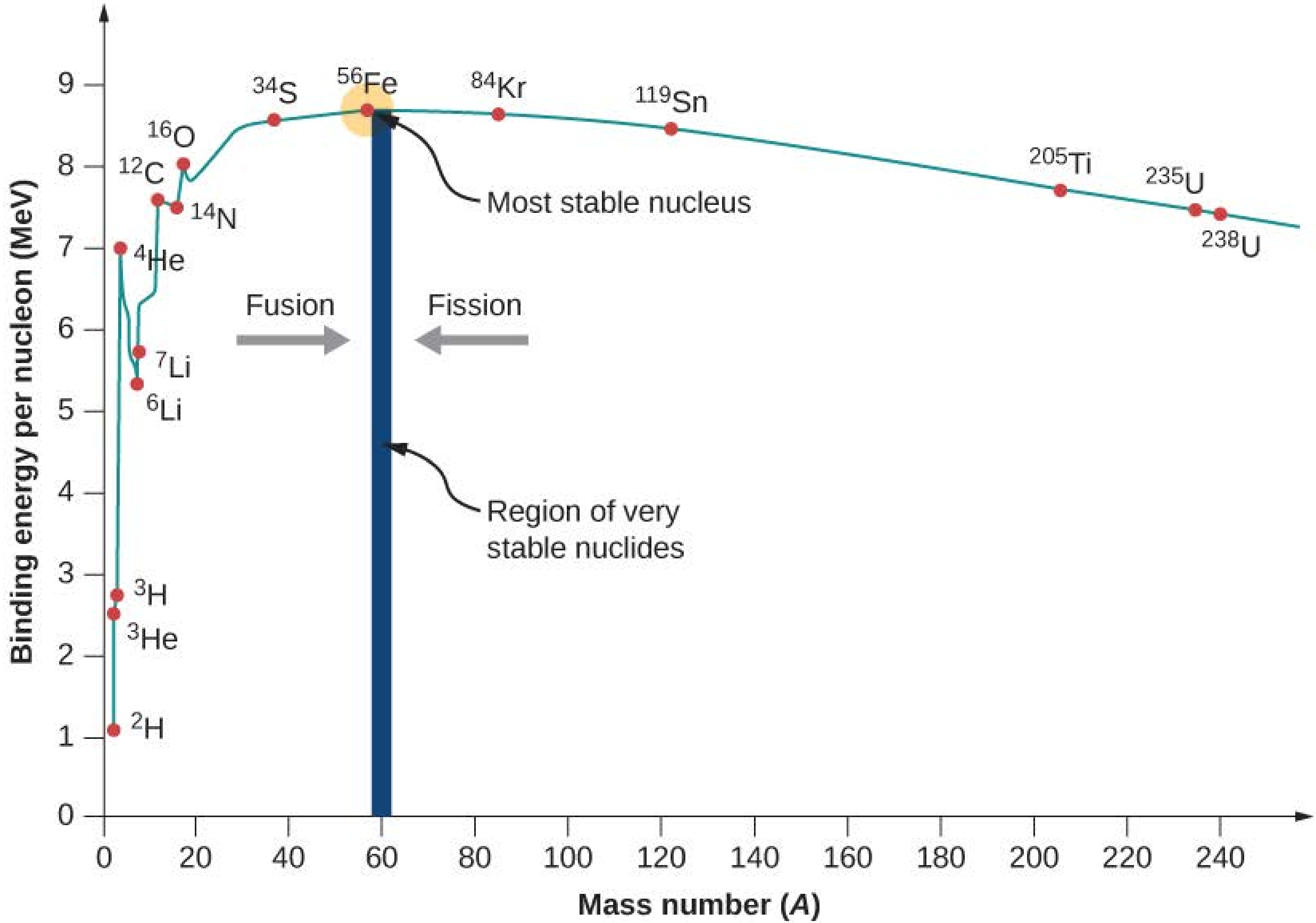
Table A.1 The conversions between the energy units employed in scattering experiments. The conversions are carried out using : $E = h\nu = \hbar\omega = \hbar ck = k_BT = \mu_BH$.

		E [meV]	ν [THz]	ω [ps^{-1}]	k [cm^{-1}]	T [K]	H [Tesla]
1 meV	=	1	0.24180	1.5193	8.0655	11.605	17.326
1 THz	=	4.1357	1	6.2832	33.356	47.994	71.655
1 ps^{-1}	=	0.65821	0.15912	1	5.3088	7.6384	11.404
1 cm^{-1}	=	0.12398	0.029979	0.18837	1	1.43883	2.1481
1 K	=	0.086170	0.020836	0.13092	0.69500	1	1.4930
1 Tesla	=	0.057717	0.013956	0.087689	0.46551	0.66980	1

The energy of a neutron is measured in meV, but it can also be characterized by its speed v, its wave length λ or its wave number k. If we use the units [meV] for energy, [km/s] for speed, [Å] for wave length and [$Å^{-1}$] for wave number, then the numerical conversions read:

$$E = 5.2267v^2 = \frac{81.799}{\lambda^2} = 2.072178k^2. \quad \text{(A.1)}$$

For example, a 4 Å neutron has an energy of about 5 meV and travels roughly at 1000 m/s.



Binding energy per nucleon (MeV)
Mass number (A)
0
1
2
3
4
5
6
7
8
9
0
20
40
60
80
100
120
140
160
180
200
220
240
2H
3H
3He
4He
6Li
7Li
12C
14N
16O
34S
56Fe
84Kr
119Sn
205Ti
235U
238U
Most stable nucleus
Region of very stable nuclides
Fusion
Fission