# Appendices

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## APPENDIX A

### **Spectroscopic Notation**

The description of "2S+1 (Molecular term)<sub>Subscript</sub>" symbol (Nassau, 2001)

- 1. 2S+1 is total spin of valence electron
- 2. Molecular term symbols (Group theory)

2.1Non – degenerate orbital

- A has a wavefunction symmetric with principle symmetry axis.
- B has a wavefunction antisymmetric with principle symmetry axis.
- 2.2 Degenerate orbital
  - E has a doubly degenerate.
  - T has a triply degenerate.
- 3. Subscript
- 1 is the mirror planes parallel to the symmetric axis.
- 2 is the mirror planes perpendicular to the symmetric axis.
- g is unchanged sign of wavefunction on inversion through a center of symmetry.
- u is unchanged sign of wavefunction on inversion through a center of symmetry.

### **APPENDIX B**

### **Trajectory Simulation in Al<sub>2</sub>O<sub>3</sub>**

Simulated by SRIM 2008 software

Target Density =  $3.9700 \text{ g/cm}^3 = 1.1724 \times 10^{23} \text{ atoms/cm}^3$ 

| Atom | Atom number | Atomic percent | Mass percent |
|------|-------------|----------------|--------------|
| Al   | - 13        | 40.00          | 52.93        |
| 0    | 8           | 60.00          | 47.07        |

Bragg Correction = 0.00%

Table B. The target depth parameters in  $Al_2O_3$ .

|                |         | Ion    | dE/dx      | dE/dx                  | Projected | Longitudinal | Lateral    |
|----------------|---------|--------|------------|------------------------|-----------|--------------|------------|
| -              | Mass    | -      |            |                        | -         | U            |            |
| Ion            |         | Energy | Electronic | Nuclear                | Range     | Straggling   | Straggling |
|                | (amu)   | (keV)  | (keV/µm)   | (keV/µm)               | (Å)       | (Å)          | (Å)        |
| $H^+$          | 1.008   | 2000   | 0.1220     | $7.428 \times 10^{-5}$ | 258600    | 10500        | 11800      |
| 0 <sup>-</sup> | 15.9995 | 23     | 0.6008     | 0.7324                 | 334       | 144          | 105        |
| $N_2^+$        | 28.006  | 50     | 0.6636     | 0.6798                 | 785       | 239          | 181        |
| $N_2^+$        | 28.006  | 70     | 0.8443     | 0.5840                 | 1103      | 307          | 244        |
| $N_2^+$        | 28.006  | 80     | 0.9243     | 0.5470                 | 1256      | 337          | 274        |
| $N_2^+$        | 28.006  | 100    | 1.045      | 0.4874                 | 1555      | 388          | 329        |
| $Ar^+$         | 39.962  | 50     | 1.003      | 2.628                  | 317       | 102          | 76         |
| $Ar^+$         | 39.932  | 70     | 1.187 —    | 2.452                  | 435       | 133          | 99         |
| $Ar^+$         | 39.962  | 80     | 1.269      | 2.370                  | 495       | 148          | 110        |
| $Ar^+$         | 39.962  | 100    | 1.516      | 2.222                  | 613       | 176          | 133        |

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# APPENDIX C

### Si(Li) X-ray Detector

The X-ray detector, Canberra, model SSL30150 is used for X-ray detection of PIXE technique. This detector is the acceptor-doped semiconductor type whose is lithium-drifted silicon for the increasing of X-ray energy measurement efficiency. Some parameters are concluded in the Table C.

Table C. The parameters of Si(Li) X-ray detector.

| Information of Canberra detector                                | SSL30150  |
|---|-----------|
| Be window thickness (cm)  | 0.0075    |
| Au layer (cm)   | 1.0E-6    |
| Si crystal thickness (cm)                                       | 1.5       |
| Target to crystal distance (cm)                                 | 10.4      |
| Ag/At cutoff energy (keV) or if<0, Si dead layer thickness (cm) | -2.2E-5   |
| maximum nominal det res at 5.9 keV                              | 190       |
| default tau (ns)  | 500       |
| Z values for window, electrode and crystal                      | 4, 79, 14 |
| Pulse dead time in µs   | 78. Ve    |
| Voigtian line shape switch with cutoff                          | F 100     |

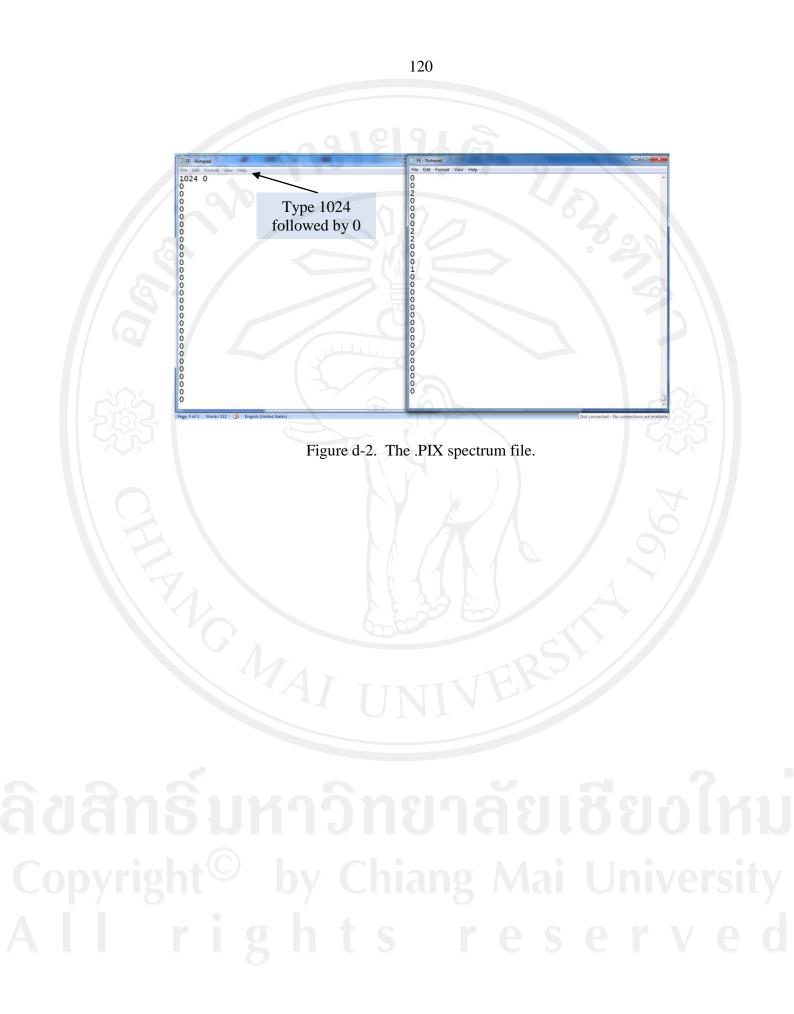
# APPENDIX D

### **Converting .SPE File to .PIX File**

The PIXE data file is collected in .SPE by MAESTRO software which has the data between channel number in the range of 0 - 1,023 and X-ray count as shown in Figure d-1. This file cannot be directly analyzed by the GUPIXWIN software. The user must erase the heading and footnote which is not related to the data. Moreover, the first line after the heading is also erased and type 1024 instead because the GUPIX software calculate the channel number at 1 to 1024. Then, spacing one times and type zero to clarify the program does not remain the old data. Eventually, the new file arrangement displays as shown in Figure d-2 which is similar to .PIX file and ready to run the spectrum for trace element concentration analysis in GUPIXWIN software.

| , Fe - Notepad  | Fe - Notepad   |
|---|--|
| The tet remark Yew, Help<br>SSPEC_ID:<br>No sample description was entered.<br>SSPEC_REM:<br>DETP# 1<br>DETDESC# TENDETRON_MCA MCB 25 Erase the<br>AP# Maestro Version 6.03<br>SDATE_MEA:<br>SDATE_MEA:<br>SDATE_MEA:<br>SMEAS_TIM:<br>DO 115 | File Edit Format View Help   |
| Erase this line   | 0  |
|   | SROI:<br>SRESETS:<br>NONE<br>0<br>SENER_FIT:<br>-0.040950 0.018932<br>SMCA_CAL:<br>3<br>-4.094970E-002 1.893220E-002 0.000000<br>SSNAP_CAL:<br>3<br>0.000000E+000 0.000000E+000 0.000000<br>+000 |
|   |  |

Figure d-1. The .SPE spectrum file.



# APPENDIX E

### **Fiber Optic Light Guide**

Table E. The information of the fiber optic light guide.

| Factor                          | Information  |
|---------------------------------|--|
| Length                          | 1.5 m  |
| Core diameter                   | 1,000 µm   |
| Jacket                          | Nylon (Temperature range $-40^{\circ}C - 100^{\circ}C$ |
| Sheathing / Cabling             | PVC  |
| Connector                       | SMA 905  |
| Fiber core                      | Pure fused silica                                      |
| Cladding                        | Doped fused silica                                     |
| Fiber profile                   | Step – index multi – mode                              |
| Operating wavelengths           | UV – VIS (200 – 750 nm)                                |
| Numerical aperture              | 0.22   |
| Recommended minimum bend radius | momentary 20 cm  |
| Recommended minimum dend radius | long term 40 cm  |

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# APPENDIX F

## **Ocean Optics S2000 Spectrometer**

Table F. The S2000 spectrometer information of Ocean Optics, Inc.

| Size                            | 141.6 mm x 104.9 mm x 40.9 mm                   |
|---------------------------------|---|
| Weight                          | 390 g   |
| Input                           | 110 mA 5 DCV (Master) ; 60 mA 5 DCV (Slave)     |
| Range of measurement            | 200 – 1,100 nm                                  |
| Light detector                  | CCD 2,048 pixels                                |
| Grating                         | 14 grating in range of UV – NIR                 |
| Income light channel            | 5, 10, 25, 50, 100 or 200 μm                    |
| Focal length                    | Input 42 mm ; Output 68 mm                      |
| Resolving power                 | 0.3 - 10.0 nm (FWHM) (depend upon the grating s |
|                                 | <0.05% at 600 nm                                |
| Loss                            | <0.10% at 435 nm                                |
|                                 | <0.10% at 250 nm                                |
| 61120                           | 86 photons/times                                |
| Sensitivity                     | 2.9 x 10 <sup>-17</sup> J/times                 |
| ri <del>cht<sup>©</sup> h</del> | 2.9 x 10 <sup>-17</sup> W/times                 |
| Connector                       | SMA 905 single – strand optical fiber (0.22 nA) |

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