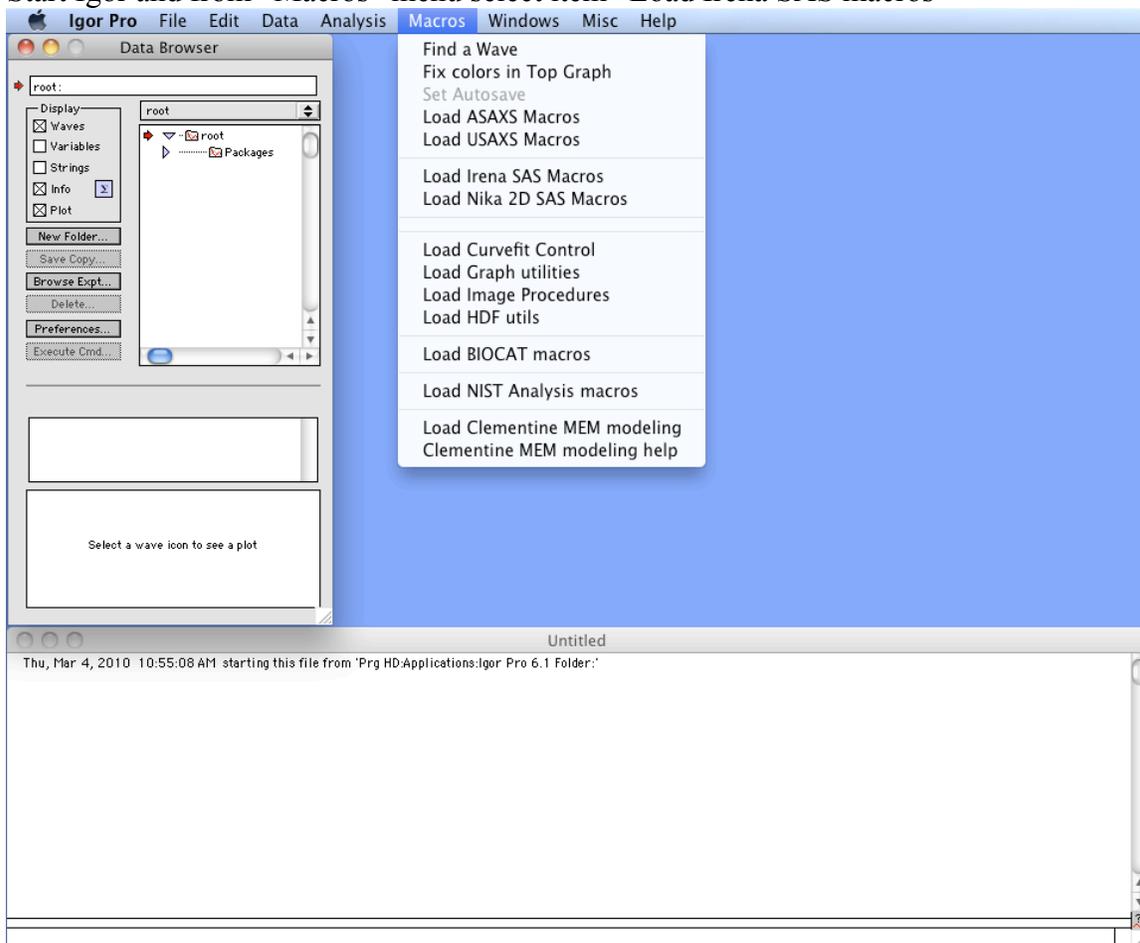


Calculation on X-ray & neutron contrast using Irena package

This handout describes how to calculate contrast for Al_2O_3 material and voids (= vacuum) in the free electron approximation. It also shows how to use Anomalous Scattering contrast calculator to calculate X-ray contrast and sample absorption at specific energy or in the range of energies.

Start Igor, load Irena macros

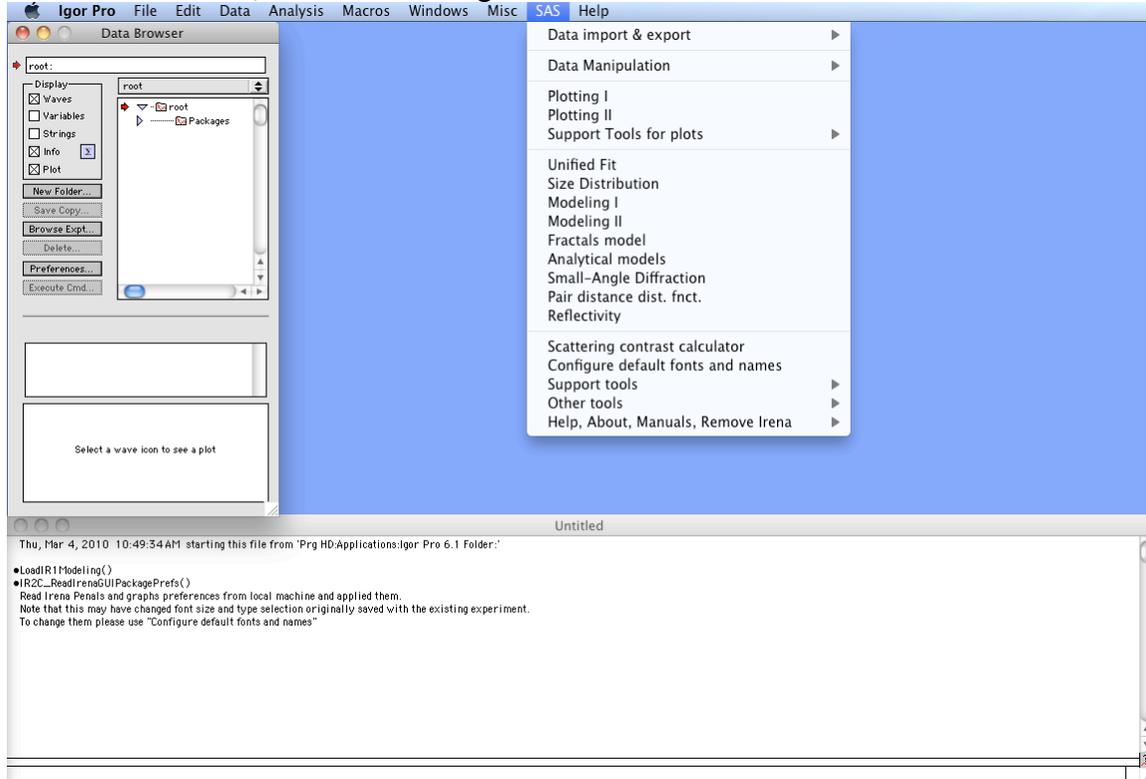
Start Igor and from “Macros” menu select item “Load Irena SAS macros”



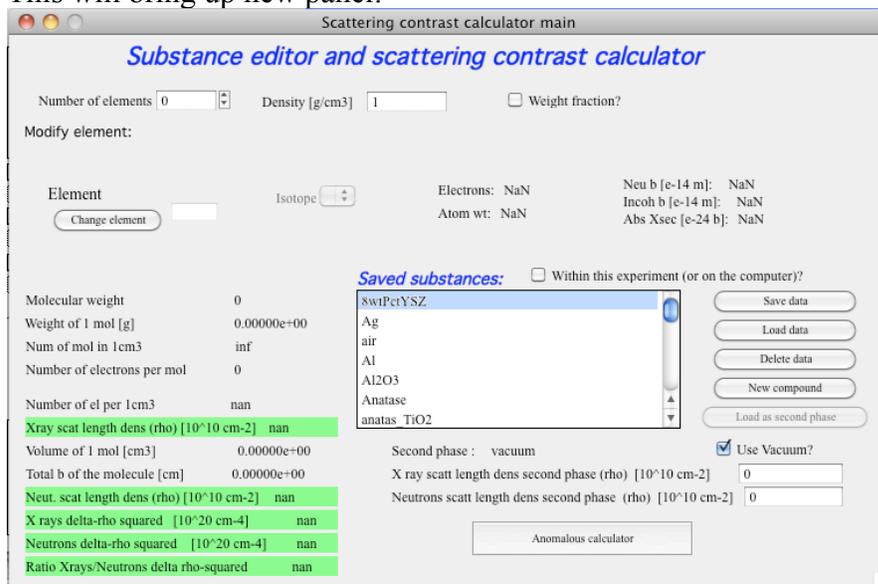
This will add new menu “SAS” in Igor.

Start the tool

In the “SAS” menu, select “Scattering contrast calculator”

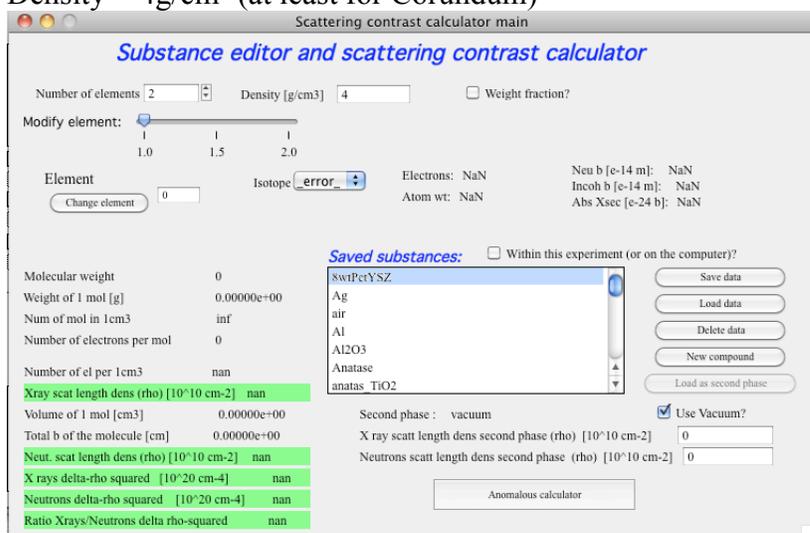


This will bring up new panel:

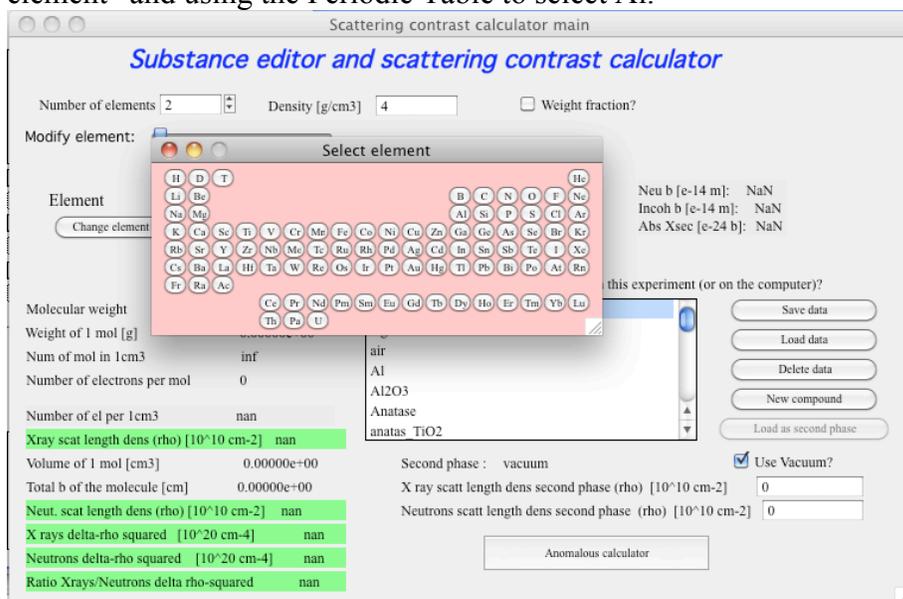


Now we need to setup the material. Follow from top:
 Number of elements = 2 (Al and O)

Density = 4g/cm^3 (at least for Corundum)



Now with slider “Modify element” pointing to 1 (first element), click on button “Change element” and using the Periodic Table to select Al.



Set next to Al value of 2 (as in Al_2O_3)

Next slide the slider “Modify element” to 2 (second element) and input O_3 .

Now check, that in the right bottom corner the checkbox “Use vacuum” is selected. This is where the second material selection is made. Vacuum is used instead of air most of the time. If we would have another material as second material, we would have to create it first, save it and then load it as second element here...

Scattering contrast calculator main

Substance editor and scattering contrast calculator

Number of elements: 2 Density [g/cm3]: 4 Weight fraction?

Modify element: 1.0 — 1.5 — 2.0

Element: O Isotope: natural Electrons: 8 Neu b [e-14 m]: 0.5803
 Atom wt: 15.9994 Incoh b [e-14 m]: 0.015
 Abs Xsec [e-24 b]: 0.000

Change element: 3

Al₂O₃

Molecular weight	101.961
Weight of 1 mol [g]	1.69311e-22
Num of mol in 1cm3	2.36252e+22
Number of electrons per mol	50
Number of el per 1cm3	1.18126e+24
Xray scat length dens (rho) [10 ¹⁰ cm ⁻²]	33.29
Volume of 1 mol [cm3]	4.23277e-23
Total b of the molecule [cm]	2.43010e-12
Neut. scat length dens (rho) [10 ¹⁰ cm ⁻²]	5.741
X rays delta-rho squared [10 ²⁰ cm ⁻⁴]	1108
Neutrons delta-rho squared [10 ²⁰ cm ⁻⁴]	32.96
Ratio Xrays/Neutrons delta rho-squared	33.62

Saved substances: Within this experiment (or on the computer)?

- 8wtPetYSZ
- Ag
- air
- Al
- Al2O3
- Anatase
- anatas TiO2

Buttons: Save data, Load data, Delete data, New compound, Load as second phase

Second phase: vacuum Use Vacuum?

X ray scatt length dens second phase (rho) [10¹⁰ cm⁻²]: 0

Neutrons scatt length dens second phase (rho) [10¹⁰ cm⁻²]: 0

Anomalous calculator

Note column of data on the left side of the tool. It lists many parameters, including X-ray scattering length density, neutron scattering length density and contrasts.

More details can be found in the manual – for example, one can select Isotope for any element which influences the neutron contrasts.

Save data

For future use, one can save the compounds as ASCII files on the computer or within the current Igor experiment. Think before you decide where to save the compounds – if they are saved on the current computer they will be available to you when any time you use this computer. But not necessarily to your colleague you send the experiment to. If they are in the Igor experiment, they are not going to be available next time you use this computer. Alternative is to save in both ☺

These operations are done through “Save data” button and other buttons right of compound listing. Here they can be also Loaded, deleted etc. Button “New compound” resets the tool to clean state...

Anomalous (energy dependence of contrast) effects

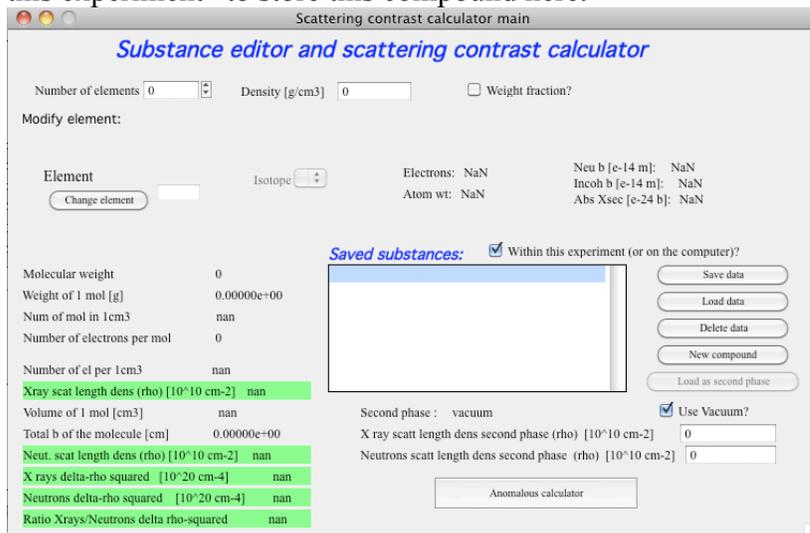
Extension of this tool uses Cromer Liberman code to calculate anomalous (energy dependent) effects. It calculates f-prime, f-double prime, absorption etc. for stored compounds. Much more details are available in included pdf manual.

Note, that this tool is VERY useful to calculate absorption of material at given energy.

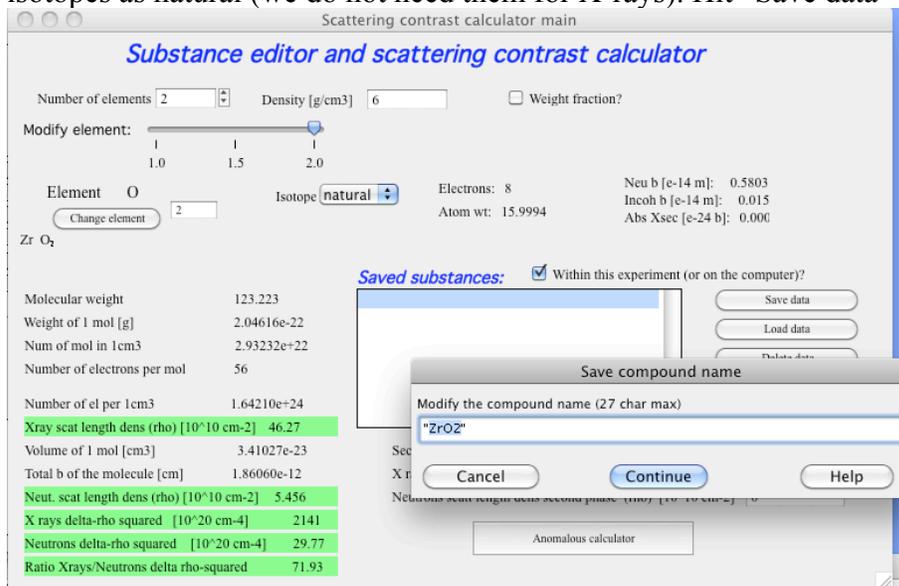
The process of using this tool is as follows:

1. Create compound(s) you want to analyze in the Main panel, as listed above. For this practice, create Zirconium Oxide ceramics as follows:

Hit button “New Compound”. This clears main panel. Switch the checkbox to “Within this experiment” to store this compound here.



Now select Number of elements as 2, density as 6g/cm³ formula ZrO₂ and leave the isotopes as natural (we do not need them for X-rays). Hit “Save data” button:



Save the compound and it should now be listed in the “Saved substances” listbox:

Scattering contrast calculator main

Substance editor and scattering contrast calculator

Number of elements: 2 Density [g/cm³]: 6 Weight fraction?

Modify element:

Element: O Isotope: natural Electrons: 8 Neutrons: 8
 Atom wt: 15.9994 Incoh b [e-14 m]: 0.5803
 Abs Xsec [e-24 b]: 0.000

Zr O₂

Molecular weight: 123.223
 Weight of 1 mol [g]: 2.04616e-22
 Num of mol in 1 cm³: 2.93232e+22
 Number of electrons per mol: 56
 Number of el per 1 cm³: 1.64210e+24

Xray scat length dens (rho) [10¹⁰ cm-2]: 46.27
 Volume of 1 mol [cm³]: 3.41027e-23
 Total b of the molecule [cm]: 1.86060e-12
 Neut. scat length dens (rho) [10¹⁰ cm-2]: 5.456
 X rays delta-rho squared [10²⁰ cm-4]: 2141
 Neutrons delta-rho squared [10²⁰ cm-4]: 29.77
 Ratio Xrays/Neutrons delta rho-squared: 71.93

Saved substances: Within this experiment (or on the computer)?

ZrO2

Save data
 Load data
 Delete data
 New compound
 Load as second phase

Second phase: vacuum Use Vacuum?
 X ray scatt length dens second phase (rho) [10¹⁰ cm-2]: 0
 Neutrons scatt length dens second phase (rho) [10¹⁰ cm-2]: 0

Anomalous calculator

Now, hit "Anomalous calculator" and new window appear:

Anomalous scattering contrast calculator

Anomalous Scattering Contrast Calculator

Select ONE or TWO stored compounds

Compounds within experiment ?

ZrO2

Calculate at single energy Calculate in energy range

Energy [keV]: 10 Q [A-1]: 0

Recalculate

Thickness [mm]: 0.1

f0 [e-]	0	f0 [e-]	0
f' [e-]	0	f' [e-]	0
f0+f' [e-]	0	f0+f' [e-]	0
f'' [e-]	0	f'' [e-]	0
Mu/Rho [cm ² /g]	0	Mu/Rho [cm ² /g]	0
Mu [1/cm]	0	Mu [1/cm]	0
1/Mu [cm]	0	1/Mu [cm]	0
exp(-Mu*T)	0	exp(-Mu*T)	0
f [10 ¹⁰ cm ⁻²]	0	f [10 ¹⁰ cm ⁻²]	0
f'' [10 ¹⁰ cm ⁻²]	0	f'' [10 ¹⁰ cm ⁻²]	0
Delta Rho Squared [10 ²⁰ cm ⁻⁴]		0	

Second phase is Vacuum

Now we have two types of questions, we may have.

Assume we have fixed energy (like tube-based instrument) with known wavelength (energy) of X-rays. Maybe Mo radiation (0.7093 Å, ~17.482 keV). And have a sample of ZrO₂ with voids and need to know the contrasts and absorption. Maybe the sample has thickness of 100 micron.

Keep the checkbox “Calculate at single energy” selected and change energy in the “Energy” to 17.482. Keep Q as 0 (for small-angle scattering, this can change if real diffraction at high Q values is done). Keep thickness to 0.1mm. Make sure the ZrO₂ is highlighted in the listbox (you can highlight up to two compounds) and the checkbox below the listbox “Second phase is vacuum” is checked. Hit button “recalculate”:

Anomalous Scattering Contrast Calculator

Select ONE or TWO stored compounds

Compounds within experiment ?

Calculate at single energy Calculate in energy range

Energy [keV]: 17.482 Q [A-1] 0

Thickness [mm] 0.1

ZrO₂ vacuum

f ₀ [e-]	18.66	f ₀ [e-]	0
f' [e-]	-1.028	f' [e-]	0
f ₀ +f' [e-]	17.64	f ₀ +f' [e-]	0
f'' [e-]	0.1899	f'' [e-]	0
Mu/Rho [cm ² /g]	11.13	Mu/Rho [cm ² /g]	0
Mu [1/cm]	66.79	Mu [1/cm]	0
1/Mu [cm]	0.01497	1/Mu [cm]	0
exp(-Mu*T)	0.5128	exp(-Mu*T)	0
f [10 ¹⁰ cm ⁻²]	43.47	f [10 ¹⁰ cm ⁻²]	0
f'' [10 ¹⁰ cm ⁻²]	0.4681	f'' [10 ¹⁰ cm ⁻²]	0
Delta Rho Squared [10²⁰ cm⁻⁴]		1890.1	

Second phase is Vacuum

And the results are in the “blue” column.

The ones of real interest usually are the “Delta Rho squared” (energy corrected contrast of voids in ZrO₂ ceramics) and the exp(-Mu*T), which can be translated for normal beings as “Transmission” at this energy and thickness... Here you see, that the sample would be about 51% transparent – reasonable experiment.

Other numbers are here mostly for information and since sometimes one actually wants to know them.

The other type of question is as: I have sample of ZrO₂ and need to decide at which energy to do my experiment. Likely you have synchrotron here ☺... Anyway, we can get also information as needed:

Select “Calculate in energy range” and panel changes:

Anomalous scattering contrast calculator

Anomalous Scattering Contrast Calculator

Select ONE or TWO stored compounds

Compounds within experiment ?

Calculate at single energy Calculate in energy range

Energy start [keV]: 10 Q [A-1] 0

Energy end [keV]: 12

Number of steps in energy: 20

Thickness [mm] 0.1

Recalculate

ZrO2 vacuum

Zr O₂

vacuum

Display f' Save f' Save f'

Display f'' Save f'' Save f''

Display f0+f' Save f0+f' Save f0+f'

Display Delta Rho squared Save Delta Rho squared

Display Mu / Rho Save Mu / Rho Save Mu / Rho

Display 1/Mu Save 1/Mu Save 1/Mu

Display exp(-Mu*T) Save exp(-Mu*T) Save exp(-Mu*T)

Second phase is Vacuum

Let's assume we have again 100 micron thick sample of ZrO₂ and need to decide where to go and what can we expect. And that we can change energy between 10 and 25 keV. We need to pick energy at which the sample has reasonable transmission. Fill Energy start as 10, Energy end as 25, set number of steps to may be 100 and thickness to 0.1. Make sure ZrO₂ is selected in the listbox and hit recalculate:

Anomalous scattering contrast calculator

Anomalous Scattering Contrast Calculator

Select ONE or TWO stored compounds

Compounds within experiment ?

Calculate at single energy Calculate in energy range

Energy start [keV]: 10 Q [A-1] 0

Energy end [keV]: 25

Number of steps in energy: 100

Thickness [mm] 0.1

Recalculate

ZrO2 vacuum

Zr O₂

vacuum

Display f' Save f' Save f'

Display f'' Save f'' Save f''

Display f0+f' Save f0+f' Save f0+f'

Display Delta Rho squared Save Delta Rho squared

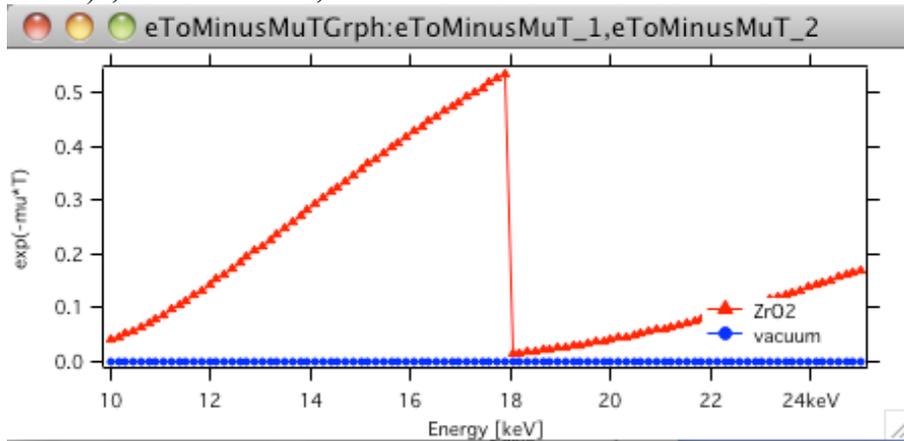
Display Mu / Rho Save Mu / Rho Save Mu / Rho

Display 1/Mu Save 1/Mu Save 1/Mu

Display exp(-Mu*T) Save exp(-Mu*T) Save exp(-Mu*T)

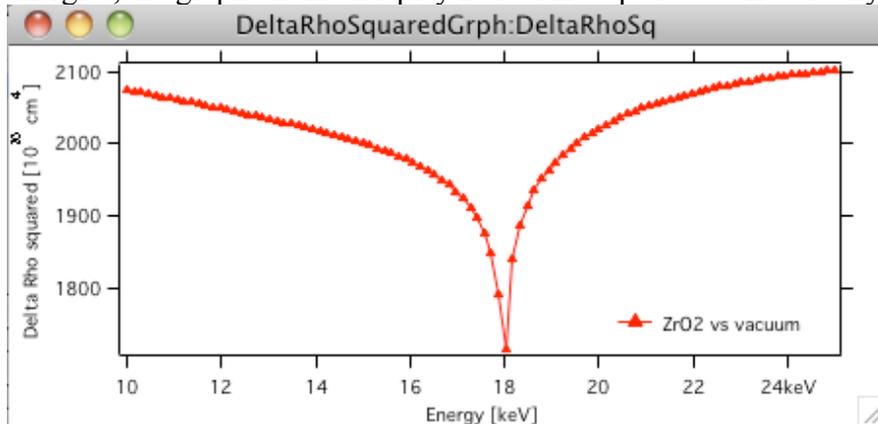
Second phase is Vacuum

There is not change in the panel, but now we can push the buttons and get results (left, grey, column of buttons) in form of graphs. Here is graph obtained from “Display exp(-Mu*T)”, as I said above, that translates to “transmission” for normal beings...



You can see, that the transmission of our 100 microns of Zirconia increases to over 50% just below the edge (around 18keV) then drops as stone and increases again to over 15% at 25keV. You would pick energy below the edge to do your experiment...

If you wanted to do anomalous experiment where you want to collect data at different energies, the graphs from “Display Delta Rho squared” can be really useful:



Note, that the contrast of Zirconia and voids in this energy range changes over all between about 2100 and nearly 1700 [10^{20} cm^{-4}]. Now you can pick energies to use as needed...

Conclusions:

This handout has shown how the Contrast calculator in Irena package can be used to calculate free electron approximation and neutron scattering contrasts using the “Main” panel. It has also shown how the included “Anomalous” calculator can be used to calculate X-ray contrast and sample absorption at one X-ray energy or in the range of X-ray energies. For more details, please, read the included manual.