

Creating input files for PENEPMA12 using CalcZAF.exe and Standard.exe

Extract the files in the PENEPMA.ZIP file to a folder on your hard disk. By default the folder should be called "Penepma12" and located in the "C:\Userdata" folder. If a different folder is to be utilized for the PENEPMA application files, the entries in the PROBEWIN.INI file must be edited to indicate the actual folders under the [software] section of the PROBEWIN.INI file in the Probe for Windows or CalcZAF application folders (usually found in "C:\Program Files\ProbeSoftware"):

PENDBASE_Path="C:\Userdata\Penepma12\Pendbase"

PENEPMA_Path="C:\Userdata\Penepma12\Penepma"

PENEPMA_Root="C:\Userdata\Penepma12"

The path for application files for creating Penepma (Penelope Monte-Carlo simulation software for EPMA) input files are specified here. The PENEPMA_Root is the folder where the base input files are stored to optimize production of characteristic x-rays, backscatter electrons, continuum or secondary x-rays.

Running CalcZAF and Standard to Create Secondary Fluorescence Profiles

First run the CalcZAF program and select the Standards | Standard Database menu to launch the Standard application. Accept the default database. From the Standard application menu click the Analytical | PENEPMA (Secondary Fluorescence Profile) Calculations menu.

Select two materials, one each for the two phases of the boundary and a third phase, usually a pure element, for calculating the k-ratio intensities. If the standard composition selected is NOT a pure element then the k-ratio intensities will be "raw" k-ratios as opposed to elemental k-ratios.

Note that material A is always on the left side of the geometry file, material B is on the right side of the geometry file and the electron beam is always incident on material A. Note that this is the opposite orientation of the normal couple.geo file used by penepma for monte-carlo calculations.

The element being fluoresced may only be in material B or it may be in both material A and material B.

If the same (compound) material is specified for both material A and material B then the fluorescence calculation merely calculated the normal sample fluorescence (from both both characteristic and continuum fluorescence).

After calculating the three material files (or selecting them using the Browse buttons), click the Penfluor and Fitall buttons to calculate the .par files for use by Fanal.exe. The default time for each .par file is 8 hours (3600 seconds for each electron energy for 8 electron energies). The default lowest electron energy is 1 keV and the highest electron energy is 50 keV.

Running CalcZAF and Standard to create PENEPMA input files

First run the CalcZAF program and select the Standards | Standard Database menu to launch the Standard application. Accept the default database. From the Standard application menu click the Analytical | PENEPMA (Monte-Carlo) Calculations menu.

To create material inputs files select up to 10 standard compositions from the standard list, enter a name for the material file and click the Create PENEPMA Material File button. The program will automatically create a material file for each composition and concatenate them into a single material file for input to the PENEPMA Material.exe program. The final material file is automatically copied from the Pendbase folder to the Penepma folder for Monte-Carlo calculations using Penepma.exe. Please be patient, the creation of the material file can take a minute or more if it contains multiple complex compositions.

To create an input file, select the production to optimize (characteristic x-rays, backscatter electrons, continuum x-ray or secondary fluorescent x-rays), a title for the input file, beam energy, beam position, etc and a material and geometry file. Note that geometry files are complicated and two example files are

supplied, bulk.geo and couple.geo. Bulk.geo describes a geometry with a simple flat disk. It can be used with any single composition material files. Generally one enters a beam position of 0, 0, 1 which has the beam position over the center of the disk with a 10 mm (1 cm) working distance.

The geometry file couple.geo is also a flat disk but consisting of two sides (half pie shapes) with different compositions. It can be used with material files that have two compositions. Generally one enters a beam position offset slightly in the x axis so that secondary fluorescent modeling can occur. Values of 1e-3, 0 and 1 would position the beam 10 um from the center of the material interface, centered in y and 10 mm above the sample.

Once the material and the input files are created, click the PENEPMA Prompt button and enter the command: "Penepma < (input file), where (input file) is the name of the input file you just created. Depending on the number of showers simulations the calculation can take up to 24 hour or longer.

Note that 4 sample production files are supplied. They are:

Cu_Cha.in	Sample characteristic x-ray production input file
Cu_Back.in	Sample backscatter electron production input file (use data column- "fractional transmitted" for backscatter intensities!)
Cu_Cont.in	Sample continuum x-ray production input file
CuFe_Sec.in	Sample fluorescent x-ray production input file

If the sample production files are edited they must be edited carefully or the program will not function properly. If that occurs it may be necessary to re-extract the sample production files to the root PENEPMA folder.

Consult the PENEPMA.PDF help file for more information.

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