Monte Carlo

1- Demonstration of Casino

Open the Casino program

Chose `File->New` (`Edit Layer` window)

Click `Add Layer`

Double click on `Undefined` (right side of the red circle)

In the composition edit box add `C` (capitalize)

Click `Done` button (`Layer Chemical Composition` window)

Click `Next` button (`Edit Layers` window)

Put `5` in the energy field

Put `2000` in the number of electrons to simulate

Click `Next` button (`Micoscope and Simulation Proprieties` window)

Click `Next` button (`Distributions` window)

Click `Next` button (`Options` window)

Click `Finish` button (`Select Physics Model` window)

Click `Yes` button (`New Simulation Request` window)

Wait for the end of the simulation

Click on automatic rescale (`View->Auto-Adjust Scale` menu)

BSE Coefficient

η = _____

You can note the max depth of the electron and radius

D_{max} = _____

R_{max} = _____

Show `Energy by Position` distribution (tree view at the left of the screen)

D_{max} = _____

R_{max} = _____

Show the phirhoz curves and note the depth and $\phi(0)$.

D_{max} = _____

$\phi(0)$ = _____

Now change the specimen for Ag and the energy to 4 keV

Menu `Simulation->Modify Sample`

Double click on `C` (right side of the red circle)

In the composition field add `Ag`

In the name field add `Ag`

Click `Done` button

Menu `Simulation->Set Up Microscope`

Change `5` keV to `4` keV

Click `Ok` button

Menu `Simulation->Run` or the green "play" button

BSE Coefficient

η = _____

You can note the max depth of the electron and radius

D_{max} = _____

R_{max} = _____

Show `Energy by Position` distribution (tree view at the left of the screen)

D_{max} = _____

R_{max} = _____

Show the phirhoz curves and note the depth and $\phi(0)$.

D_{max} = _____

$\phi(0)$ = _____

2- Incident Energy Variation

Simulate for `Ag` specimen with energies between 5 to 30 keV with a 5 keV step

Menu `Simulation->Set Up Microscope`

Click `Simulate Multiple Energies`

Change `4` keV to `5` keV in `Start`, `30` keV in `End` and `Step` to `5` keV

Click `Ok` button

Menu `Simulation->Run` or the green "play" button

Energy (keV)	η	D_{max} e^-	R_{max} e^-	D_{max} *x-ray*	ϕ***(0)***
		nm	nm	nm	
5					
10					
15					
20					
25					
30					

Simulate for C specimen with energies between 5 to 30 keV with a 5 keV step

Menu Simulation->Modify Sample

Double click on Ag (right side of the red circle)

In the composition field add C

In the name field add C

Click Done button

Menu Simulation->Run or the green "play" button

Energy (keV)	η	D_{max} e^-	R_{max} e^-	D_{max} ***x-ray***	$\phi(0)$
		nm	nm	nm	
5					
10					
15					
20					
25					
30					

3- Atomic Number Variation

Simulate for C, Al, Cu, Ag, and Au specimen with energy of 10 keV at 0°

Element	η	D_{max} e^-	R_{max} e^-	D_{max} ***x-ray***	$\phi(0)$
C					
Al					
Cu					
Ag					
Au					

4- Incident Electron Angle

Simulate for Al specimen with energies between 5 keV at 0°, 20°, and 60°

Menu Simulation->Modify Sample

Double click on Au (right side of the red circle)

In the composition field add Al

In the name field add `Al`

Click `Done` button

Menu `Simulation->Set Up Microscope`

Change the `Tilt` of the specimen to `20°`

Click `Ok` button

Menu `Simulation->Run` or the green “play” button

Tilt (°)	η	D_{max} ***e***$^-$	R_{max} ***e***$^-$	D_{max} ***x-ray***	ϕ***(0)***
0					
20					
60					

Look also at the `Energy by Position` distribution

Microanalysis

1- Demonstration of Win X-Ray

Open the Win X-Ray program

Chose `File->New`

Change `Incident Energy Start` to `10` keV

Set the `number of electrons` to `500`

Check `X-Ray Compute` and `Compute Characteristic`, and `Compute Background`

Click `Next` button (`Option Simulation` window)

Click on `Set Element for All Regions` button (`Option Specimen` window)

Change the atomic number `Z` to `29`, or `Symbol` to `Cu`

Click `Ok` button (`Option element for the region 1` window)

Click `Next` button (`Option Specimen` window)

Click `Next` button (`Option X-Ray` window)

Click `Next` button (`Advanced Option` window)

Click `Next` button (`Physics Model` window)

Click `Next` button (`Result General Option` window)

Click `Next` button (`Result Trajectory Option` window)

Click `Finish` button (`Result Distribution Option` window)

Wait for the end of the simulation

Click on + to expand the tree view

Click on the `trajectory +`

Click on the `interaction volume` and adjust the new windows as you wish

Move the mouse over the picture to find the max depth and radial

Change the `X-Z Plane` to `X-Y Plane`

Click on the `X-Ray +`

Click on the `Intensity` to shows the intensity generated (`I Gen`) and emitted (`I Emi`) (with specimen absorption) for each line in number of photons.

Click on `Spectrum` to show the complete spectrum with the effect of the detector

Click on the `Y Axis Log`

Check and uncheck `Background`, `Characteristic`, and `Total`

Move the mouse to read energy and intensity at the cursor.

Without Y log scale, zoom on the K-Lines (8 keV) by left click + move down and right with the mouse to select the zoom region.

To reset the view left-click + move up and left with the mouse.

Now click on PRZ Curves

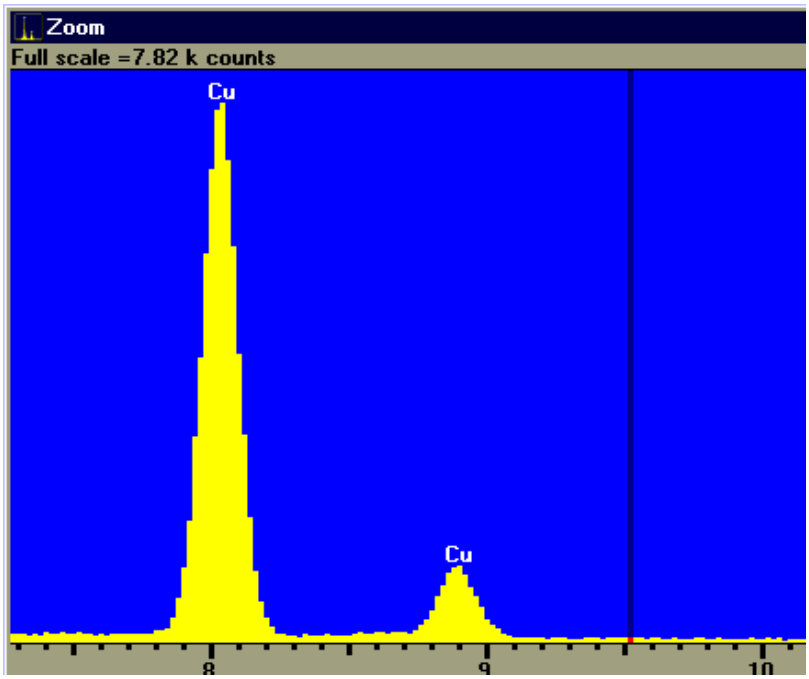
Click on Ka1 of the Cu, you have to click on + Cu first.

Click on La of the Cu, you should see the effect of the specimen absorption

Click on lines, Cu

Click on Ka1 and Ka2

Click on La and Lb1



2- L lines from Ag

Select in the menu Option->Option Specimen

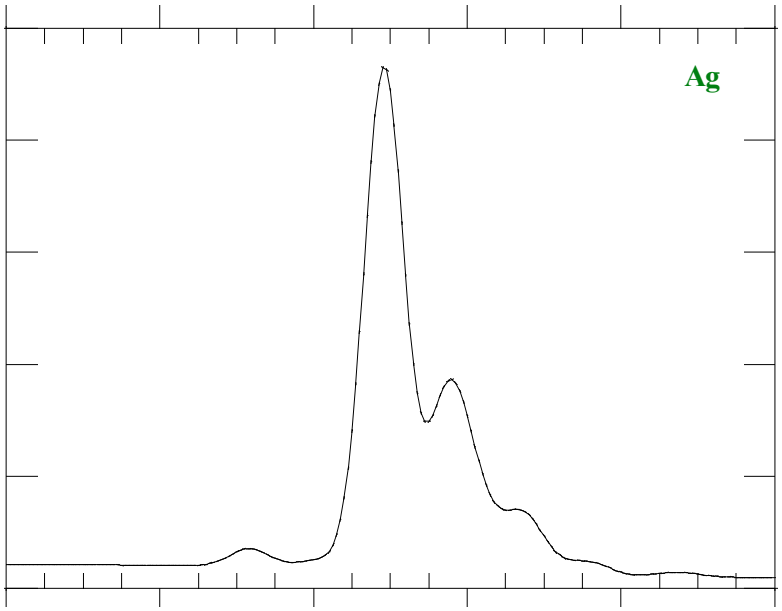
Click on Set Element for All Regions button

Change the atomic number Z to 47, or Symbol to Ag

Click Ok button

Click on Simulation->Run or the green “play” button

Look at the Spectrum for the L-lines



3- M lines from W

Select in the menu `Option->Option Specimen`

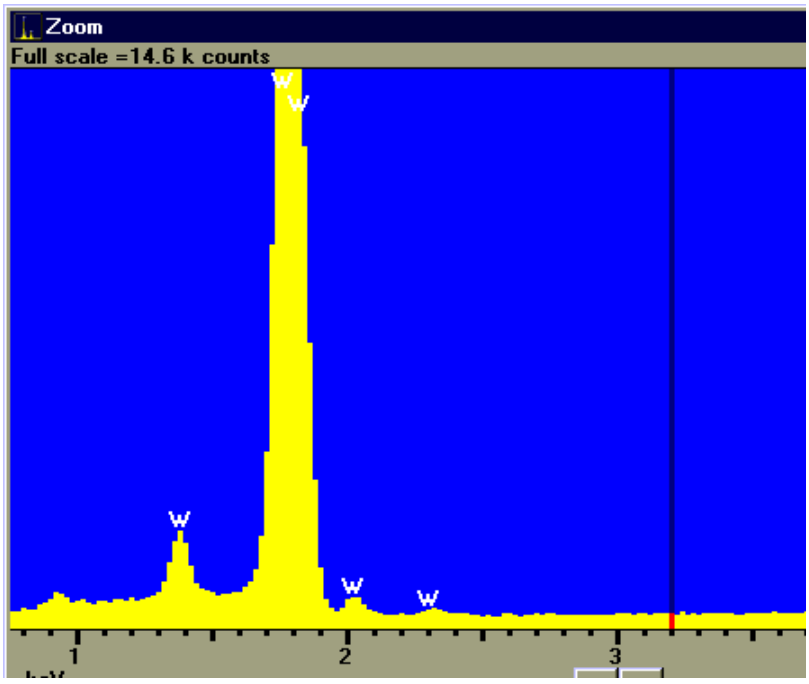
Click on `Set Element for All Regions` button

Change the atomic number `Z` to `74`, or `Symbol` to `W`

Click `Ok` button

Click on `Simulation->Run` or the green “play” button

Look at the `Spectrum` for the W-lines



4- k-ratio Calculation

Open `WinX-Ray`

Menu `Option->Option Simulation`

Set the energy to `15` keV

Check `Compute X-Ray`

Set the `number of electrons` to `500`

Simulate for pure `Au`, note the intensity of L_α line

Simulate for pure `Cu`, note the intensity of $K_{\alpha 1}$ line

Menu `Option->Option Specimen`

Click `Set Element for All Regions`

Set the number of elements at `2` (click on up arrow)

Set element 1 to `Au`

Set element 2 to `Cu`

Set `Weight Fraction` to `0.8` and `0.2` respectively

Click `Ok` button

Click on `Simulation->`Run or the green "play" button

Note the intensity for Au La and Cu Ka1

Change the `Weight Fraction` to `0.6` and `0.4` and re simulate

Concentration of Au (%)	***I L_α Au***	***k ratio Au***	***I $K_{\alpha 1}$ Cu***	***k ratio Cu***
100				
80				
60				
40				
20				
0				

If k ratio is equal to 0.62 gold and 0.35 for Cu,

what it is the concentration of this alloy? _____

5- Thin Film on Substrate

Open Casino

Open `Simulation->Set Up Microscope`

Put `20` keV of `Energy` and `2000` for the `Number of electrons to simulate`

Open Simulation->Modify Sample

Select Multi-Layer

Click Add Layer button

Click to change it to Cu

Click Add Layer button

Click to change it to Si

Change the thickness of Cu to 10 nm

Click Done

Click on Simulation->Run or the green "play" button

Pure Cu Intensity = _____

Pure Si Intensity = _____

Thickness of Cu (nm)	*I K Cu*	*k ratio Cu*	*I K Si*	*k ratio Si*
10				
50				
100				
500				
1000				
1500				

6- Particles in Matrix

Open Casino

Open Simulation->Set Up Microscope

Click Simulate Multiple Energies

Put to 1 keV in Start, 10 keV in End and Step to 1 keV

Put 2000 for the Number of electrons to simulate

Open Simulation->Modify Sample

Select Multi-Layer

Click Add Layer button

Click to change it to Ti

Click Add Layer button

Click to change it to Si

Click Add Layer button

Click to change it to Ti

Change the `thickness` of `Ti` to `100` nm (in the first layer)

Change the `thickness` of `Si` to `100` nm

Click `Done`

Click on Simulation->Run or the green “play” button

Simulate pure Ti

Simulate pure Si

Incident Energy (keV)	***I L Ti***	***Pure Ti***	***k ratio Ti***
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

Incident Energy (keV)	***I K Si***	***Pure Si***	***k ratio Si***
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

How to Solve Problems with Simulations

1- Vertical Interface C Au

Open Casino

Open Simulation->Modify Sample

Select Grain Boundary

Click Add Layer button

Click to change it to C

Click Add Layer button

Click to change it to Au

Click Done button

Open Simulation->Set Up Microscope

Put 20 keV for Energy and 2000 for the Number of electrons to simulate

Click on Simulation->Run or the green "play" button

2- Scanning a Vertical Interface

Open Simulation->Set Up Microscope

Check Scan the beam to create an image

From: -400 nm, To: 400 nm, step: 200 nm

Click on Simulation->Run or the green "play" button

Position	η
-400	
-300	
-200	
-100	
0	
100	
200	
300	
400	

Contrast = _____

3- Scanning a Vertical Interface part 2

Open Casino

Open Simulation->Modify Sample

Select Grain Boundary

Click `Add Layer` button

Click to change it to `GaAs`

Click `Add Layer` button

Click to change it to `AlAs`

Click `Add Layer` button

Click to change it to `GaAs`

Change the thickness of `AlAs` to `5` nm

Click `Done`

Open `Simulation->Set Up Microscope`

Put `15` keV for `Energy` and `2000` for the `Number of electrons to simulate`

Put a beam diameter of `2` nm

Check `Scan the beam to create an image`

`From: -10` nm, `To: 10` nm, `step: 2` nm

Click on `Simulation->`Run or the green "play" button

Position	η
-10	
-8	
-6	
-4	
-2	
0	
2	
4	
6	
8	
10	

Contrast = _____

Change the energy to 1 keV with a beam diameter of 5 nm and re simulate

Position	η
-10	
-8	
-6	
-4	
-2	
0	
2	
4	
6	
8	
10	

Contrast = _____