Appendices

Appendix A

Isotopes of Selected Elements

Table A.1, on the next two pages, lists all stable, naturally occurring isotopes of elements observed in the various spectra shown or discussed in this thesis. Elements are listed in order of increasing mass. Naturally occurring radioactive nuclides, such as ^{40}K and ^{180}Ta, generally have very small natural abundances, and were not included in this table. The information in this table is taken from *Nuclides and Isotopes, Fifteenth Edition*, General Electric Nuclear Energy, 1996.

Element	Nuclide	Atomic mass, amu	Natural abundance, %
Hydrogen	^{1}H	1.0078	99.985
	^{2}H	2.0141	0.015
Lithium	^{6}Li	6.0151	7.5
	^{7}Li	7.0160	92.5
Carbon	^{12}C	12.000	98.90
	^{13}C	13.003	1.10
Oxygen	^{16}O	15.995	99.76
	^{17}O	16.999	0.04
	^{18}O	17.999	0.20
Sodium	^{23}Na	22.990	100.00
Magnesium	^{24}Mg	23.985	78.99
	^{25}Mg	24.986	10.00
	^{26}Mg	25.983	11.01
Aluminum	^{27}Al	26.982	100.00
Silicon	^{28}Si	27.977	92.23
	^{29}Si	28.976	4.67
	^{30}Si	29.974	3.10
Sulfur	^{32}S	31.972	95.02
	^{33}S	32.971	0.75
	^{34}S	33.968	4.21
	^{36}S	35.967	0.02
Potassium	^{39}K	38.964	93.26
	^{41}K	40.962	6.73

Table A.1. Natural abundances and masses of stable isotopes of selected elements.

Element	Nuclide	Atomic mass, amu	Natural abundance, %
Calcium	^{40}Ca	39.963	96.94
	^{42}Ca	41.959	0.647
	^{43}Ca	42.959	0.135
	^{44}Ca	43.955	2.086
	^{46}Ca	45.954	0.004
	^{48}Ca	47.953	0.187
Chromium	^{50}Cr	49.946	4.35
	^{52}Cr	51.941	83.79
	^{53}Cr	52.941	9.50
	^{54}Cr	53.939	2.36
Iron	^{54}Fe	53.940	5.85
	^{56}Fe	55.935	91.75
	^{57}Fe	56.935	2.12
	^{58}Fe	57.933	0.28
Copper	^{63}Cu	62.930	69.17
	^{65}Cu	64.928	30.83
Molybdenum	^{92}Mo	91.907	14.84
	^{94}Mo	93.905	9.25
	^{95}Mo	94.906	15.92
	^{96}Mo	95.905	16.68
	^{97}Mo	96.906	9.55
	^{98}Mo	97.905	24.13
	^{100}Mo	99.907	9.63
Tantalum	^{181}Ta	180.948	99.988

Table A.1, continued. Natural abundances and masses of stable isotopes of selected elements.

Appendix B

Ion Definitions Used in Simulations

SIMION ion trajectory software, versions 6.0 and 7.0 (by David A. Dahl, Idaho National Engineering and Environmental Laboratory, Idaho Falls, 83415), were used extensively both in testing possible designs and in evaluating the working design. In order to make full use of SIMION's ion definition capabilities, I wrote a spreadsheet to estimate the properties of positive ions emerging from an impact-generated plasma. The ion properties generated using the spreadsheet were loaded into SIMION and used for various simulations. This appendix contains the details of the spreadsheet. It is hoped that it may be useful for anyone trying to run similar impact-ionization simulations.

SIMION requires ion definition files to be of the following ASCII format, in which each line represents an individual ion:

TOB, MASS, CHARGE, X, Y, Z, AZ, EL, KE, CWF, COLOR

TOB is the ion's time-of-birth. X, y, and z refer to the coordinates at which the ion originates. AZ and EL are the azimuth and elevation angles, respectively, along which the ions are initially moving with an initial kinetic energy, KE. Figure B.1 shows the coordinate system in which ions are defined. CWF is the charge-weighing factor, which is used in certain ion-ion repulsion calculations (default 1), and color is the color with which the ion appears on the screen.

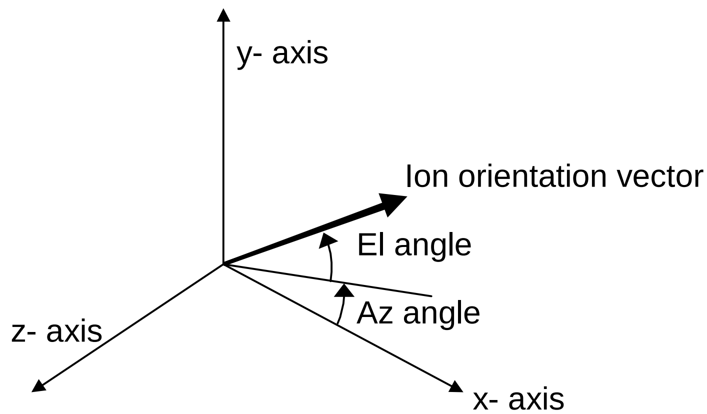

Figure B.1. Coordinate system and angular orientations of ions used in SIMION. Azimuthal angle lies along the xz plane, in the negative z direction. Elevation angle is in the direction of y.

Below is a section from the first page of the spreadsheet. This ion definition spreadsheet produces a file of ion definitions with the following properties. First, the initial kinetic energies of ions are a Gaussian-random distribution about a specified mean, with a specified standard deviation. Second, the spatial distribution of the ions can be specified as either isotropic, *cos* θ, or cos^2 θ about the normal to the target plate. Ions can originate at the same point, at varying points, or from a small distribution of points about some location. Although time-of-birth and CWF could be modified, I never needed to do so. Mass and charge are easily specified as needed for each simulation. Values in the first six columns are input directly. The values of Az, El, and KE for each ion were calculated using the process described in the following pages.

Ion definition template Page 1

Gaussian Distribution
ions come off of plate in y-z plane, directed right, parallel to x-axis

average energy	40 eV	39.72 actual energy average
stdev	25 eV	25.00 actual energy stdev

			initial ion location			off of x along z	off of x-z along y			
TOB	mass	charge	x	y	z	az	el	KE	CFW	color
0	56	1	5.001	0	0	3.532	-7.027	57.328	1	1
0	56	1	5.001	0	0	-67.596	-20.620	81.120	1	1
0	56	1	5.001	0	0	1.397	-61.068	25.415	1	1
0	56	1	5.001	0	0	77.802	29.052	36.501	1	1
0	56	1	5.001	0	0	23.623	-9.895	29.929	1	1
0	56	1	5.001	0	0	17.240	7.263	9.368	1	1
0	56	1	5.001	0	0	-7.732	22.263	26.998	1	1
0	56	1	5.001	0	0	45.324	-6.879	43.903	1	1
0	56	1	5.001	0	0	33.316	9.824	60.822	1	1
0	56	1	5.001	0	0	-66.266	-42.192	36.443	1	1
0	56	1	5.001	0	0	35.487	51.647	72.173	1	1
0	56	1	5.001	0	0	-13.153	45.889	18.502	1	1
0	56	1	5.001	0	0	-53.510	-5.973	-8.664	1	1
0	56	1	5.001	0	0	-47.595	-30.520	66.578	1	1

Below is a section of the second page of the spreadsheet, in which a set of random values in a Gaussian distribution was generated. Each value in the leftmost column is the sum of 50 random numbers, each of which has an average value of zero. The average and standard deviation for the entire column of sums are calculated and displayed at the top of the page. The kinetic energy of the nth ion is determined by the formula:

$$KE_n = KE_0 + \left(\frac{\sigma_0}{\sigma_n}\right)(N_n), \quad (1)$$

where KE_0 is average kinetic energy specified on the first page, σ_0 is the specified standard deviation from the first page, σ_n is the standard deviation of the random sums from the second page, and N_n is the nth random sum on the second page.

Gaussian distribution generator				Page 2. Uses sum of 50 randomly-generated numbers to give a random normal distribution				
average	0.0406							
stdev	1.8012							
	1	2	3	4	5	6	7	8
-1.741	-0.378	-0.25	0.0034	0.1944	-0.072	0.177	-0.269	-0.052
2.331	0.0863	0.1353	-0.028	0.3569	0.394	0.3474	0.0121	0.2424
1.159	-0.441	0.4716	0.2117	-0.062	0.0559	0.3325	-0.49	0.0371
-0.518	0.2131	0.473	0.0592	0.1735	0.1904	-0.382	-0.464	-0.25
-3.383	0.3217	-0.32	-0.415	0.0408	-0.293	-0.189	-0.307	0.1735
-1.132	-0.439	-0.289	-0.046	-0.367	0.2571	-0.172	0.2115	-0.078
-1.533	-0.364	0.1838	-0.047	-0.287	0.481	-0.095	0.2088	0.3166
1.527	0.3773	-0.173	-0.33	-0.467	0.4798	0.4888	-0.286	-0.344
-0.412	0.3966	0.4396	-0.065	0.1112	0.0811	-0.044	-0.205	-0.295
2.833	0.0981	0.221	-0.047	-0.154	0.4053	0.0631	0.1409	0.2108
-3.165	0.3621	-0.039	-0.458	0.1486	0.2067	-0.498	-0.187	-0.037

Below is a sample from page three of the spreadsheet. This page generates the x-, y-, and z-directional components with which the azimuth and elevation angles of each ion are calculated. In the first three columns, three random numbers define a directional vector. R is the magnitude of this vector. In the next column, vectors which fall inside a positive-x hemisphere with radius 0.5 are assigned a value of 1 (eventually retained). Vectors outside this hemisphere are assigned a value of zero, and will not be used. Zero-sets are deleted, and the remaining coordinates are randomly sorted and tabulated. The az and el values for defined ions are then

$$\mathrm{Az}_n = \tan^{-1}\left(\frac{z_n}{x_n}\right) \tag{2}$$

$$\mathrm{El}_\mathrm{n} = \tan^{-1}\left(\frac{y_n}{\sqrt{x_n^2 + z_n^2}}\right). \tag{3}$$

The resulting angles are converted from radians into degrees, which are the units used by SIMION.

isotropic distribution								Page 3		
				sphere				isotropic distribution		
rand x	rand y	rand z	R	R<0.5	x	y	z	x	y	z
0.388	0.291	-0.097	0.494	1	0.3878	0.2909	-0.097	0.0602	-0.284	-0.062
0.061	0.080	0.414	0.426	1	0.0612	0.0801	0.4137	0.2014	0.2275	-0.08
0.278	-0.387	0.420	0.635	0	0	0	0	0.2868	0.3441	-0.181
0.428	-0.204	0.048	0.477	1	0.4281	-0.204	0.0477	0.0368	0.1188	0.2317
0.138	-0.224	-0.370	0.455	1	0.1385	-0.224	-0.37	0.3012	0.1318	0.0102
0.327	0.157	0.210	0.419	1	0.3272	0.1574	0.2095	0.091	0.0955	0.2684
0.400	-0.378	-0.191	0.582	0	0	0	0	0.2717	-0.26	0.0394
0.397	0.432	0.305	0.662	0	0	0	0	0.4287	-0.162	0.1489
0.368	0.157	-0.376	0.549	0	0	0	0	0.2436	0.4002	0.0278
0.466	0.421	0.428	0.760	0	0	0	0	0.2838	0.2779	-0.022
0.169	0.115	0.443	0.488	1	0.1694	0.1148	0.4433	0.0661	-0.267	0.0205
0.342	0.052	-0.080	0.355	1	0.3423	0.0517	-0.08	0.0139	-0.087	-0.288

Below is a sample from page four of the spreadsheet, which generates a cosine distribution of ions. X-, y-, and z-components are chosen randomly, similar to the isotropic distribution. Vectors outside of the r=0.5 hemisphere are excluded. The angle θ of each vector is calculated, and if the value of *cos* θ is greater than a random number, the vector is rejected. Note that θ is being defined as the angle away from the normal (in this case, the positive x-axis), and is not the same as the Az or El angles used in the ion definition file. The calculation of the cos^2 θ distribution is similar, except that cos^2 θ is compared to the random number. The resulting list of vectors is sorted, zero values eliminated, and vectors are ordered randomly into the list used to calculate Az and El for the ions. The Az and El calculations are the same as for the isotropic distribution.

cosine distribution										Page 4	
rand x	rand y	rand z	theta	R	sphere R<0.5	prob	rand	P>rand	x	y	z
0.307	-0.018	0.081	15.2	0.32	1	0.965	0.317	1	0.3069	-0.018	0.0814
0.012	-0.034	-0.133	85.0	0.14	1	0.087	0.969	0	0	0	0
0.018	0.442	0.221	87.9	0.49	1	0.037	0.337	0	0	0	0
0.053	0.131	0.220	78.3	0.26	1	0.203	0.745	0	0	0	0
0.430	-0.189	0.427	47.3	0.63	0	0.678	0.429	1	0	0	0
0.487	0.338	-0.141	37.0	0.61	0	0.799	0.313	1	0	0	0
0.334	-0.062	-0.162	27.4	0.38	1	0.888	0.627	1	0.3344	-0.062	-0.162
0.143	0.067	-0.411	71.1	0.44	1	0.324	0.326	0	0	0	0
0.399	0.090	0.030	13.4	0.41	1	0.973	0.242	1	0.399	0.0904	0.0304
0.226	0.176	0.109	42.6	0.31	1	0.736	0.969	0	0	0	0
0.457	0.280	0.216	37.7	0.58	0	0.791	0.987	0	0	0	0
0.276	-0.215	0.193	46.3	0.40	1	0.691	0.078	1	0.2758	-0.215	0.1927
0.122	0.364	0.161	72.9	0.42	1	0.294	0.555	0	0	0	0

Figures B.2, B.3, and B.4 show typical populations of ions generated using the above method, and compare the angular (spatial) distributions to ideal isotropic, *cos* θ, and cos^2 θ distributions. For these plots, θ for each ion (from groups of 5000 ions) was calculated as the angle in degrees from the normal to the surface at which ions originated. The number of ions with a given value of θ (rounded to the nearest integer) was then divided by *sin* θ to yield a surface density (effectively the density on the surface of a sphere to which the ion vectors had been projected) which was normalized. This normalized density as a function of θ is shown in the plots.

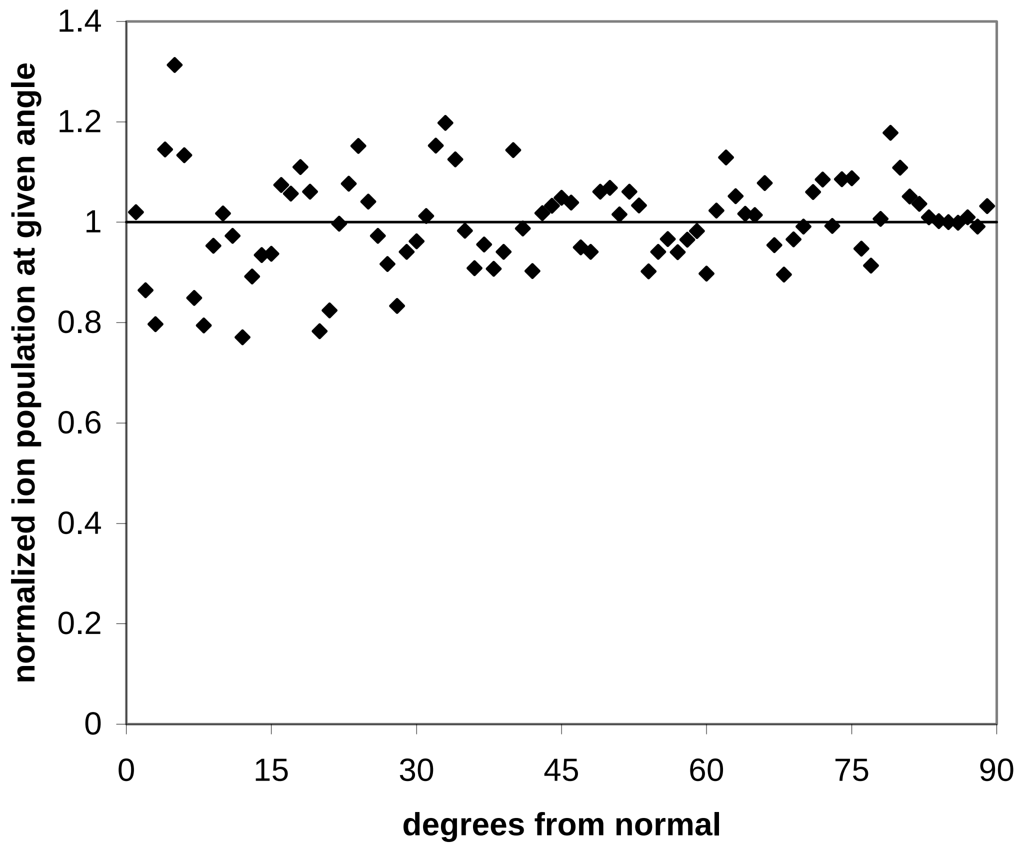

Figure B.2. Typical isotropic ion distribution as function of angle from normal.

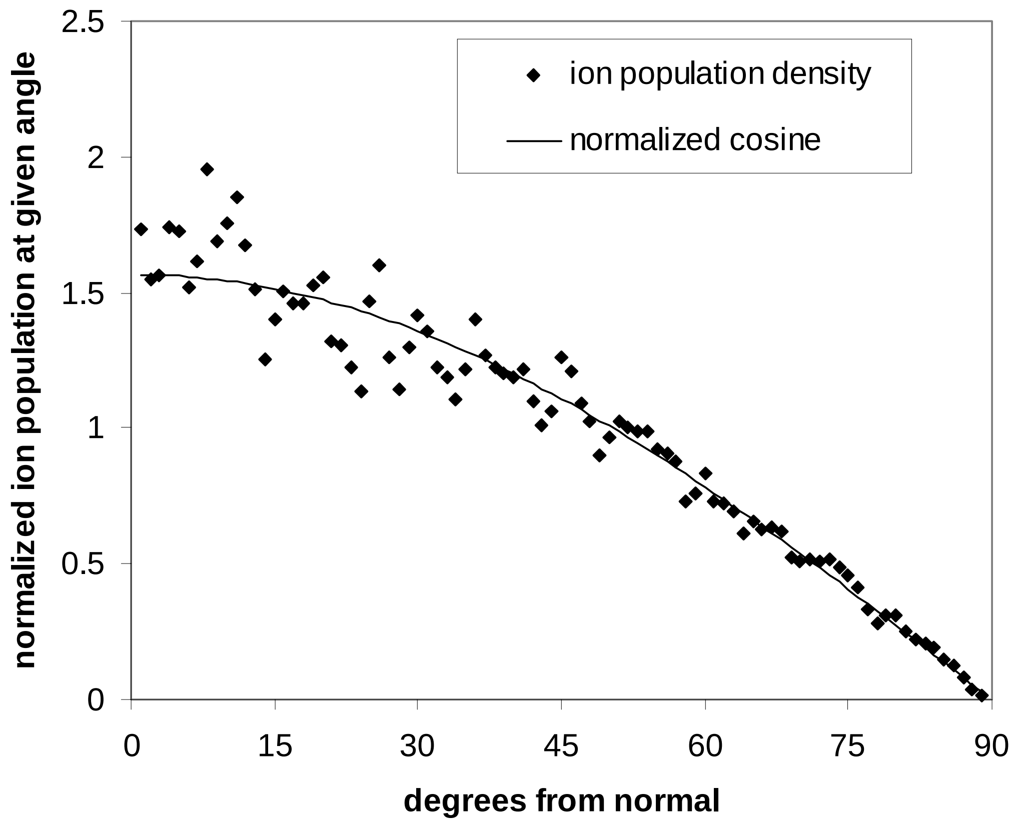

Figure B.3. Typical cosine ion distribution as function of angle from normal.

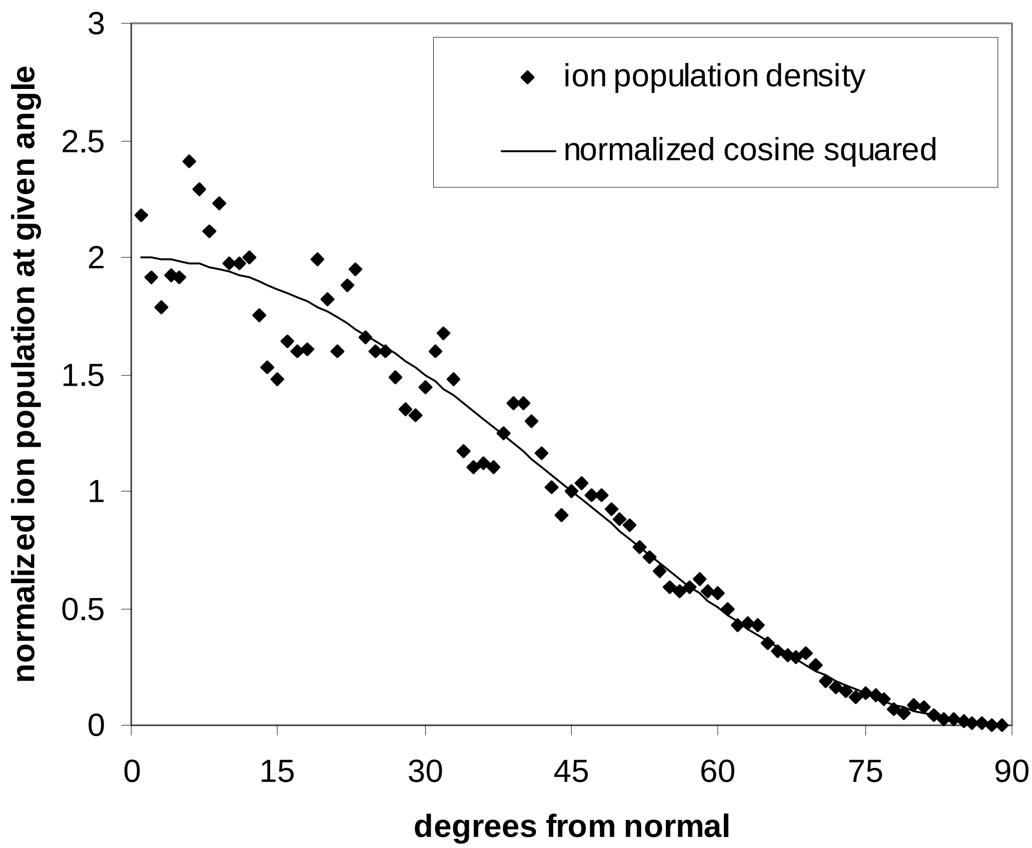

Figure B.4. Typical cosine-squared ion distribution as function of angle from normal.