How to use DYNA, a matricial formalism to analyze x-ray magnetic reflectivity curves

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M. Elzo *et al.* JMMM **324**, 105-112 (2012), http://neel.cnrs.fr/spip.php?article2575

20-09-2018

Outline

I. **Principle of XRMR**

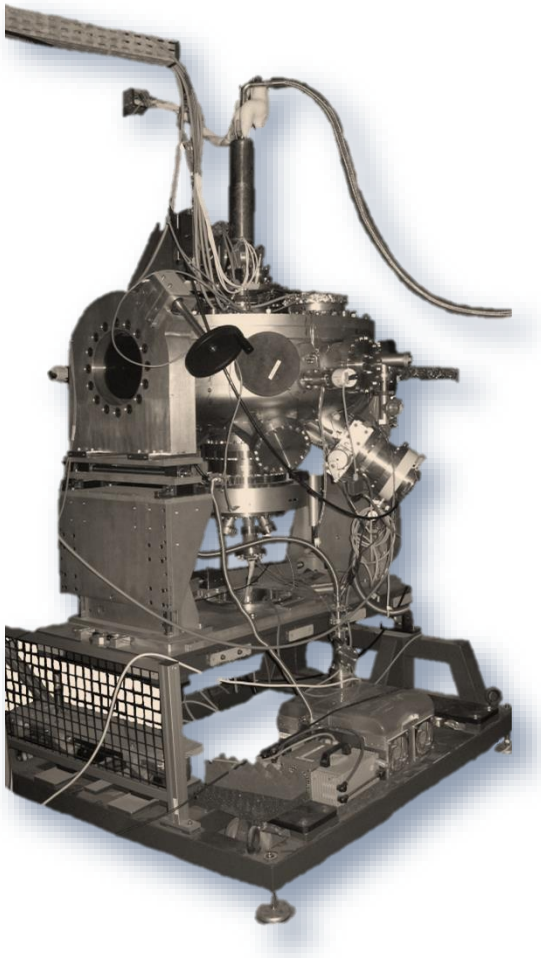
II. **Formalism**

1. **Generality**
2. **Kinematic**
3. **Dynamic, what is Dyna doing**

III. **How to use DYNA a matricial dynamic formalism**

1. **Entry: Optical constant / Parameter**
2. **Starting: Build a layer / Set the configuration**
3. **Fitting : Add experimental data / play with the parameter**

IV. **Conclusions and Outlook**

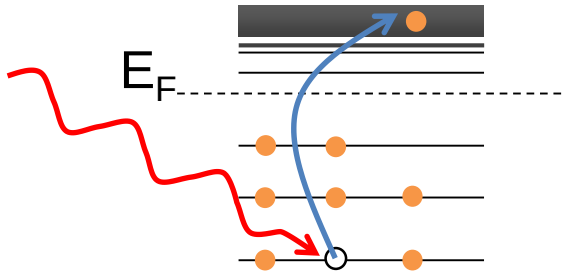


I. Principle of XRMR (1/3)

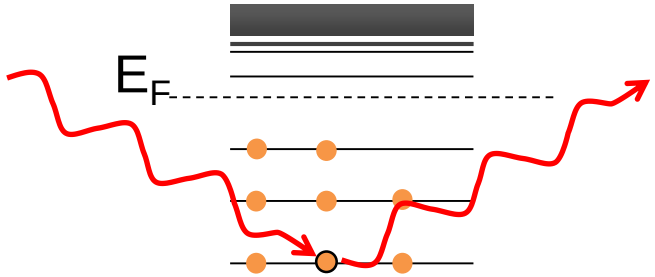
When use X-ray:

- Magnetic sensitivity
- Spatial resolution
- Element selectivity

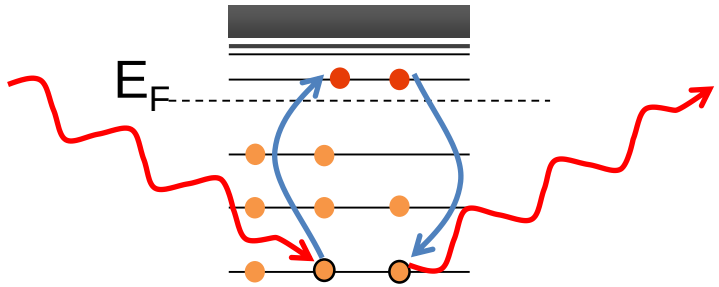
Absorption spectroscopy



Scattering

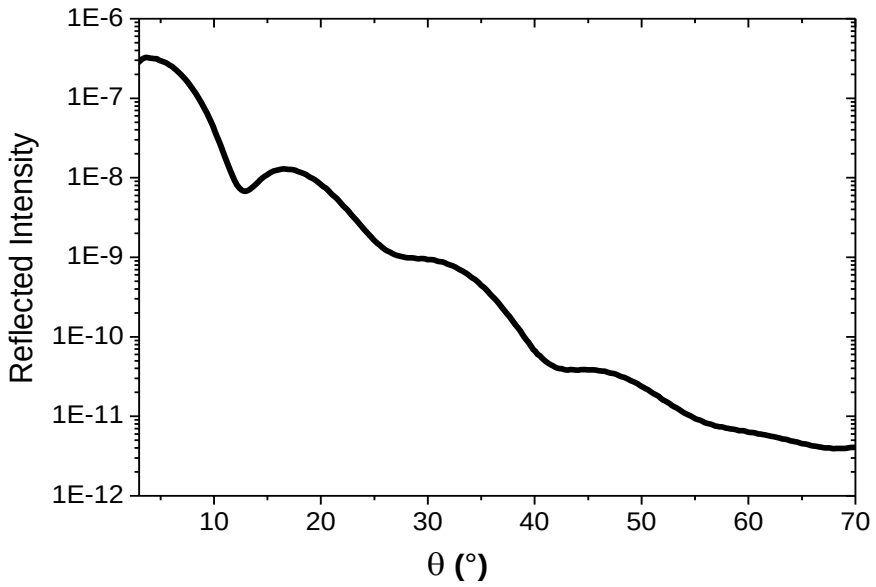


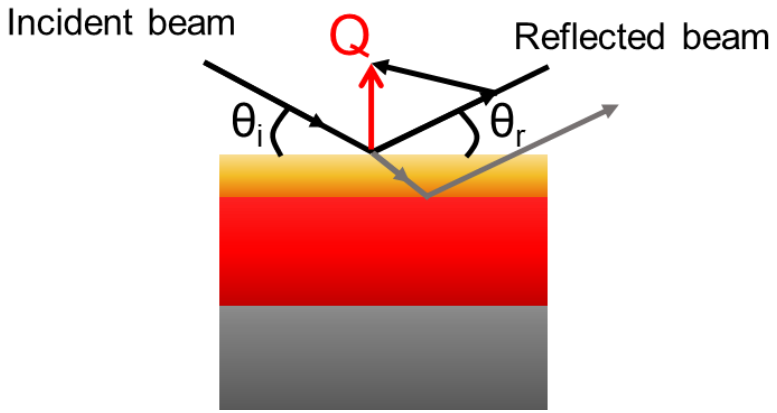
Resonant Scattering



I. Principle of XRMR (2/3)

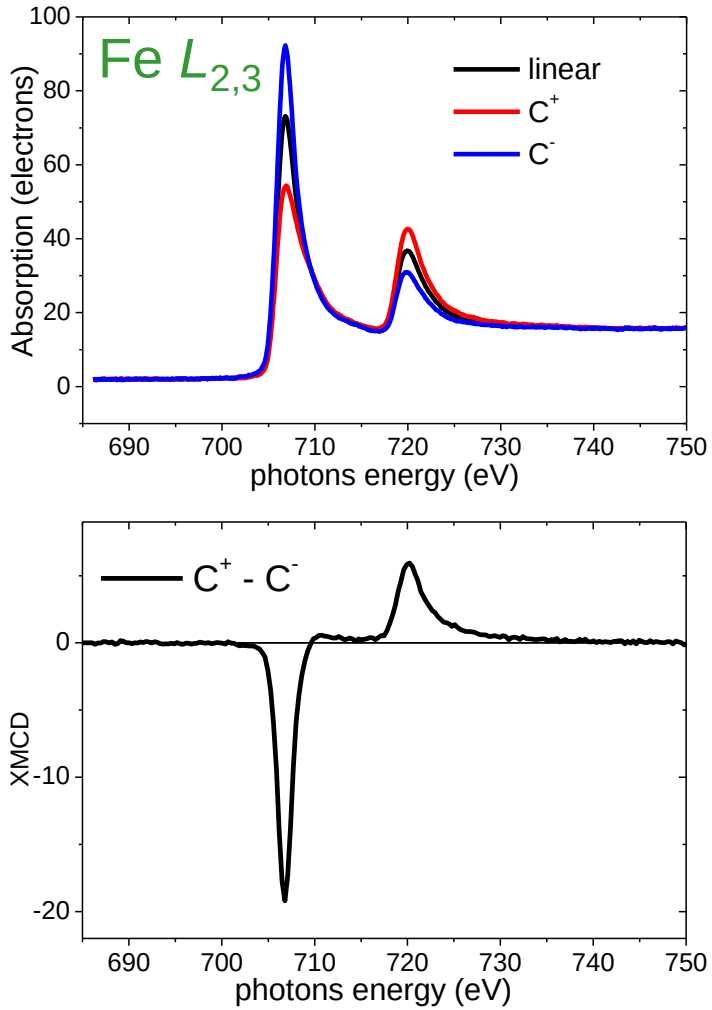
- Interaction x-ray – Matter:
  - Specular Reflectivity
  - Spectroscopy : XMCD*





$$n = 1 - \delta + i\beta$$

$$\beta \propto \text{Absorption}$$

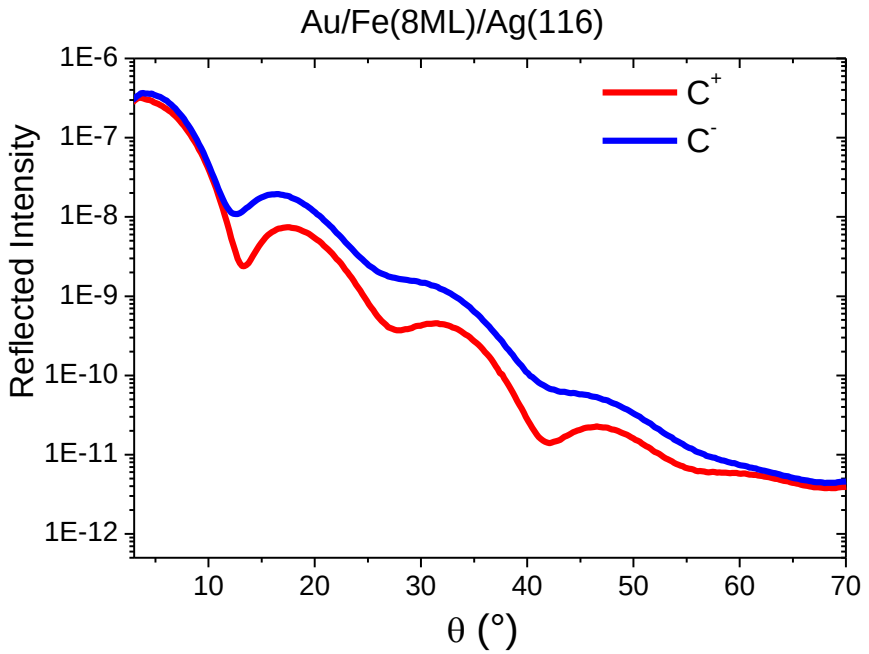


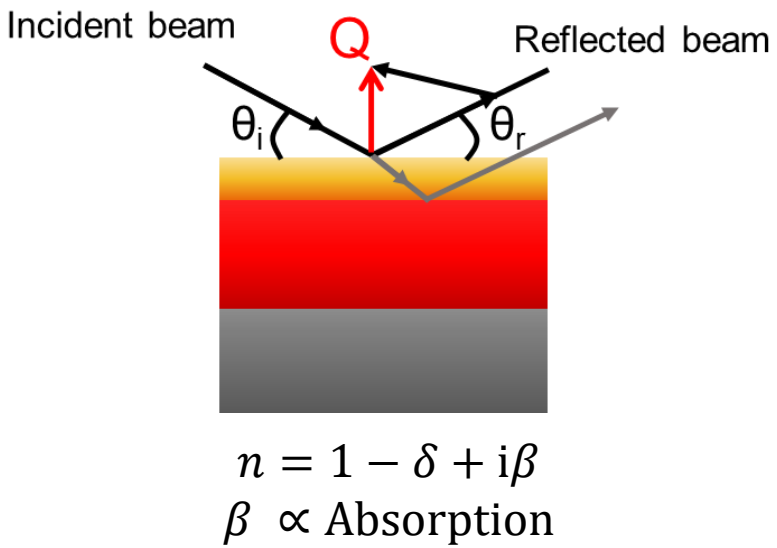
* X-ray Magnetic Circular Dichroism

I. Principle of XRMR (2/3)

- Interaction x-ray – Matter:
  - Specular Reflectivity
  - Spectroscopy : XMCD*

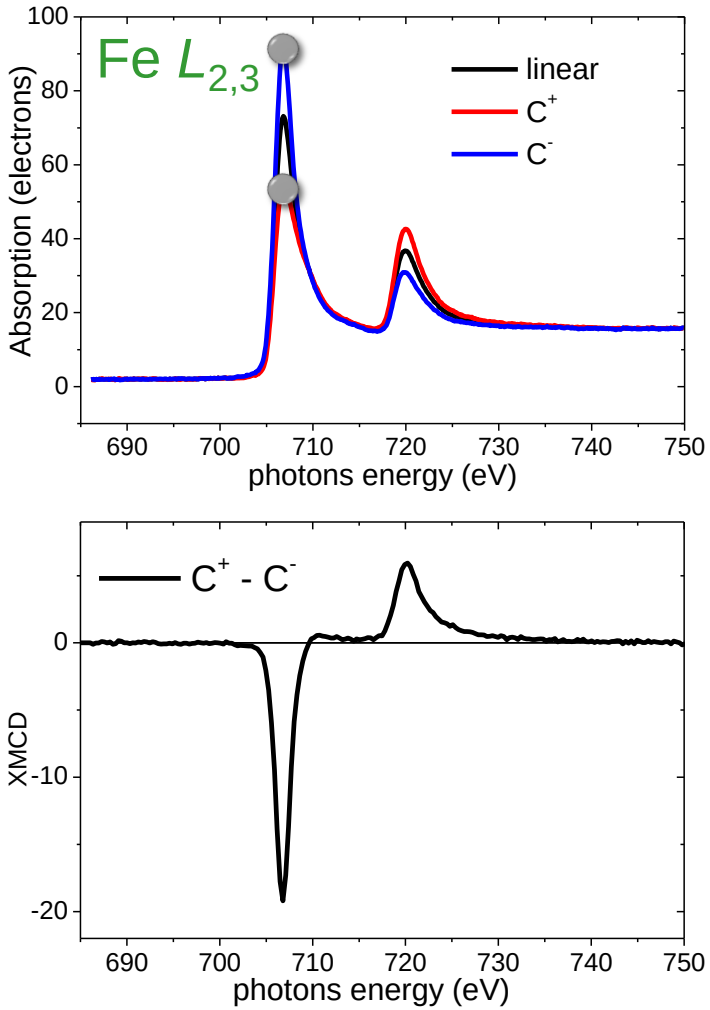
} X-ray Resonant Magnetic Reflectivity (XRMR)





$n = 1 - \delta + i\beta$

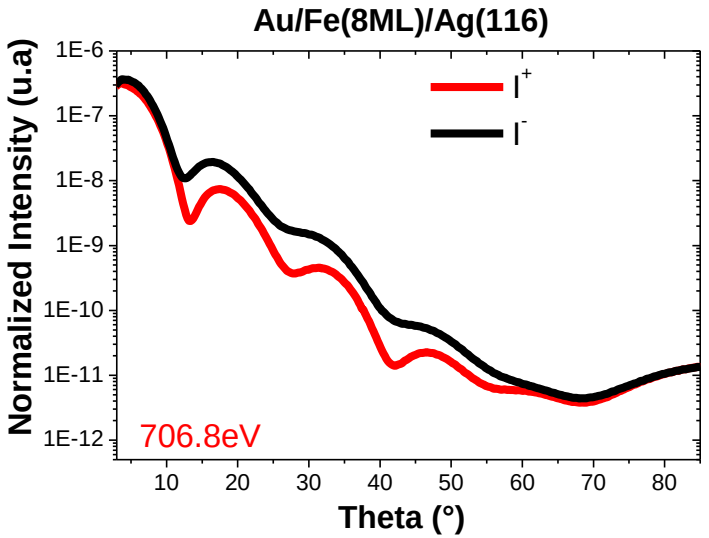
$\beta \propto$ Absorption

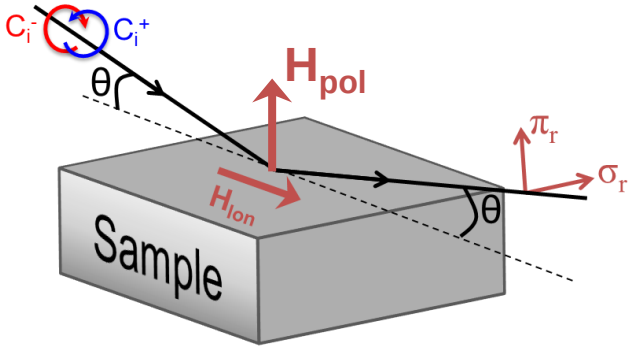


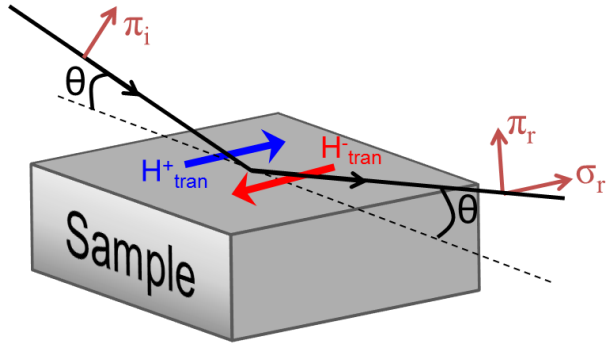
* X-ray Magnetic Circular Dichroism

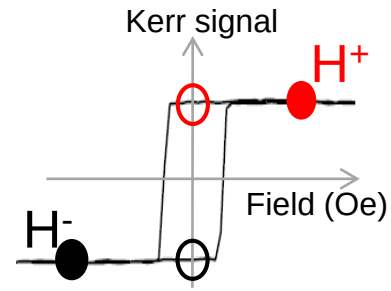
I. Principle of XRMR (3/3)

- 2 ways to obtain I^+ and I^-:
  - By reversing the polarization
    - Cpm configuration
  - By reversing the applied field.
    - Hpm configuration and Π configuration









- The field can be:
  - In the 3 directions : longitudinal, transverse and polar
  - At saturation or at remanence

Outline

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1. **Generality**
2. **Kinematic**
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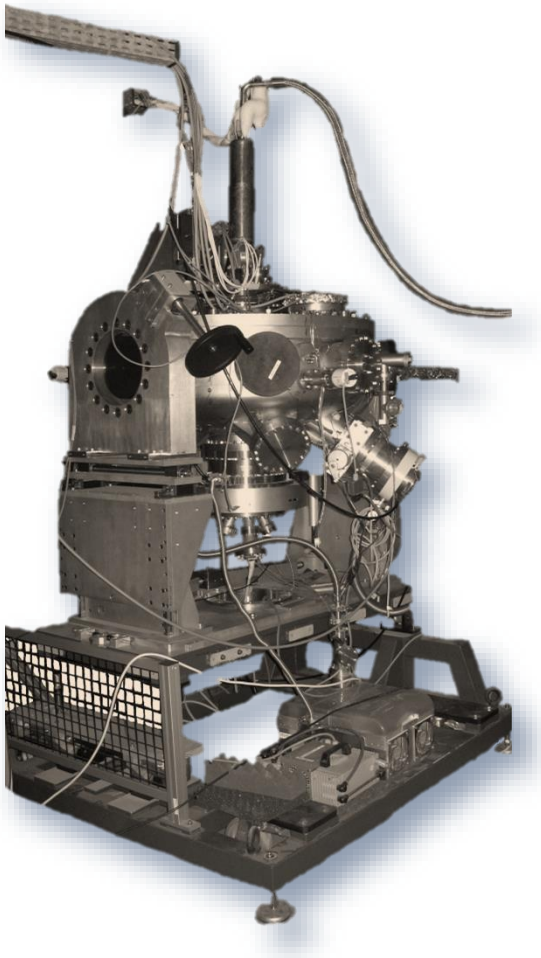
IV. Conclusions and Outlook



II. Formalism: Generality

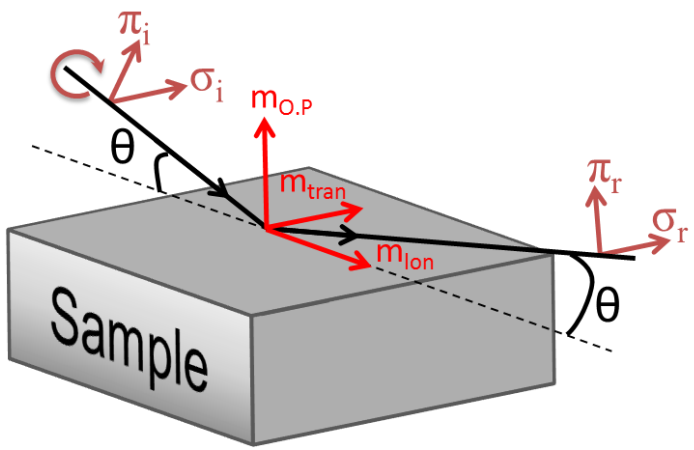
Diffracted intensity and Resonant atomic scattering factor, f: Hannon *et al.* PRL **61**, 1245 (1989)

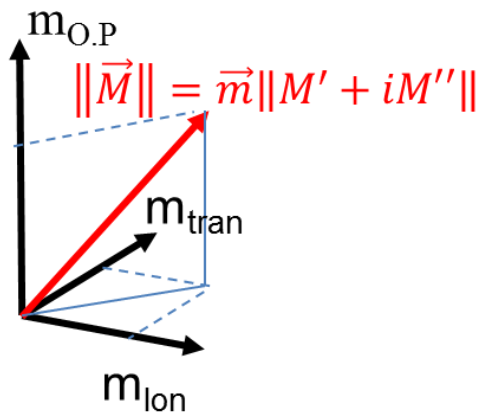
$$I \propto \left| \sum_j f_j e^{i\vec{Q}\cdot\vec{r}_j} \right|^2 \qquad f(E) = (\mathbf{e}_r^* \cdot \mathbf{e}_i)(f_0 + F'(E) + iF''(E)) - i(\mathbf{e}_r^* \times \mathbf{e}_i)\cdot\mathbf{m}(M'(E) + iM''(E))$$

Charge scattering = F_c

1st order magnetic scattering = F_m

$$I^{\pm} \propto C^2 \pm 2MC$$





Matrix expression based on the σ, π polarization states:

F. De Bergevin *et al*, Acta Cryst. **A37**, 314 (1981)
J. P. Hill and D. F. McMorrow, Acta Cryst. A **52**, 236 (1996)

$$f(E) = F_c \begin{pmatrix} 1 & 0 \\ 0 & \cos(2\theta) \end{pmatrix} - iF_m \begin{pmatrix} 0 & m_{lon}\cos(\theta) + m_{O.P}\sin(\theta) \\ -m_{lon}\cos(\theta) + m_{O.P}\sin(\theta) & -m_{tran}\sin(2\theta) \end{pmatrix}$$

See Annex for details

II. Formalism: kinematic (1/2)

$$I \propto \left| \sum_j f_j e^{i\vec{Q}\cdot\vec{r}_j} \right|^2$$

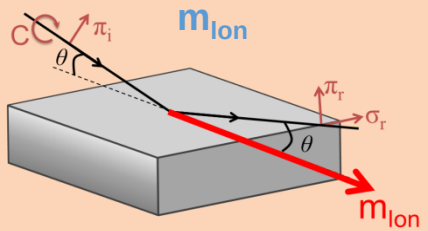
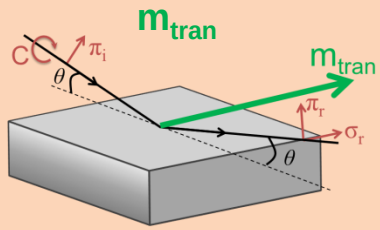
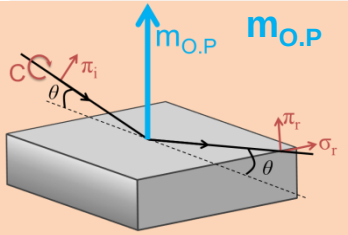
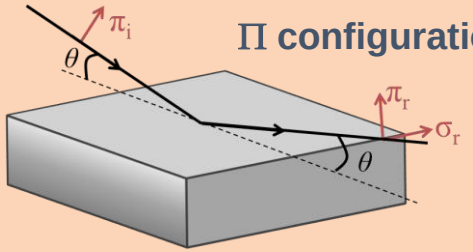
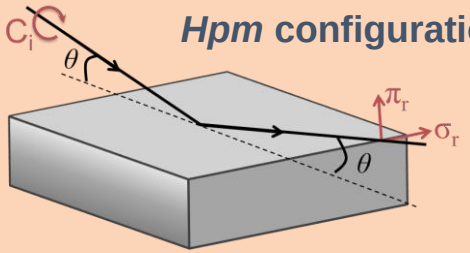
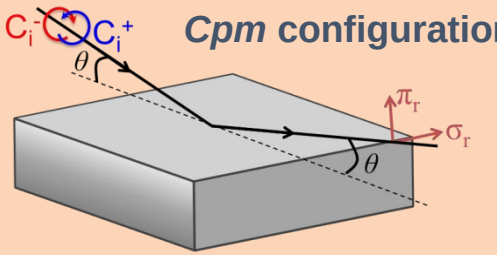
$$I^{\pm} \propto C^2 \pm 2MC$$

$$A = \frac{I^+ - I^-}{I^+ + I^-}$$

$$A \propto \frac{M}{C}$$

$$FM_1 = F''M' - F'M''$$

$$FM_2 = F'M' + F''M''$$

Experimental Configurations \ Magnetic component			
 Π configuration	0	$\frac{m_{tran}\sin(4\theta)FM_1}{\cos(2\theta)^2\,\lvert F_c\rvert^2}$	0
 *Hpm* configuration	$\frac{-4\,m_{lon}\cos\theta^3\,FM_2}{[1+\cos(2\theta)^2]\lvert F_c\rvert^2}$	$\frac{m_{tran}\sin(4\theta)FM_1}{[1+\cos(2\theta)^2]\lvert F_c\rvert^2}$	$\frac{4\,m_{O.P}\sin\theta^3\,FM_2}{[1+\cos(2\theta)^2]\lvert F_c\rvert^2}$
 *Cpm* configuration		0	

See Annex for details

II. Formalism: kinematic (2/2)

$$I \propto \left| \sum_j f_j e^{i\vec{Q}\cdot\vec{r}_j} \right|^2$$

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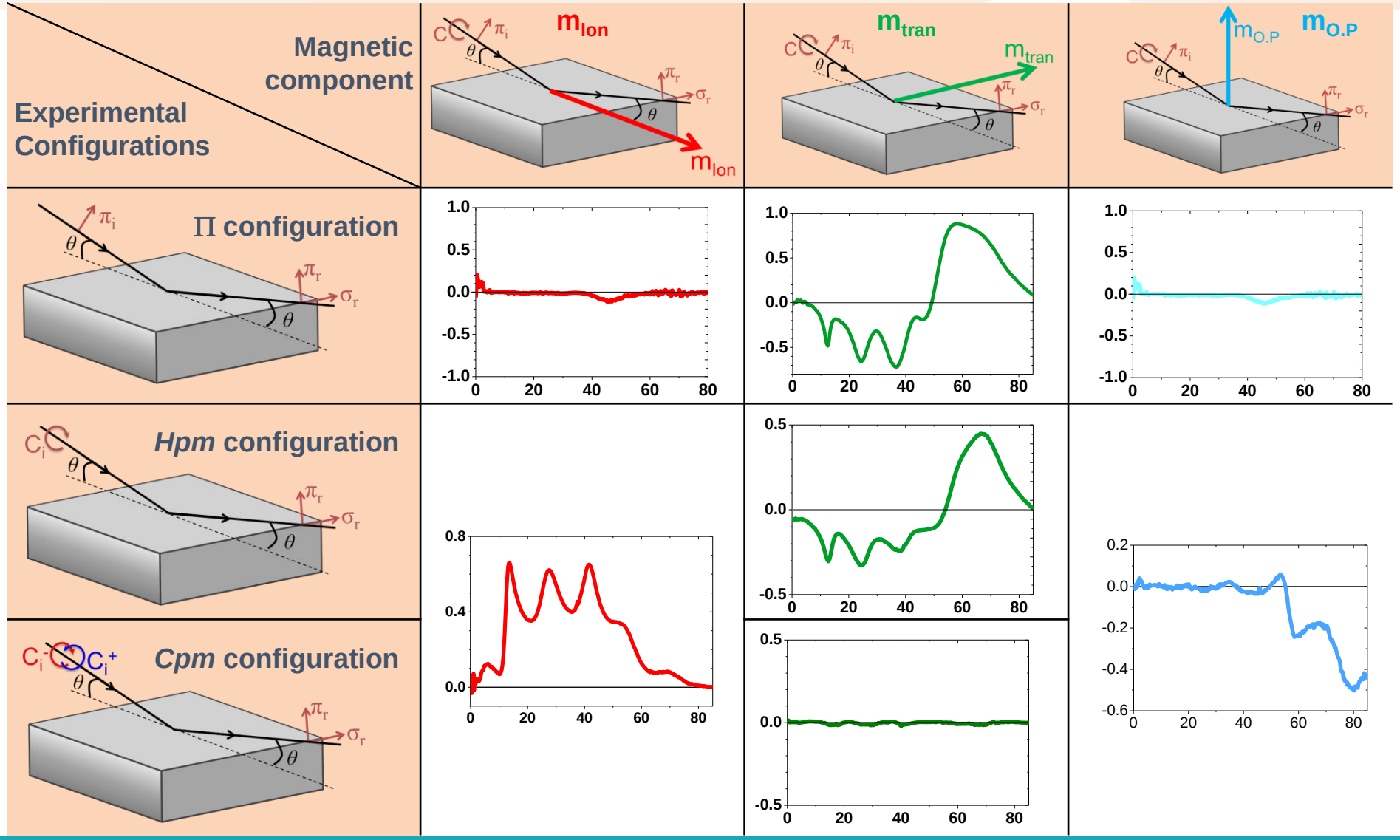


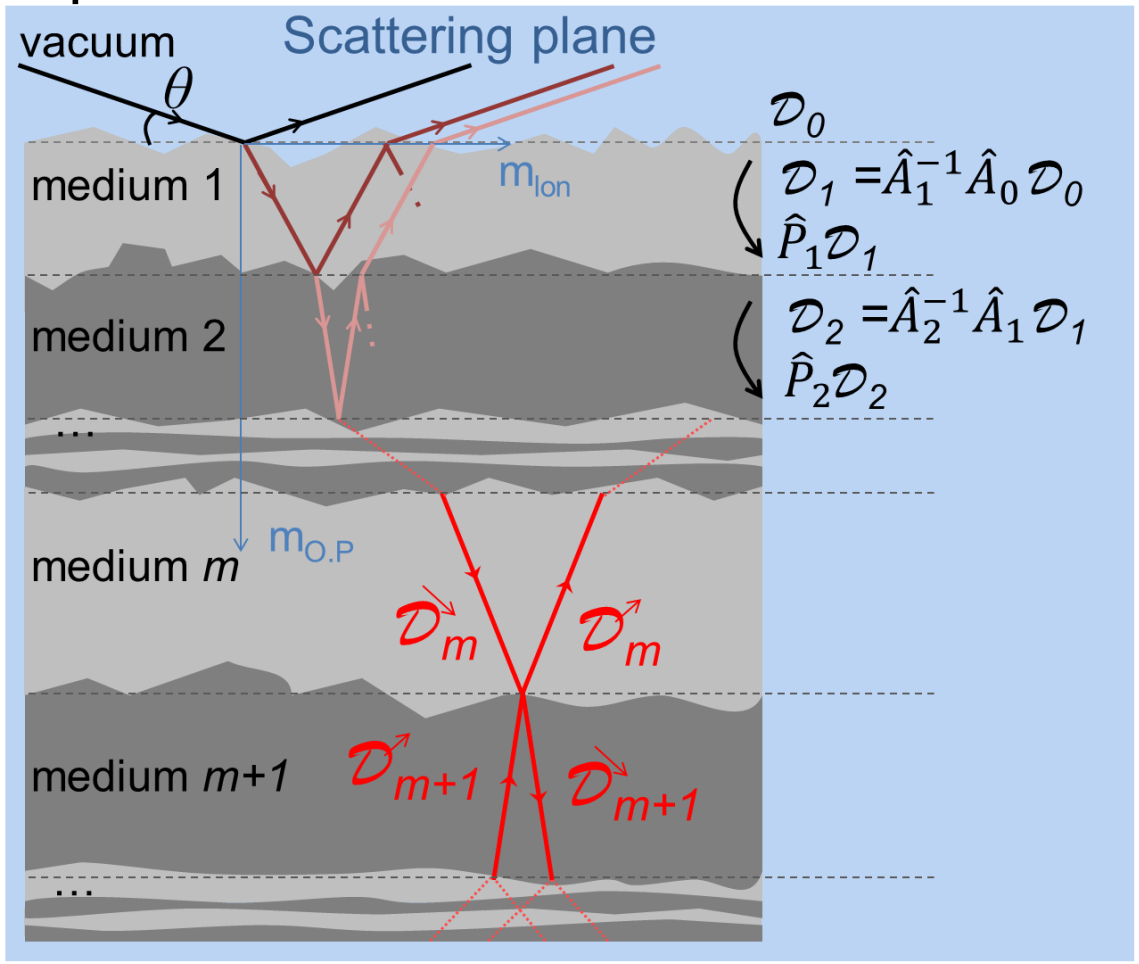
II. Formalism: dynamic = matrix formalism (1/3)

For this formalism, take the optics point of view

- The propagation of electro-magnetic waves in a medium is described by Maxwell equations
  - The electric displacement **D** is related to the electric field **E** thanks to the tensorial dielectric permittivity $\hat{\varepsilon}$: **D = $\hat{\varepsilon}$.E**
  - The magnetic field **B** is related to the magnetizing field **H** thanks to scalar magnetic permability μ
- Link between the permittivity, and the scattering factors
  - $\hat{\varepsilon} = 1 + \frac{r_0 \lambda^2}{\pi} \sum_i \rho_i \hat{f}_i$ where r_0 est electron radius and ρ_i is the density of the ith element.
- Solve Maxwell equation
  - The eigenwaves propagating in a magnetic medium are circularly polarized waves (in the incident wave basis)
  - Refractive index linked with optical factor F_c and F_m :
    - $n^{\pm} \approx 1 + \frac{r_0 \lambda^2 \rho}{2\pi} (F_c \mp (\cos\theta m_{lon} + \sin\theta\, m_{O.P}) F_m)$

II. Formalism: dynamic = matrix formalism (2/3)

The propagation of electro-magnetic waves in a medium is described by Maxwell equations : Circular basis.



The wave is therefore described in the circular basis and for each medium there is 2 waves represented by the electric displacement **D**, one incident (transmitted) and one reflected. So the electric displacement can be written:

$$\mathcal{D}_0 = \begin{pmatrix} i^+ \\ i^- \\ r^+ \\ r^- \end{pmatrix}$$

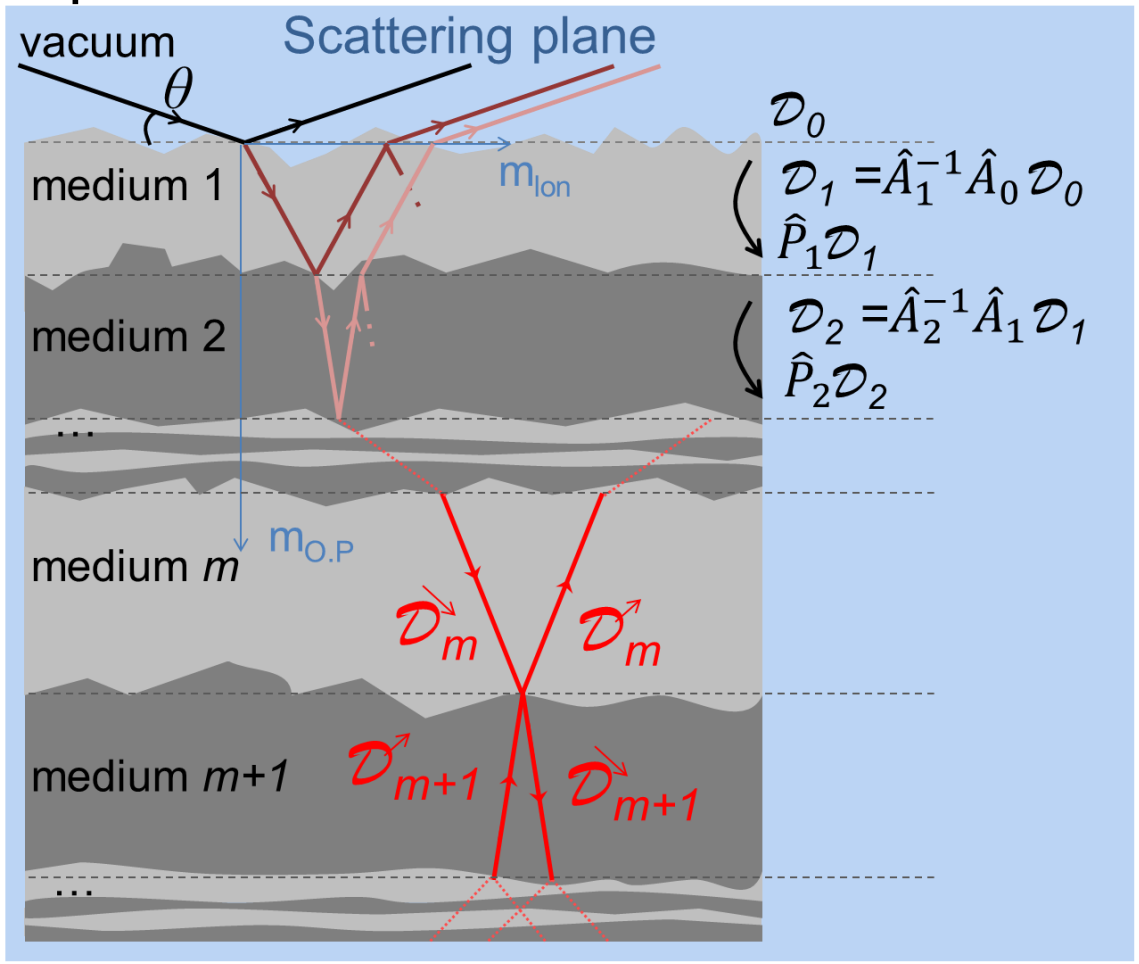
At each interface, the boundary condition are taken into account thanks to the boundary matrix $\hat{A}_i$.

$$\hat{A}_0\mathcal{D}_0 = \hat{A}_1\mathcal{D}_1 \text{ so } \hat{A}_1{}^{-1}\hat{A}_0\mathcal{D}_0 = \mathcal{D}_1$$

The roughness is treated by multiplying the matrix element $\hat{A}_1{}^{-1}\hat{A}_0$ by an exponential simulating the roughness as a Gaussian with a certain width σ. The magnetic roughness is not taken into account

II. Formalism: dynamic = matrix formalism (3/3)

The propagation of electro-magnetic waves in a medium is described by Maxwell equations : Circular basis.



Then the wave is propagating through the medium which is modeled by a the matrix $\hat{P}_i$. At the end of the first medium $\mathcal{D}_1' = \hat{P}_1\mathcal{D}_1 = \hat{P}_1\hat{A}_1{}^{-1}\hat{A}_0\mathcal{D}_0$ and at the start of the new medium $\mathcal{D}_2 = \hat{A}_2{}^{-1}\hat{A}_1\hat{P}_1\hat{A}_1{}^{-1}\hat{A}_0\mathcal{D}_0$. So at the end

$$\mathcal{D}_f = \hat{A}_f{}^{-1}\left(\prod_m \hat{A}_m\hat{P}_m\hat{A}_m{}^{-1}\right)\hat{A}_0\,\mathcal{D} = \hat{M}\mathcal{D}_0$$

Where $\mathcal{D}_0 = \begin{pmatrix} i^+ \\ i^- \\ r^+ \\ r^- \end{pmatrix}$ and $\mathcal{D}_f = \begin{pmatrix} t^+ \\ t^- \\ 0 \\ 0 \end{pmatrix}$ (0)

By solving this system we obtain the reflectivity in function of the incident wave. Since $\hat{P}_i$ and $\hat{A}_i$ depend on the angle θ, the wavelength λ, the refractive index n and the permittivity $\hat{\varepsilon}$, those last 2 depending on magnetization, one can derive the magnetization, thickness and roughness of each layer.

II. Formalism: Summary

Magnetic dichroïsm + Reflectivity = depth magnetic sensibility

Qualitative Analysis

Direct
- Circular polarization
  - Asymmetry low angles = m_{lon}
  - Asymmetry high angles = $m_{O.P}$
- Linear polarisation → Asymmetry = m_{tran}

Quantitative Analysis

Complex: Matricial formalism+ fit = determination of depth magnetic profile

M. Elzo and E. Jal *et al.* JMMM **324**, 105-112 (2012)

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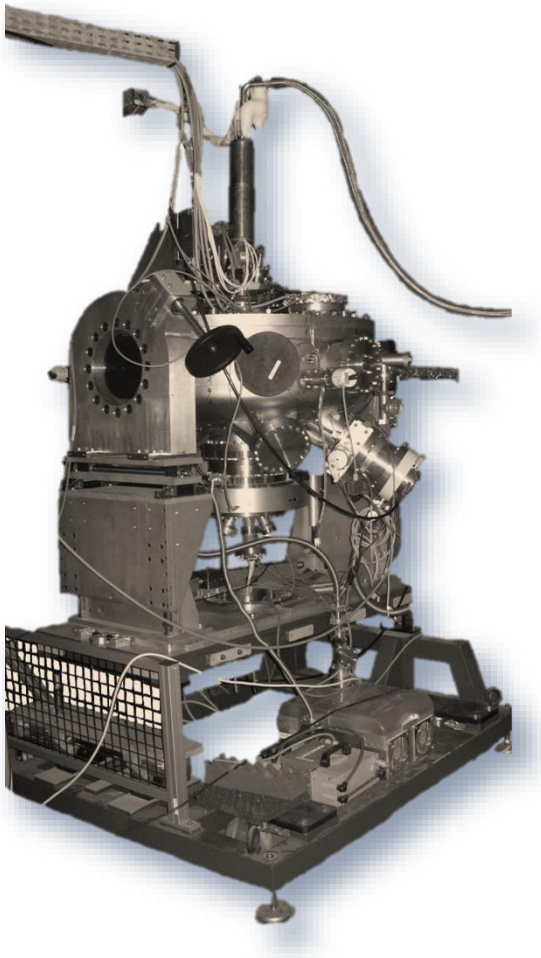
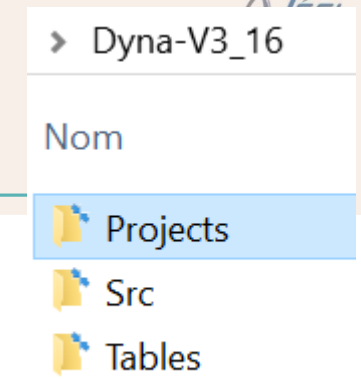
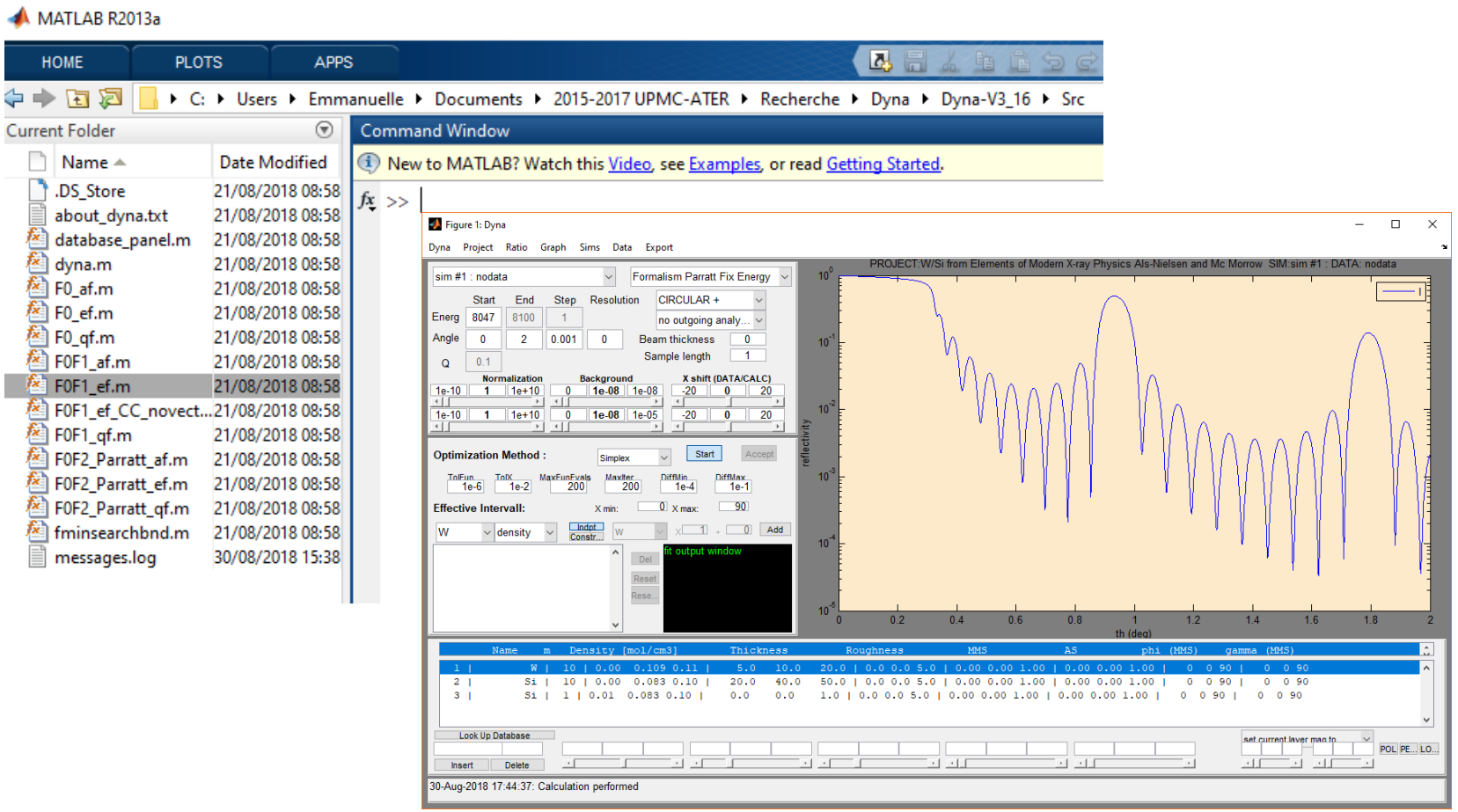


III. How to use DYNA

In a folder download the “sources” and “datas” folder, from here http://neel.cnrs.fr/spip.php?article2575 and create a “projects” folder





Open Matlab

- go to the path of you main folder/sources (e.g. Dyna-v3_16/Src)
- type dyna and press enter
- This window open

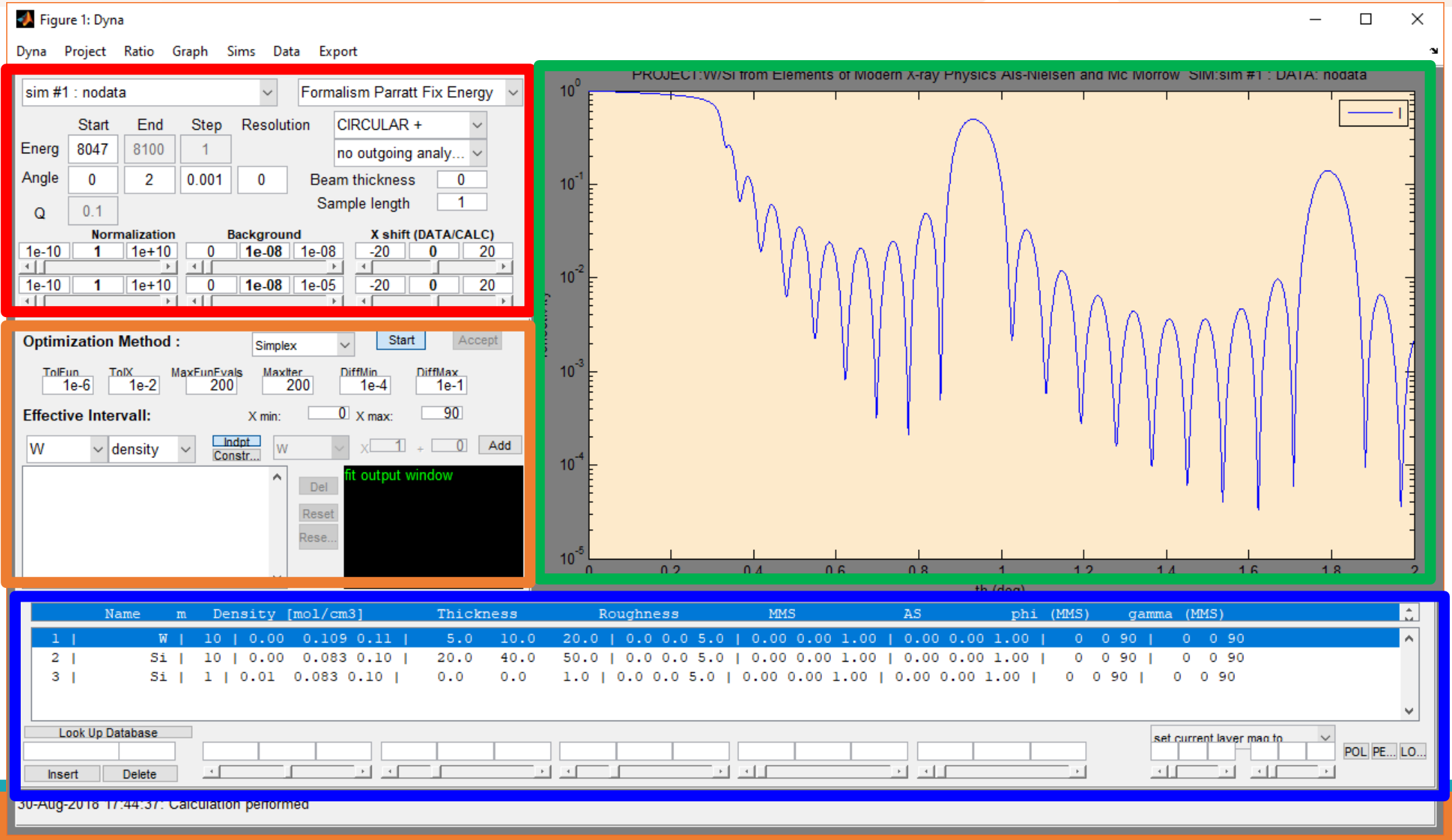
III. How to use DYNA

Experimental parameter

Sample composition

Result of the formalism

Fitting window

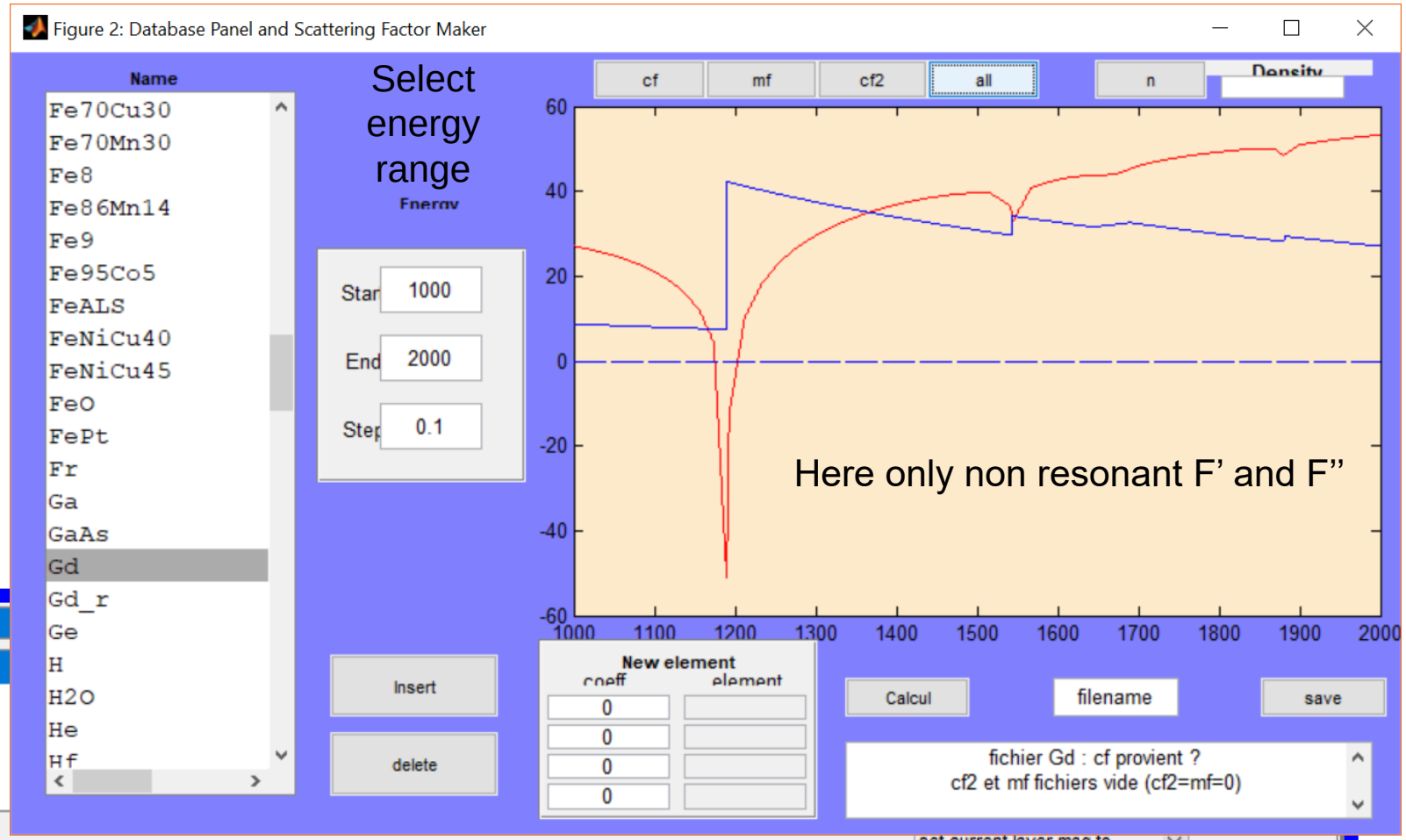


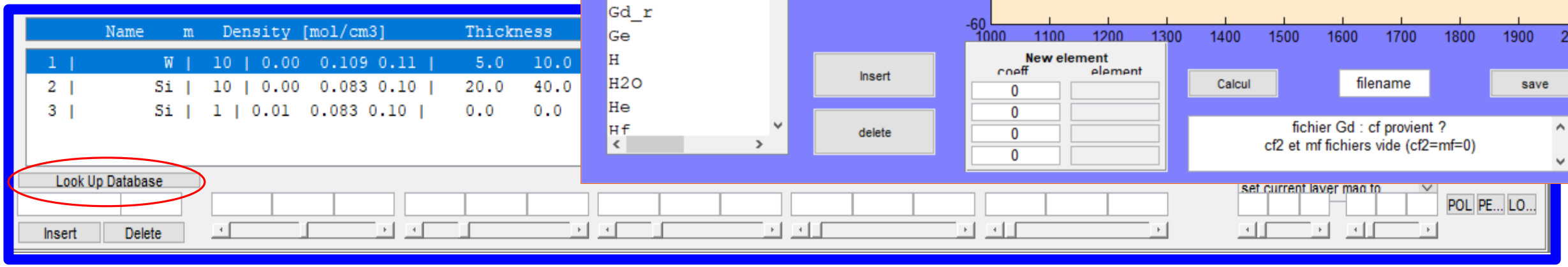
III. How to use DYNA: Optical constant (1/3)

Need to know the absorption, and XMCD to determine

- The absorption and dispersive factor, F' and F''
- The XMCD/2 and magnetic dispersive factor, M' and M''

Check that they exist in the table (select energy range)

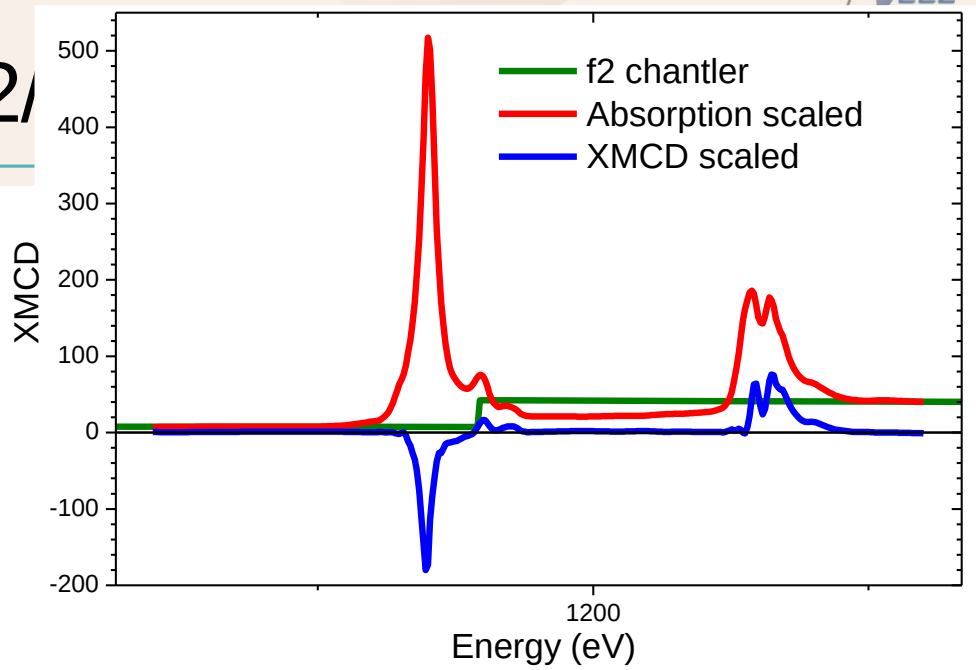


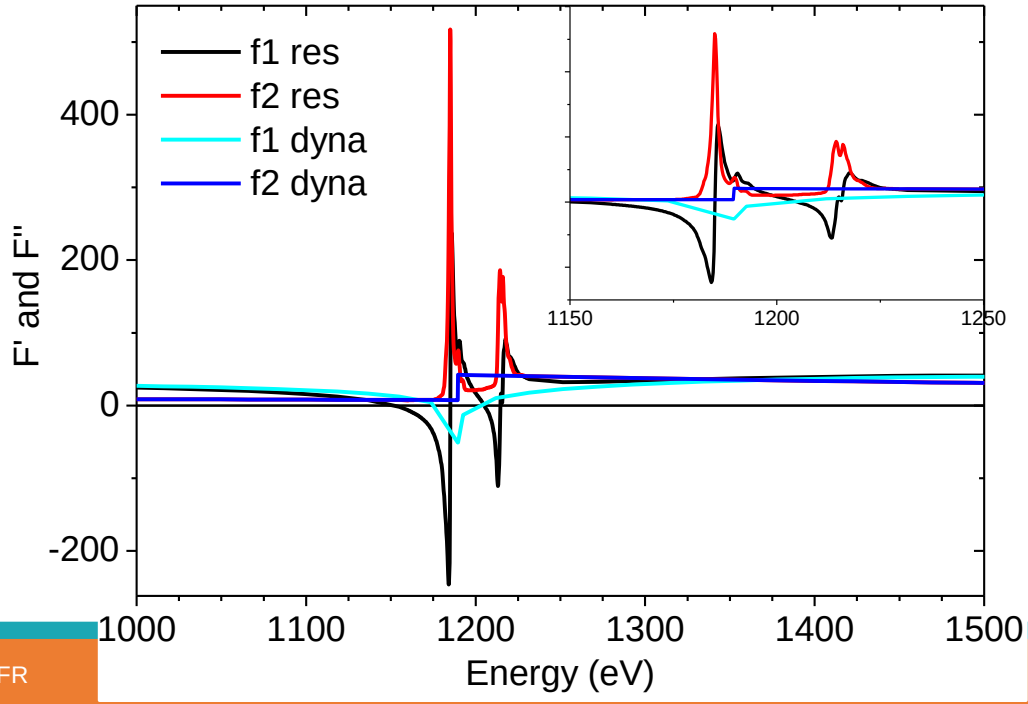


III. How to use DYNA: Optical constant (2/

If the complete resonant optical constant doesn't exist

- From an article or measurement extract XAS (F") for both polarization
- Be careful we need F" and not β ($\beta = cste.\lambda^2.F''$)
- Scale it far from the edge to Chantler table and Derive the scaled XMCD/2 (https://physics.nist.gov/PhysRefData/FFast/html/form.html)
- You have the resonant part of F" and M", the imaginary part
- Add this resonant part to the non-resonant file in order to use Kramers Kronig relation to derive the real part F' and M'



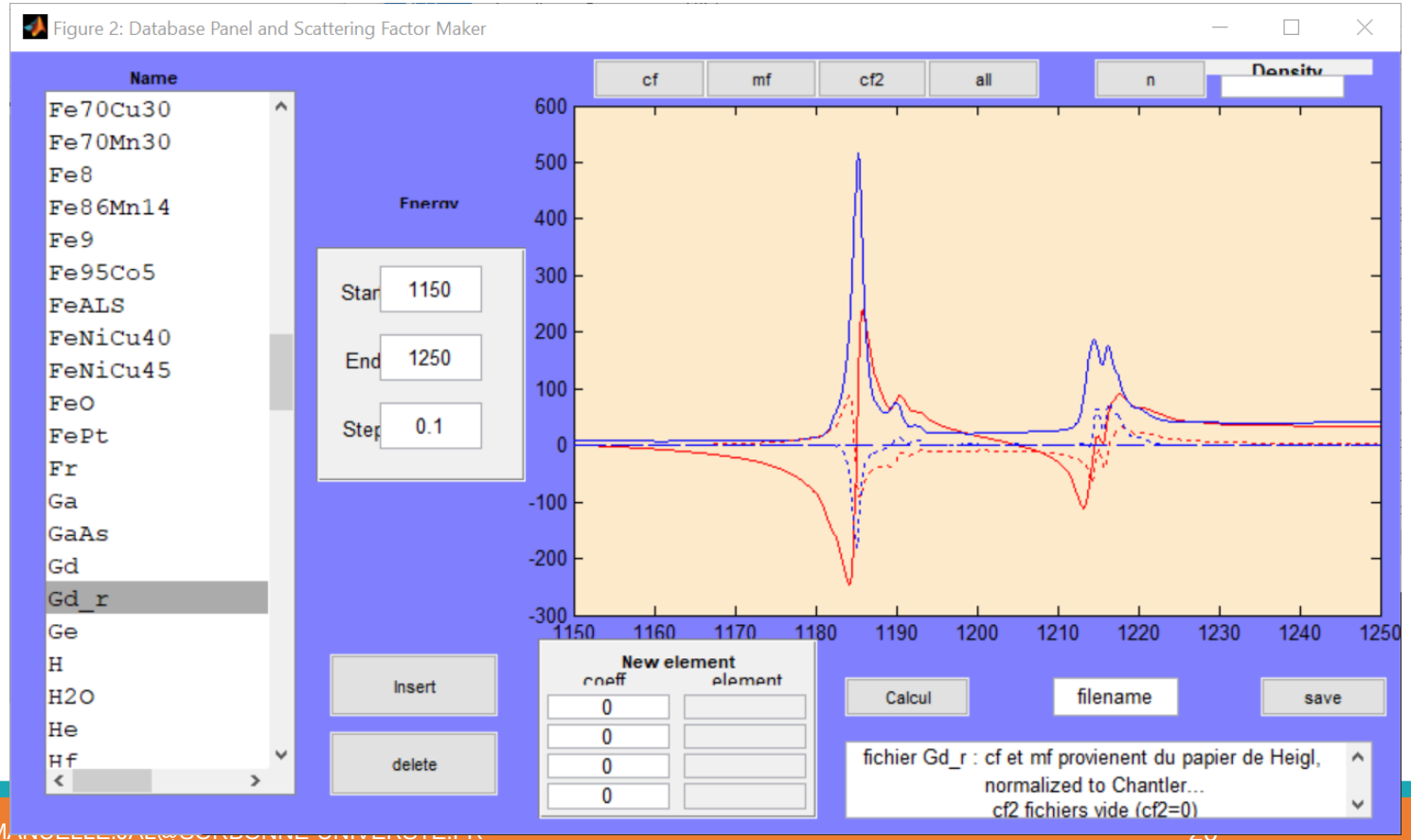


III. How to use DYNA: Optical constant (3/3)

If the complete resonant optical constant doesn't exist

- Export Energy (eV), F', F'' in one .cf folder and the same for the magnetic part (E(eV), M', M'') in a .mf folder. Need to create an associate .cf2 file (=0) and a note (.txt) file where you can write where does those data come from.

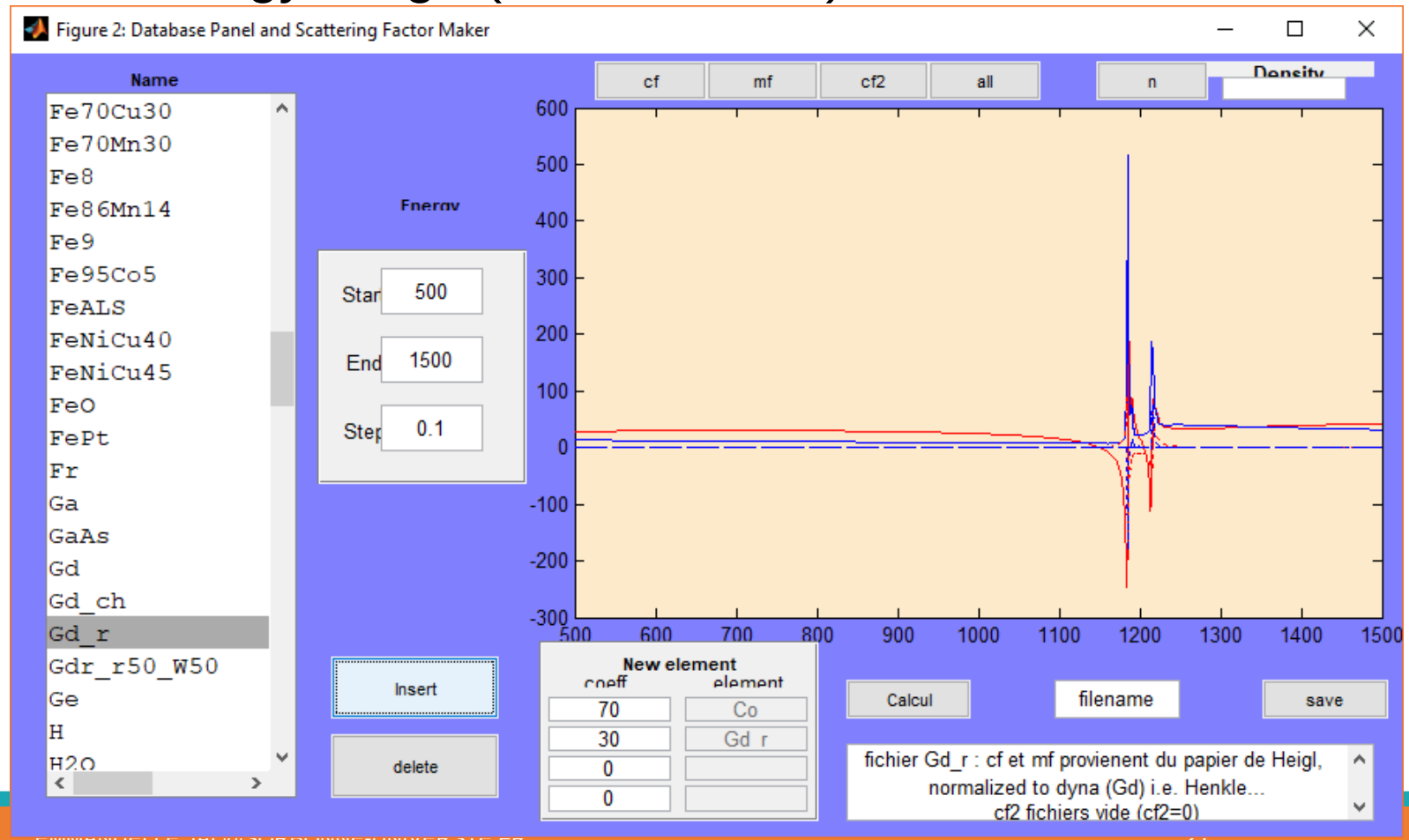
- You can plot them from the program



III. How to use DYNA: Optical constant for alloy (1/2)

If for an alloy you do not have any measured or tabulated optical constant, you can create an artificial alloy from the dyna database panel. To create an alloy $Co_{70}Gd_{30}$

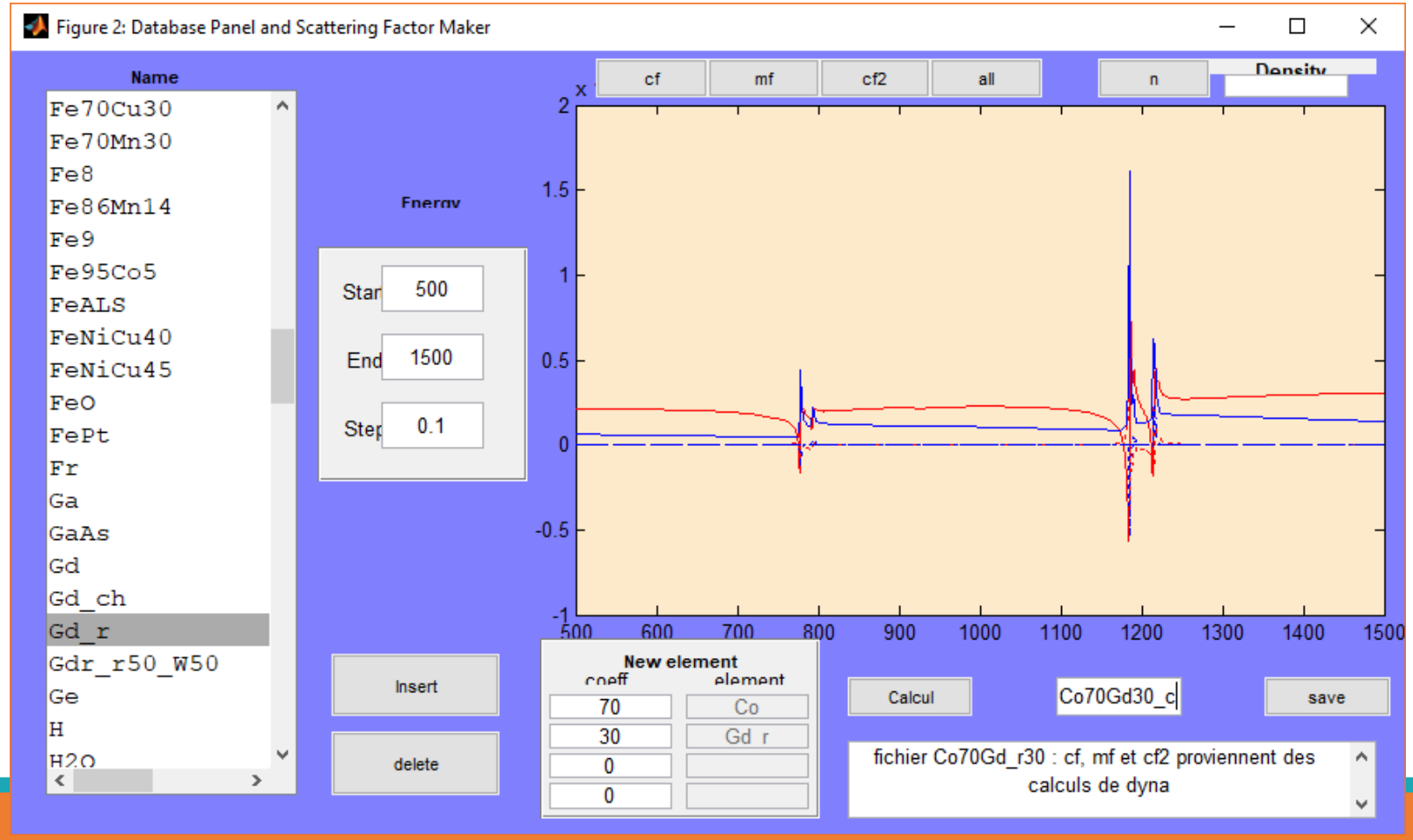
- In the database panel, select the energy range (500-1500 eV) and click on the Co element.
- Press insert, it will appears in the new element case
- Select the Gd element and press insert. You have now 2 elements
- Put the alloy coefficient (70-30)



III. How to use DYNA: Optical constant for alloy (2/2)

If for an alloy you do not have any measured or tabulated optical constant, you can create an artificial alloy from the dyna database panel. To create an alloy $Co_{70}Gd_{30}$

- Press Calcul, it will give you the the optical constant with the stoichiometric coefficient you have entered
- Type a filename (eg: Co70Gd30_c, c for calculated)
- Enter the comment in the comment window
- You can save those data and use the filename for one layer in the main panel

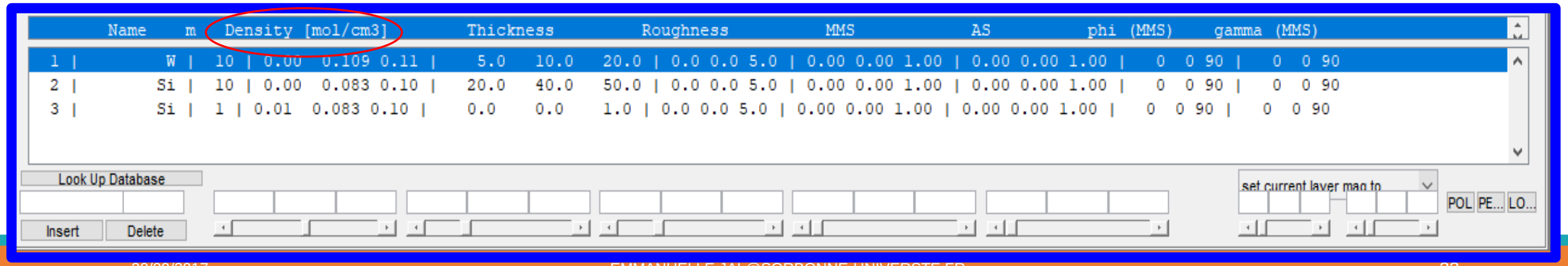


III. How to use DYNA: parameter

Once you have the optical constant for all your chemical component, need to calculate the density in mol/cm^3 .

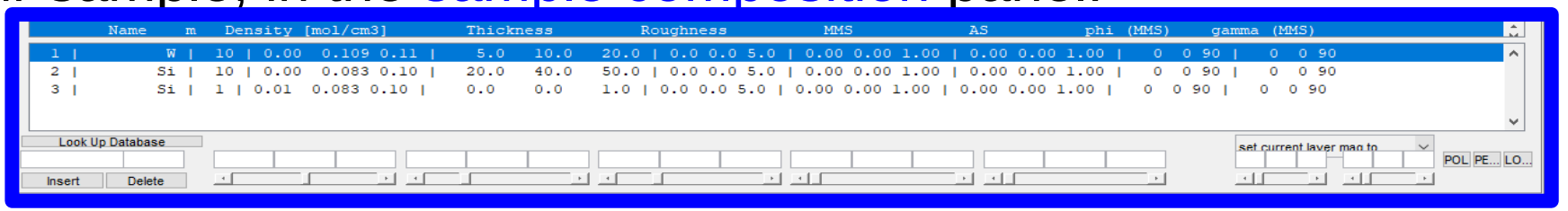
- From a periodic table (https://www.webelements.com/), know the density in g/cm^3 and the atomic mass in g/mol, and divide them.
- Here the principal element

	Fe	Ni	Co	Si	Al	Pt	Gd	Tb	Ta	Cu	Al2O3
Densite g/cm^3	7.874	8.908	8.9	2.33	2.7	21.09	7.901	8.219	16.650	8.920	4
Masse atomique g/mol	55.845	58.6934	58.933	28.0855	26.98	195.084	157.23	158.925	180.95	63.546	101.961
Densite mol/cm^3	0.141	0.152	0.151	0.083	0.100	0.108	0.0502	0.0517	0.092	0.1404	0.039

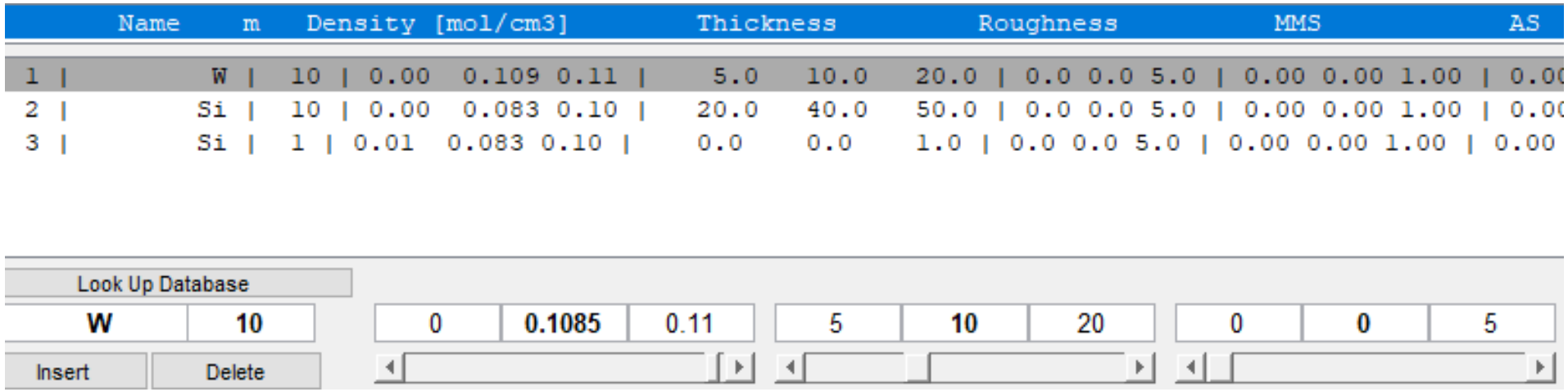


III. How to use DYNA: Build a layer/sample (1/2)

To build your sample, in the sample composition panel:



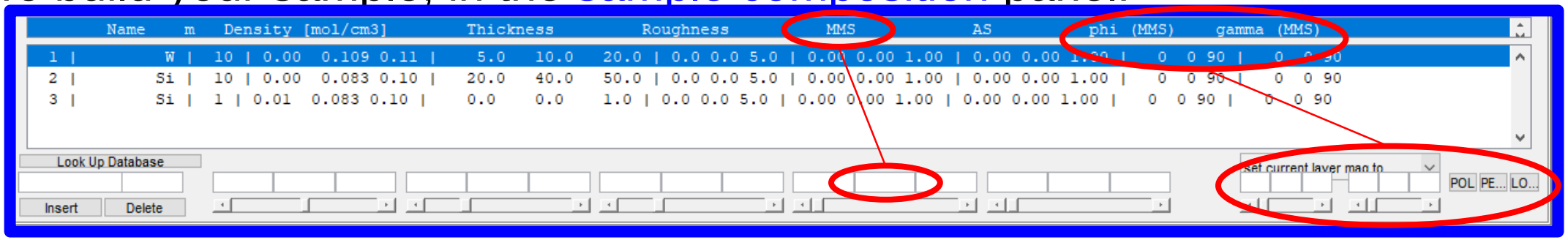
- Select a line
  - Enter the name
  - m=nb of repetition of a multilayer stack
  - Density
  - Thickness
  - Roughness



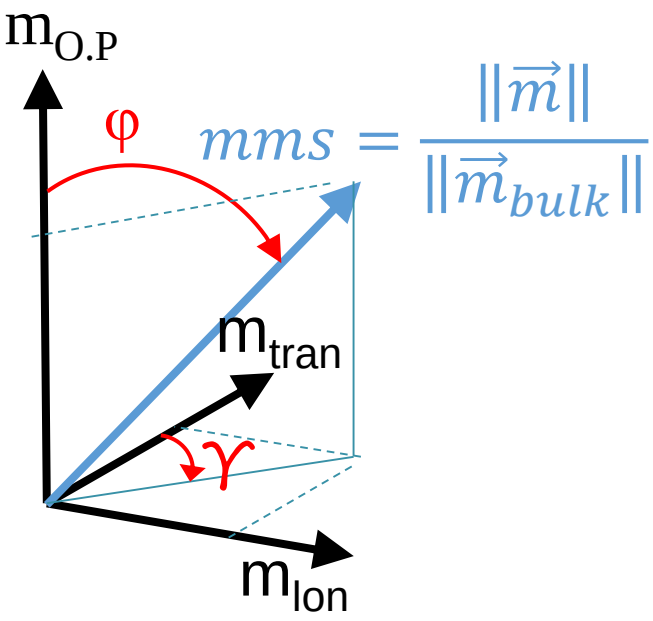
- Do the same for the other layer of your sample
- Do not forget to adjust the lower and upper limit
- If you want to add a layer or delete one, use the button “insert” and “delete” in the left-bottom corner.

III. How to use DYNA: Build a layer/sample (2/2)

To build your sample, in the sample composition panel:



- Then take care of the magnetic part
  - Put 1 for mms, it will give a magnetic moment proportional to the magnetic optical constant.
  - Adjust both angles phi and gamma for the direction
  - There is 3 registered useful direction
  - If you want several mms, you need to divide your magnetic layer but we will do that after the structural fit (slide 44)

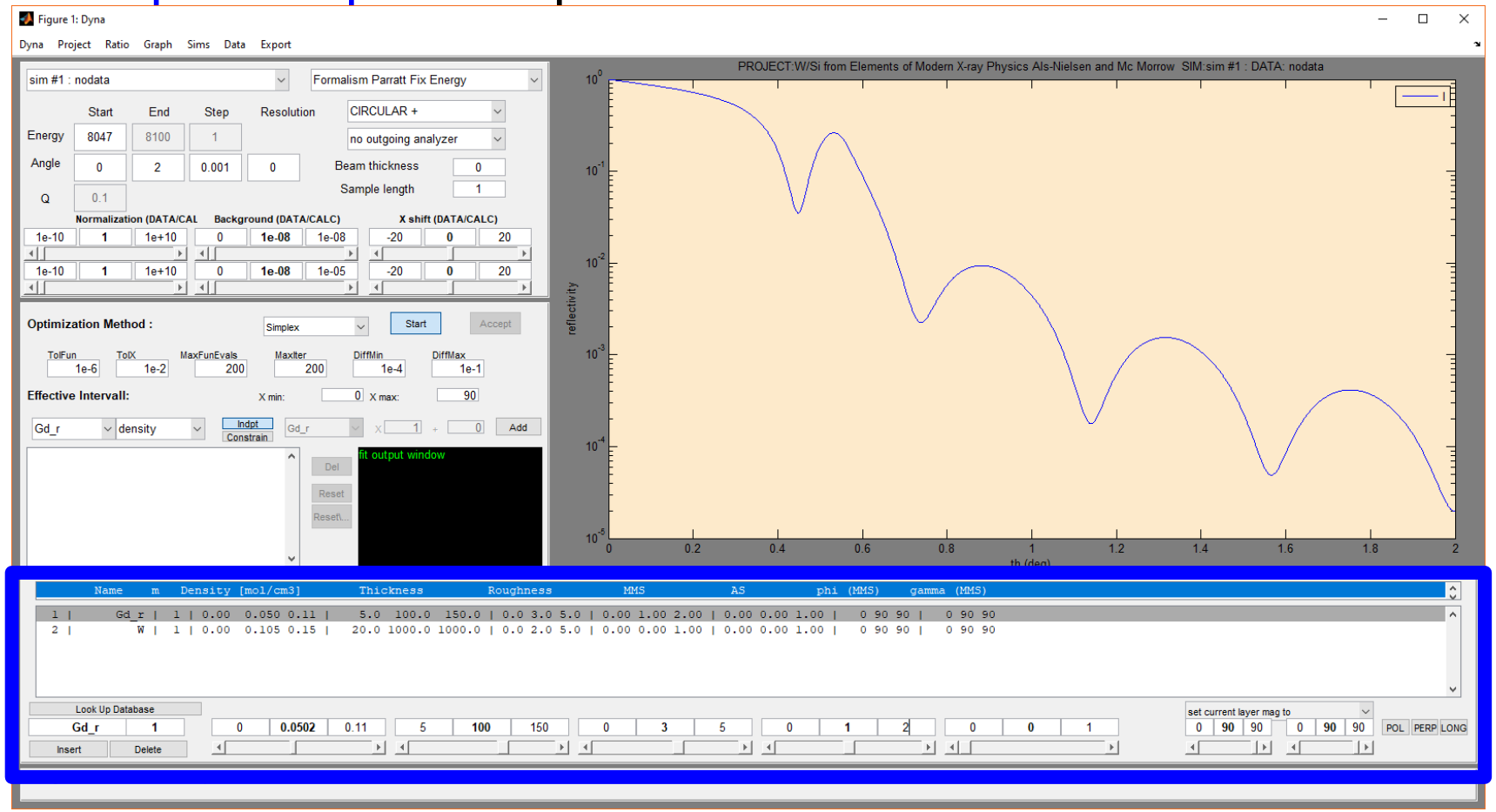


- Do not take into account AS => for anisotropic ferrimagnetic

III. How to use DYNA: Set experimental parameter (1/2)

To build your sample, in the sample composition panel:

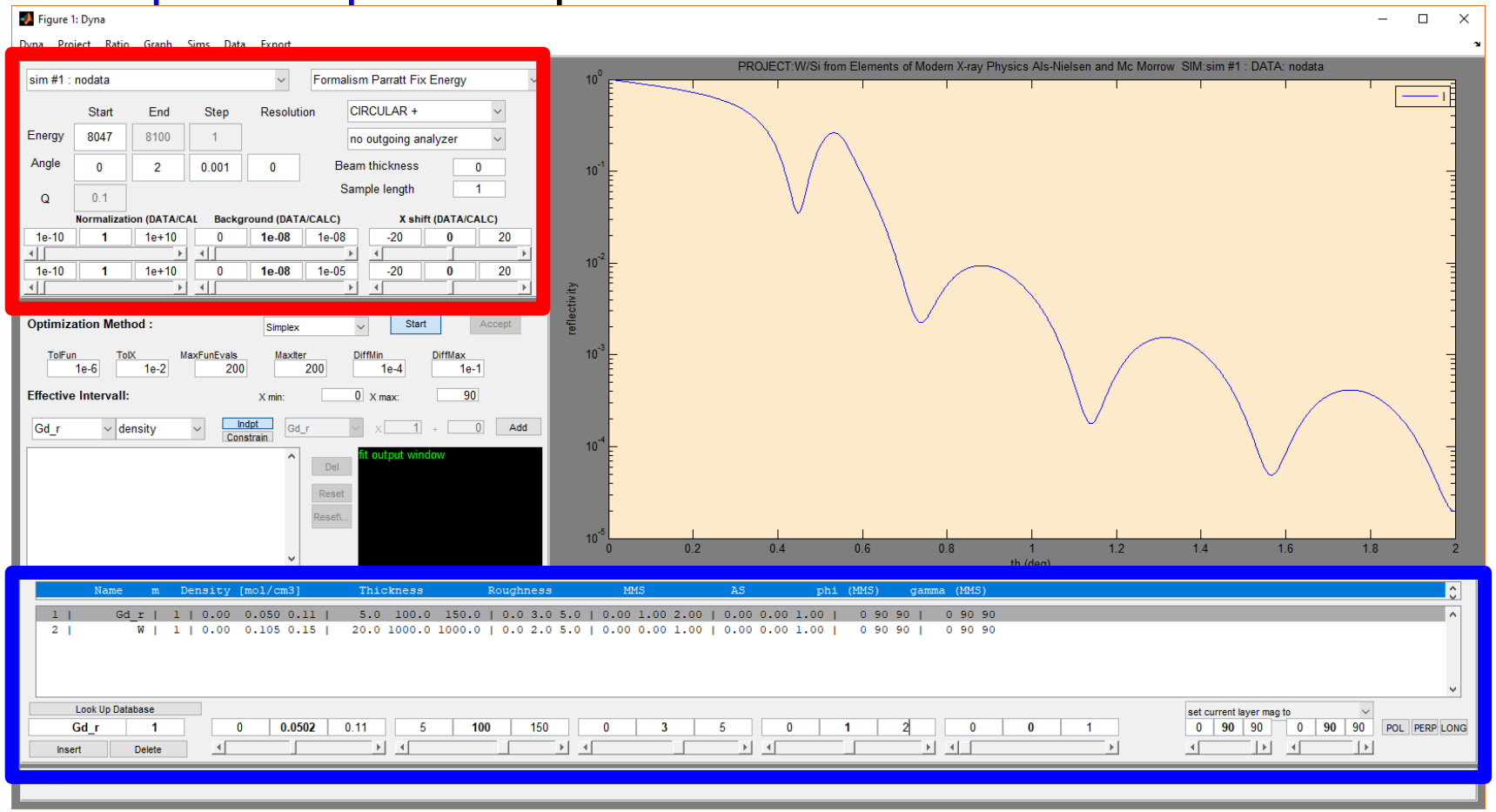
- You should obtain that



III. How to use DYNA: Set experimental parameter (1/2)

To build your sample, in the sample composition panel:

- You should obtain that



Now you need to adjust the experimental parameter

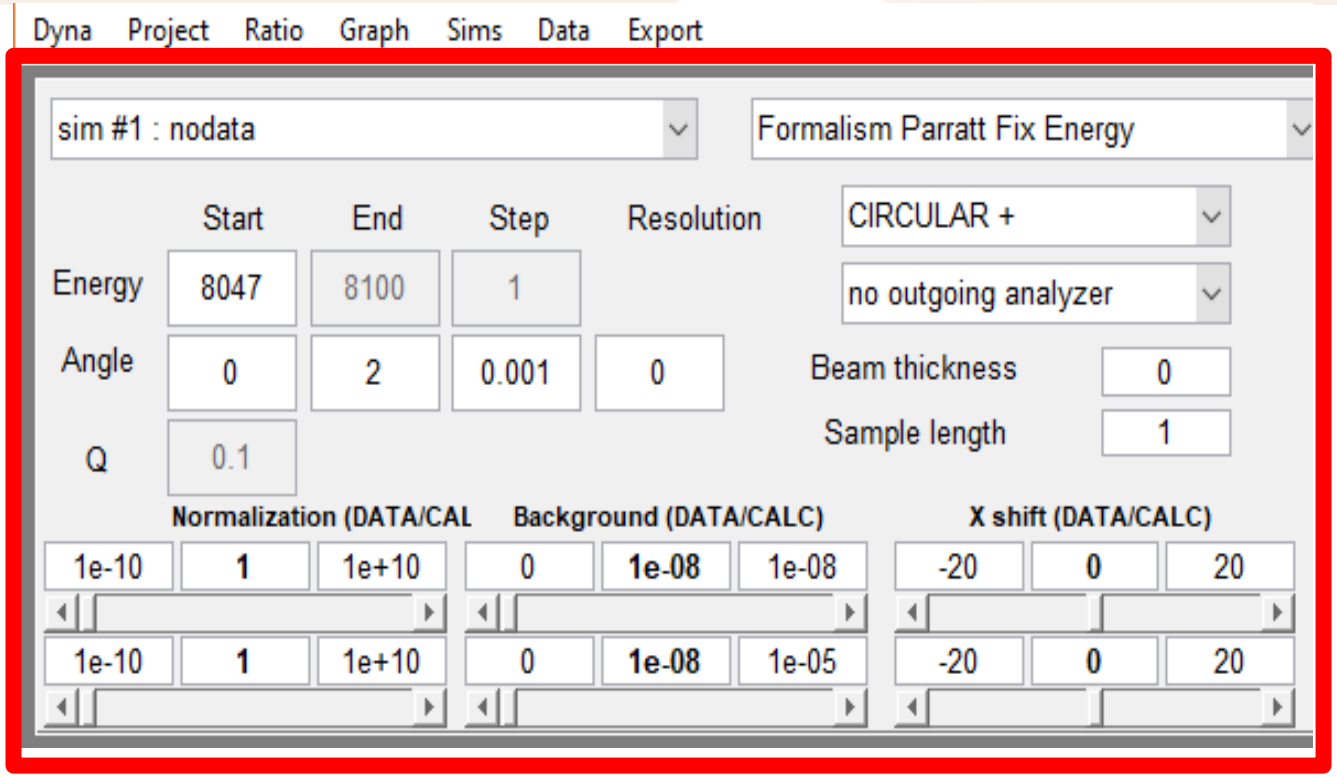
III. How to use DYNA: Set experimental parameter (2/2)

Adjust the experimental parameter

- Type of Formalism

(top right slide menu)

  - Paratt (only structyre)
  - Magnetism (structure + magnetism)
  - Anisotropy (structure + anisotropy)
  - For each, fix energy / fix angle / fix Q



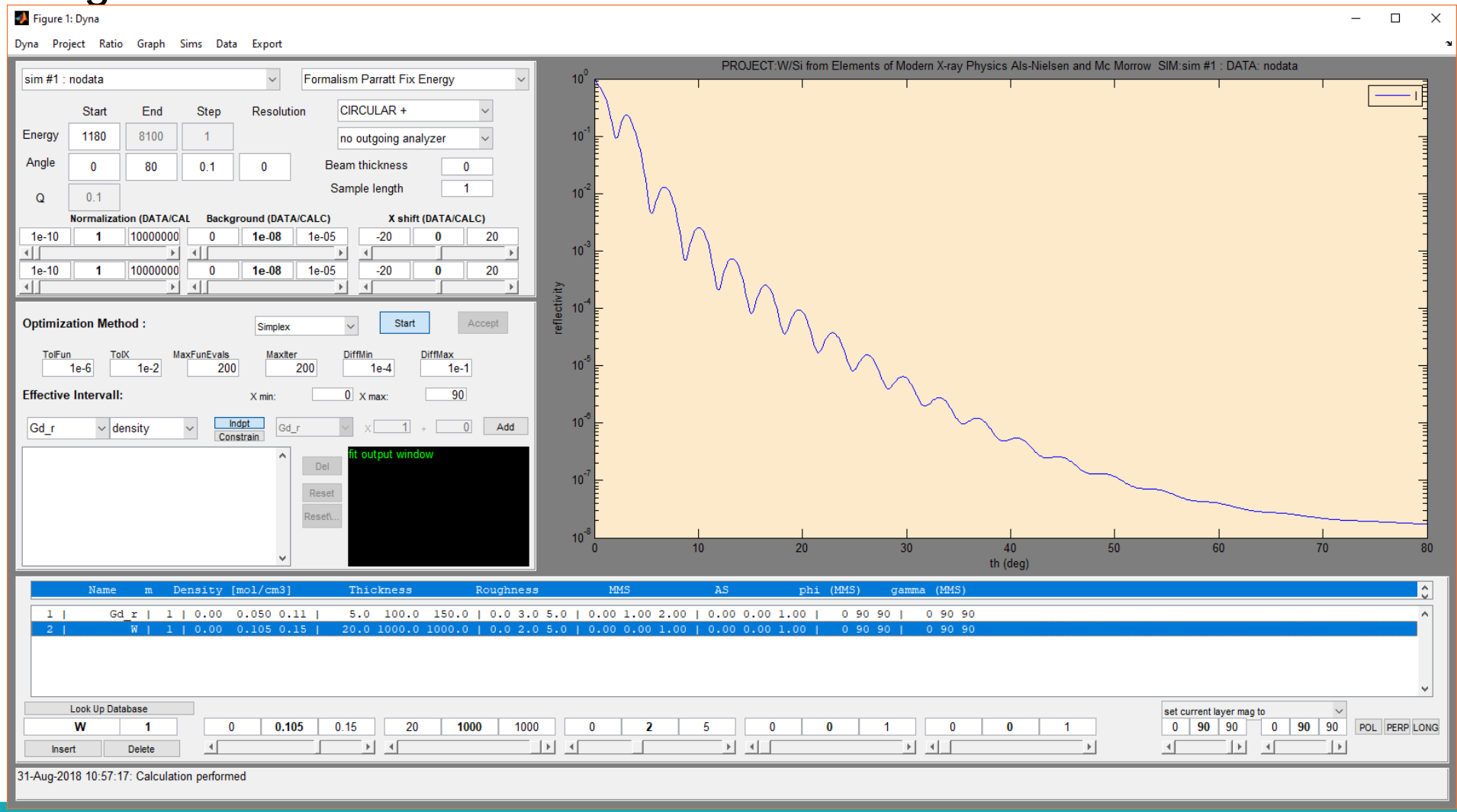
- Energy / Angle
- Polarization (no outgoing analyzer
- All the other variable will be adjusted to mimic the experimental data
- You can add a simulation by going to the Sims menu (at the top). The sample panel will be the same between the different simulation, but all the parameter of the experimental are independent from one simulation to the other.

III. How to use DYNA: Import experimental data

You should get something like that

You want to compare this calcul to your data.

- Your data should be in a txt file in a 2 column format
- In the data menu Select import data
- Go to your data folder and select your data file



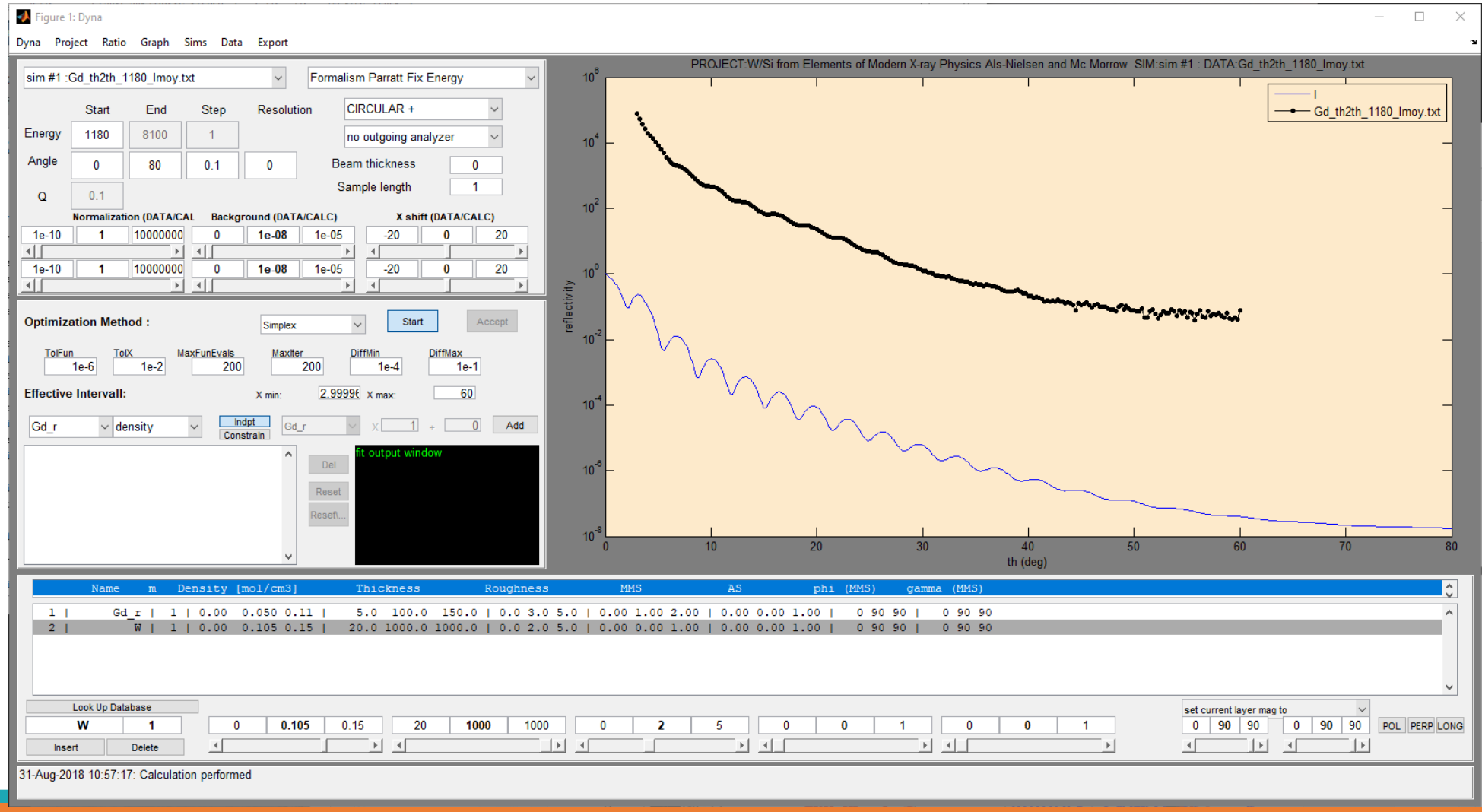
III. How to use DYNA: Play with experimental parameter (1/3)

You should get something like that

You want to adjust roughly your calculation to the data by playing with the experimental parameter

- Normalization
- Background
- X-shift (not for angle scan)

I usually only play with the calc parameter



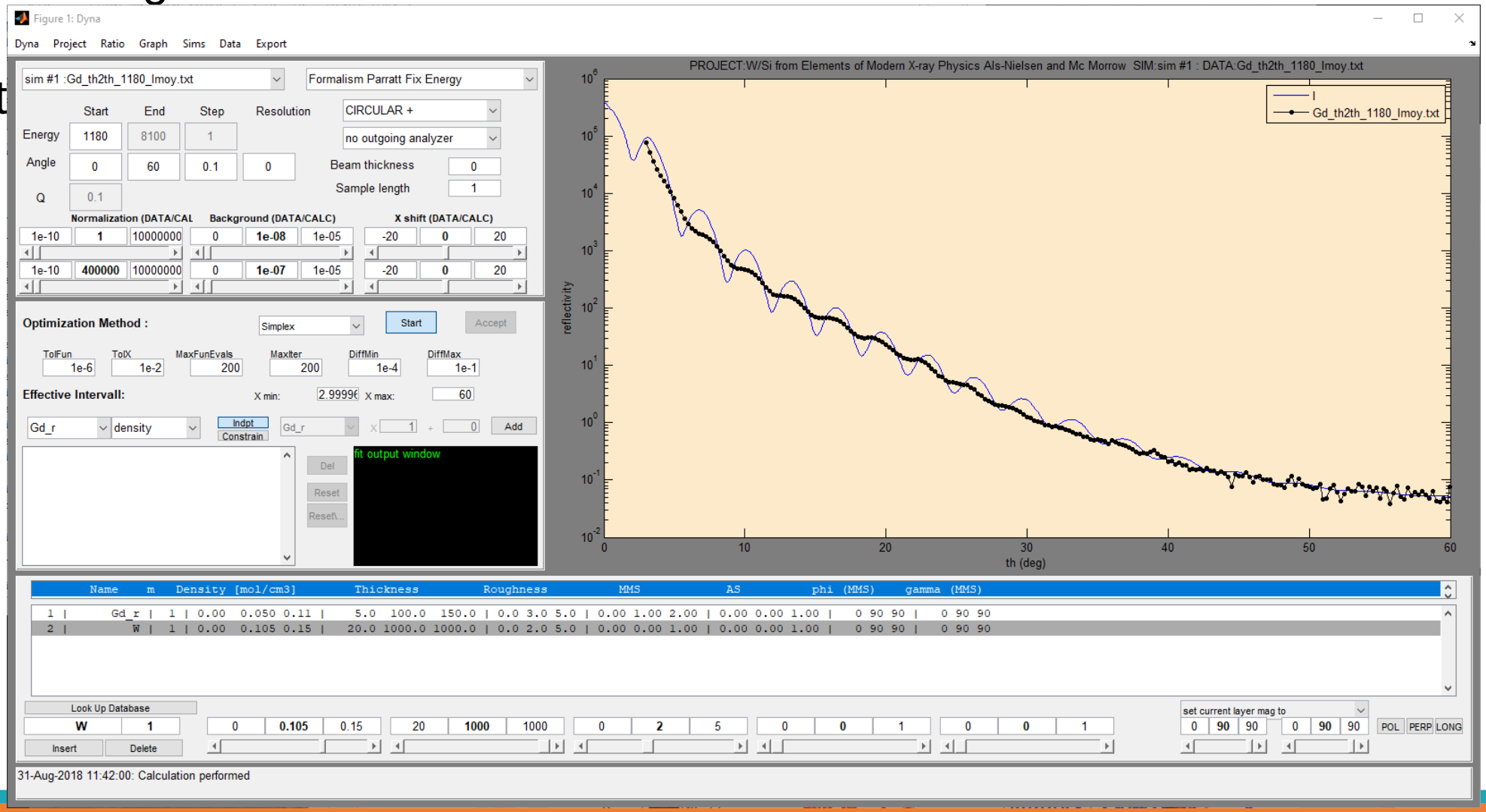
III. How to use DYNA: Play with experimental parameter (2/3)

You should get something like that

You want to adjust roughly your calculation to the data by playing with the experimental parameter

- beam thickness
- Sample length
- Resolution

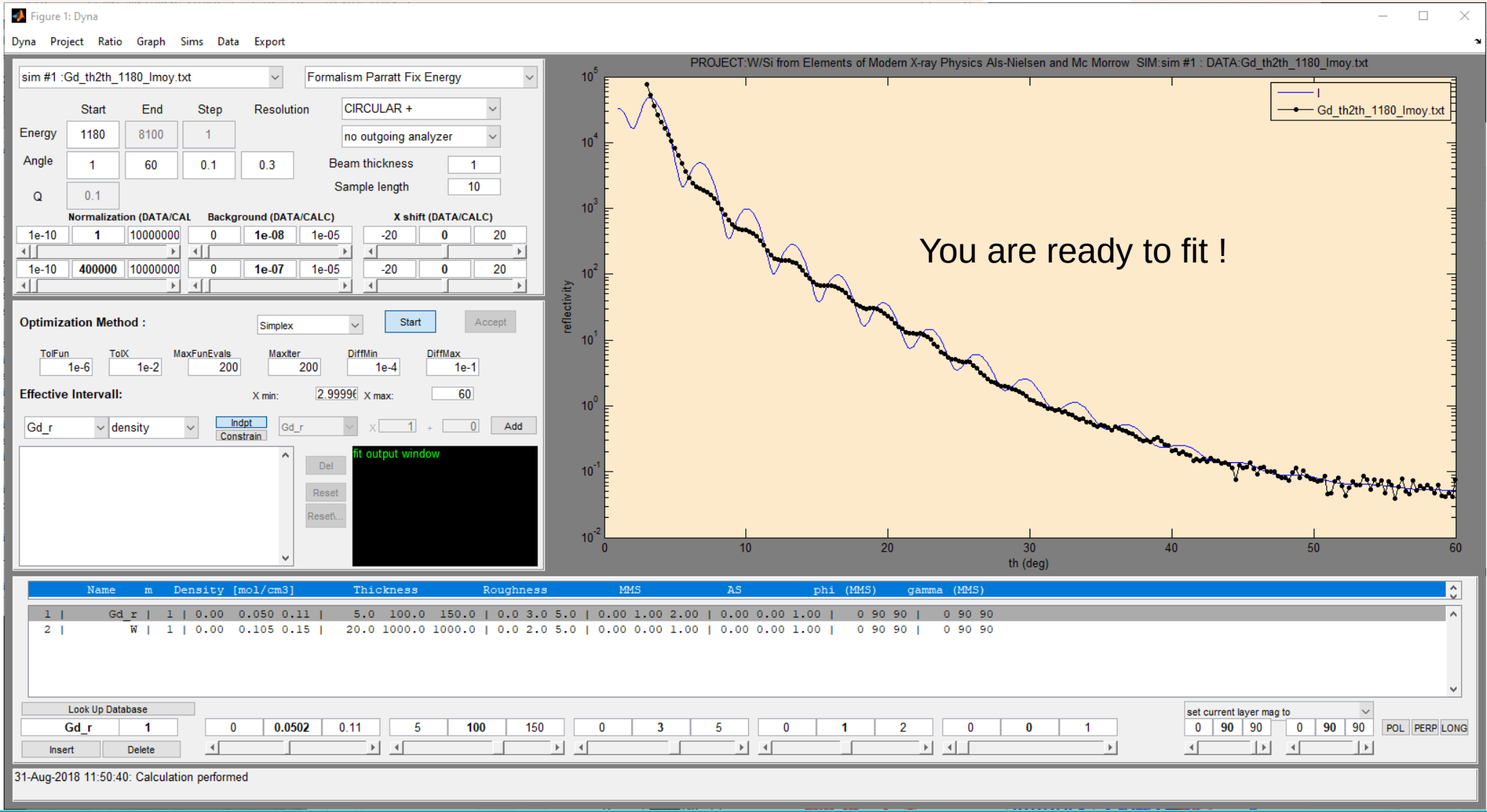
Warning, the resolution and the roughness have a similar effect…



III. How to use DYNA: Play with experimental parameter (3/3)

To save your project and export your simulation:

- Use the Project menu to save and load your project
- Use the export menu to export your simulation



III. How to use DYNA: Fitting generality / strategy (1/2)

In DYNA you can only fit the sample parameter (and not the experimental one)

Since there is a lot of parameter to play with, you need to be careful. Here are some rules and trick I am following

- Do not fit all the parameters together
- Start by structural parameter and Paratt formalism (Use laverage) far from resonance and then at resonance
  - Only thickness
  - Only roughness

  } Do not hesitate to re-iterate those steps
  - Both
  - Density
- Without changing the structure, fit the magnetic parameter with magnetism formalism (Use Asymetry)
  - Only mms, 1 layer
  - Depending on the qualitative analysis, fit the angles
  - Try to divide the magnetic layer

III. How to use DYNA: Fitting generality / strategy (1/2)

- Use several experiment set up at the same time:
  - several energy
  - Reflectivity and asymmetry
- Do not forget to adjust the experimental parameter if you do not succeed to fit properly the roughness

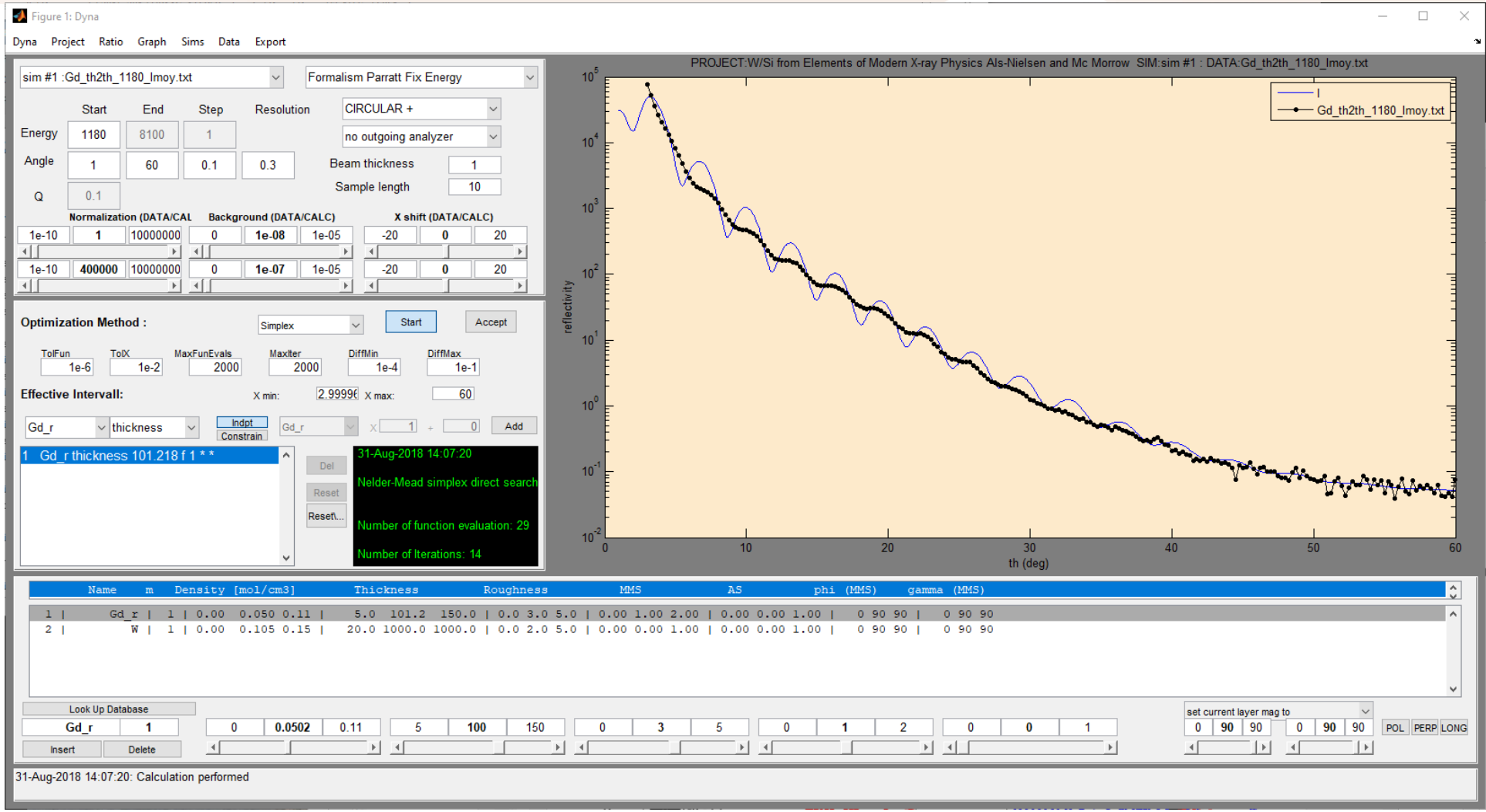
Here a summary on how the parameters influence the most the results

- The thickness plays on the oscillation periodicity
- The roughness plays on the amplitude of the oscillation and decreasing shape
- The density plays on the slope, mainly at small angle
- The mms plays only on the amplitude of the asymmetry.
- The angle plays on the shape accordingly to the kinematic formalism
- If do not succeed to fit the asymmetry at large angle but quite good at low angle, try to make interface magnetic layer.

III. How to use DYNA: Fit example Gd 10 nm on W: structure (1/3)

Fit the thickness of Gd

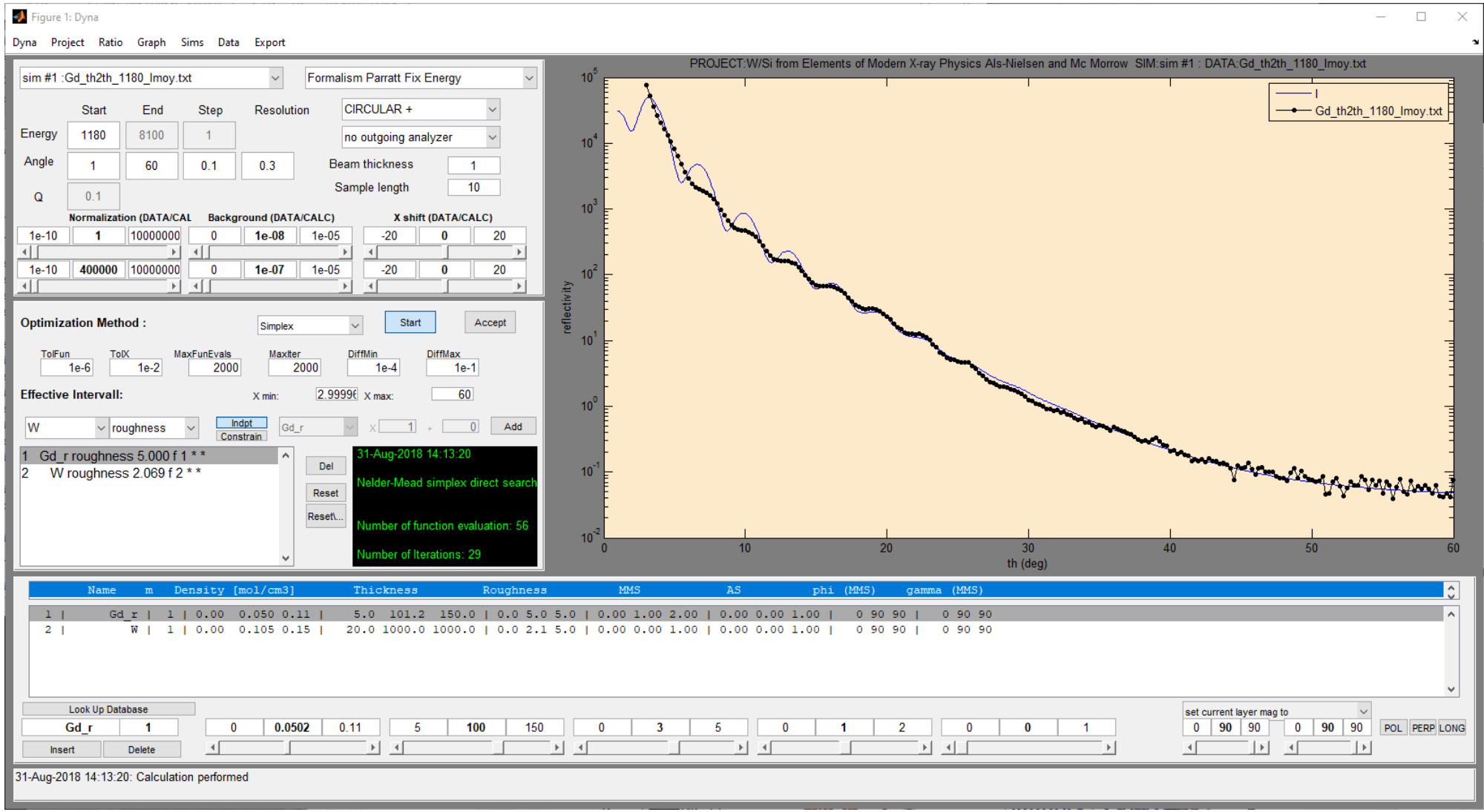
- In the fitting window, select the layer, the parameter, press “add”
- Then “start”, when finished, “accept” or “reset all”
- Increase the “MaxIter” and “MaxFunEvals” if needed



III. How to use DYNA: Fit example Gd 10 nm on W: structure (1/3)

Fit the Roughness

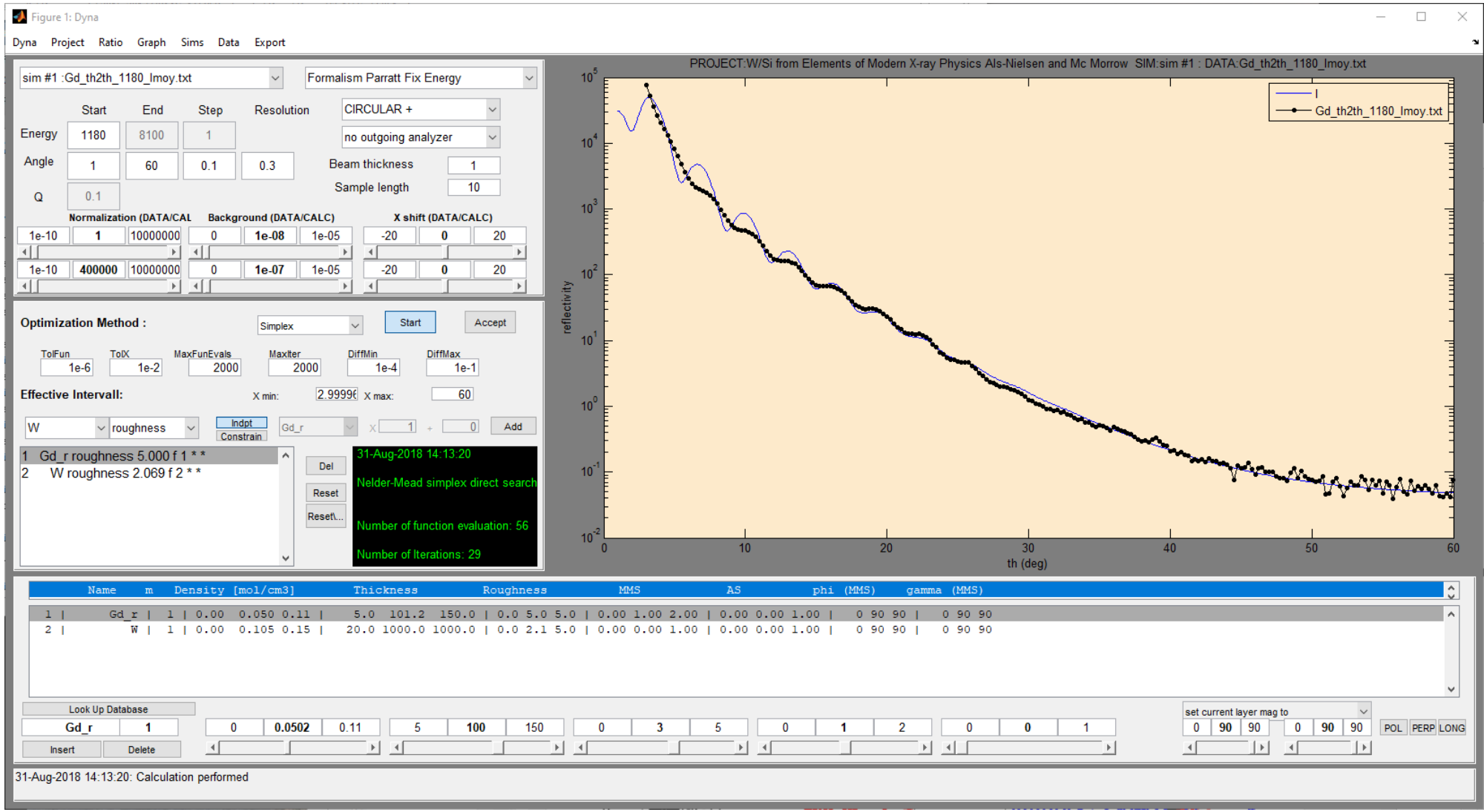
- Delete the fitting parameter thickness
- Add Roughness of Gd_r and W
- Fit



III. How to use DYNA: Fit example Gd 10 nm on W: structure (1/3)

Fit the Roughness

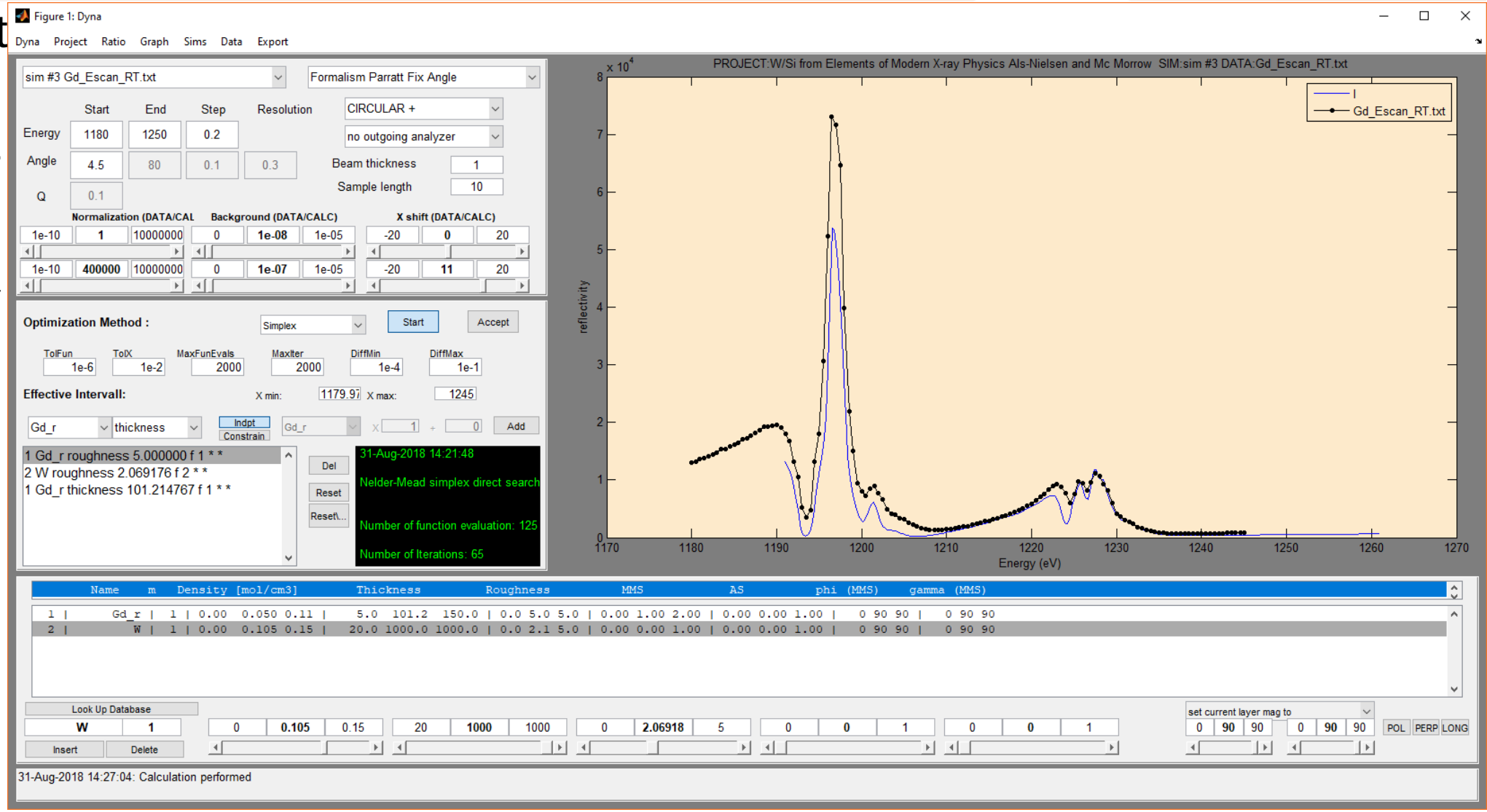
- Delete the fitting parameter thickness
- Add Roughness of Gd_r and W
- Fit, Accept
- Fit both roughness and thickness but looks worst, reset all
- Since oscillations week, Add an energy



III. How to use DYNA: Fit example Gd 10 nm on W: structure (1/3)

Add an energy at resonance

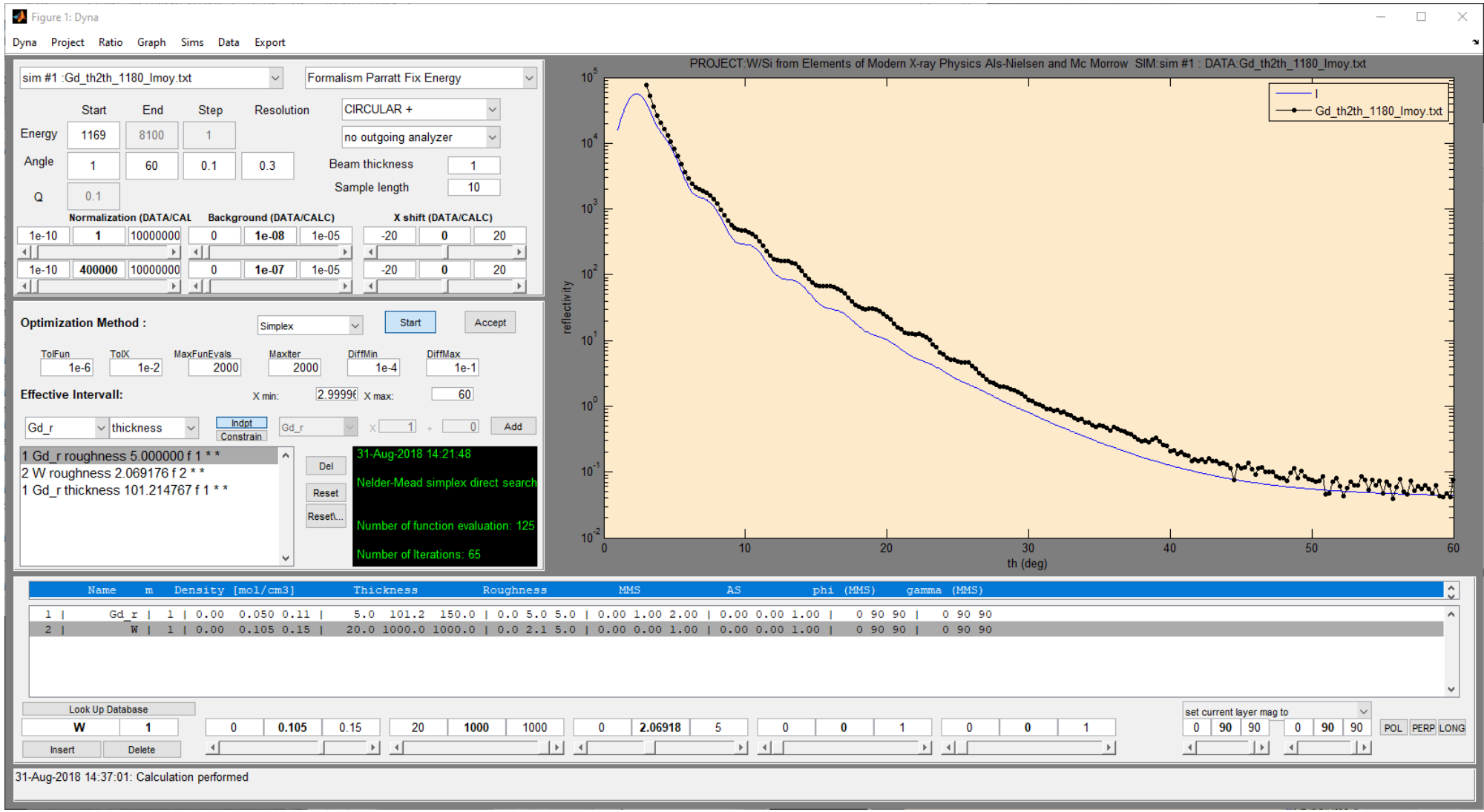
- check the shift in energy!
- 11 eV shift => substarct 11 eV to the experience



III. How to use DYNA: Fit example Gd 10 nm on W: structure (1/3)

Add an energy at resonance

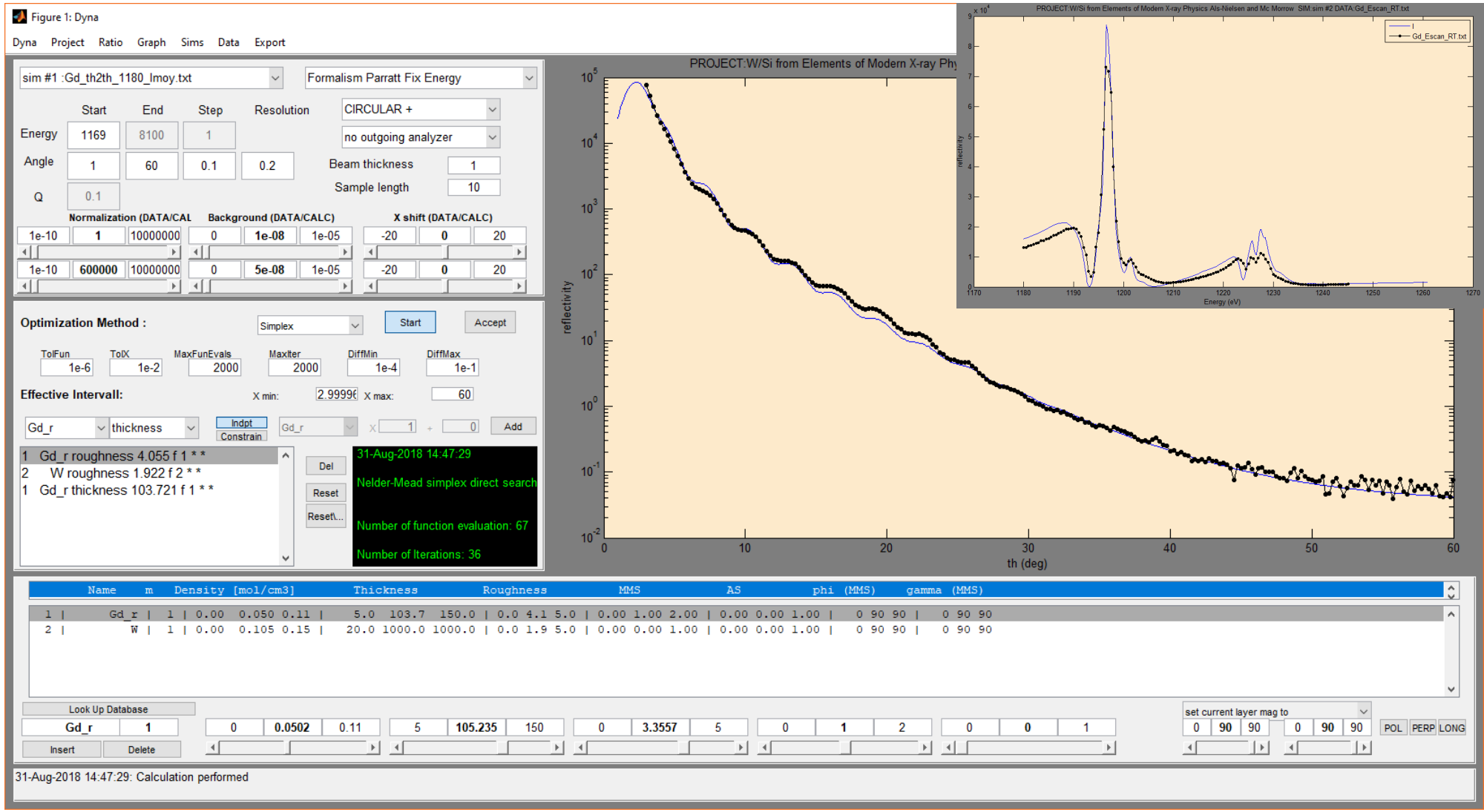
- check back 1180eV (1169 in DYNA)
- Much better!



III. How to use DYNA: Fit example Gd 10 nm on W: structure (1/3)

Add an energy at resonance

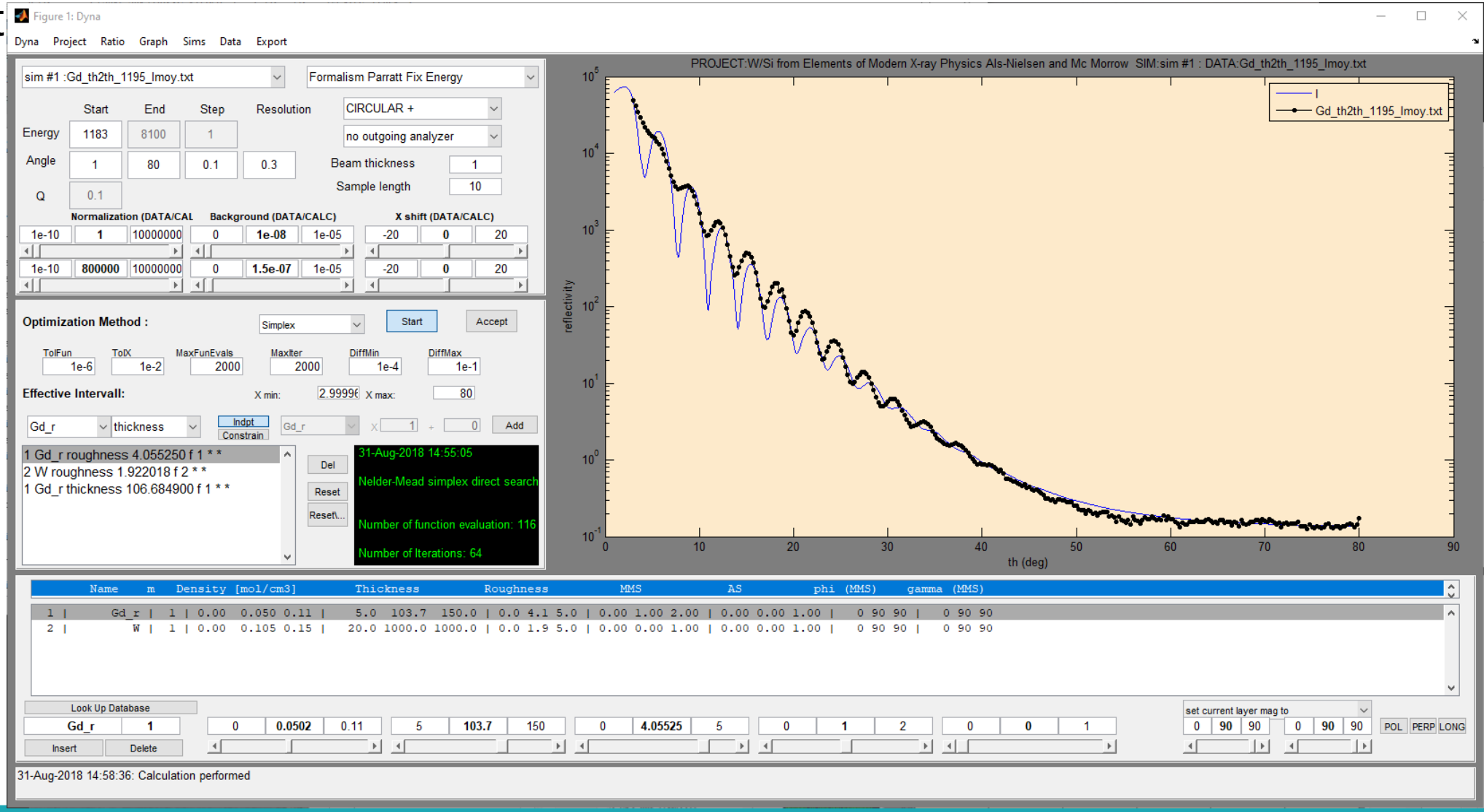
- 1180eV (1169 in DYNA)
- Adjust the normalization and redo fit roughness and normalization



III. How to use DYNA: Fit example Gd 10 nm on W: structure (1/3)

Add an energy at resonance

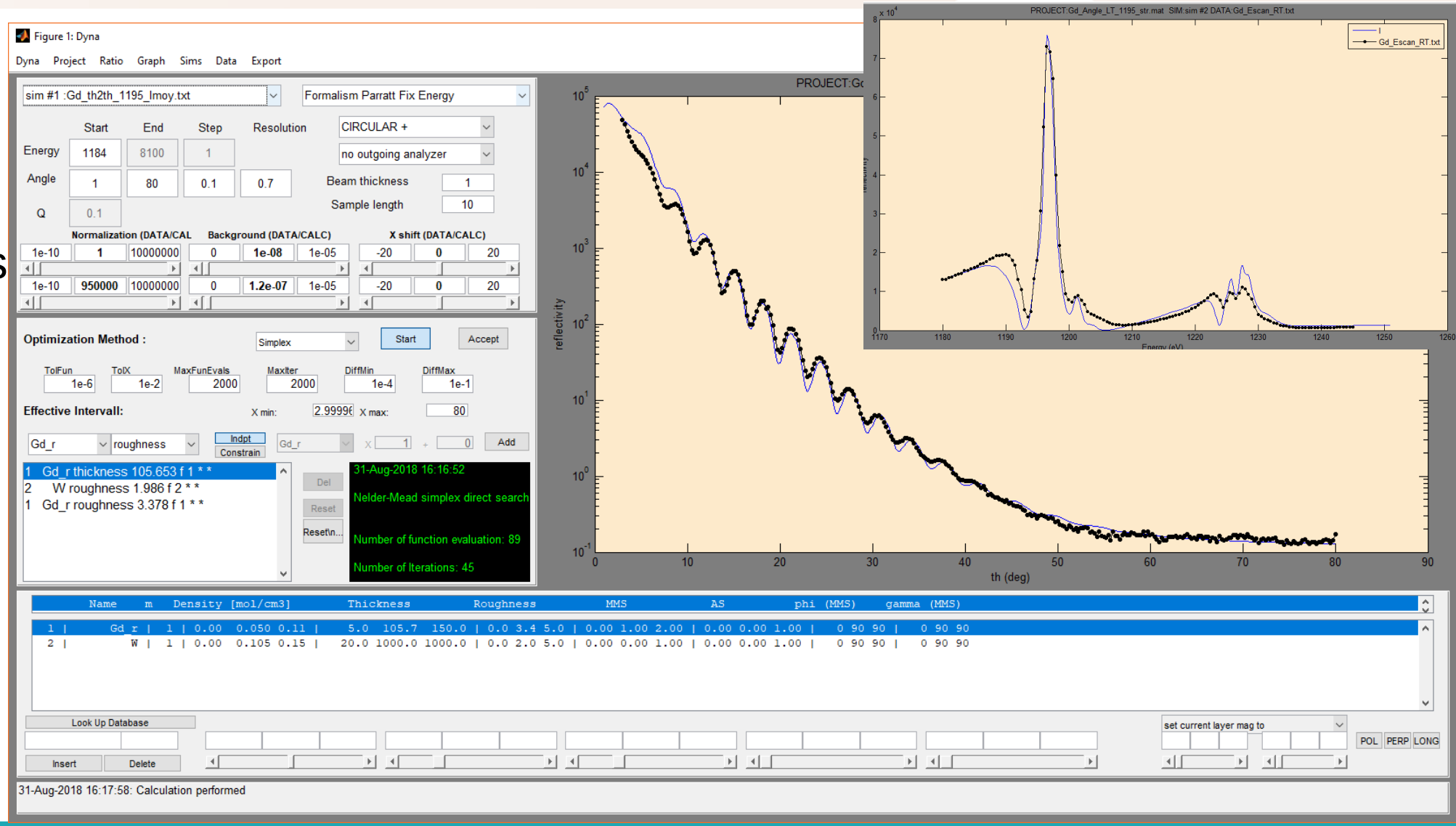
- 1195 eV (1183eV Dyna)
-



III. How to use DYNA: Fit example Gd 10 nm on W: structure (1/3)

Add an energy at resonance

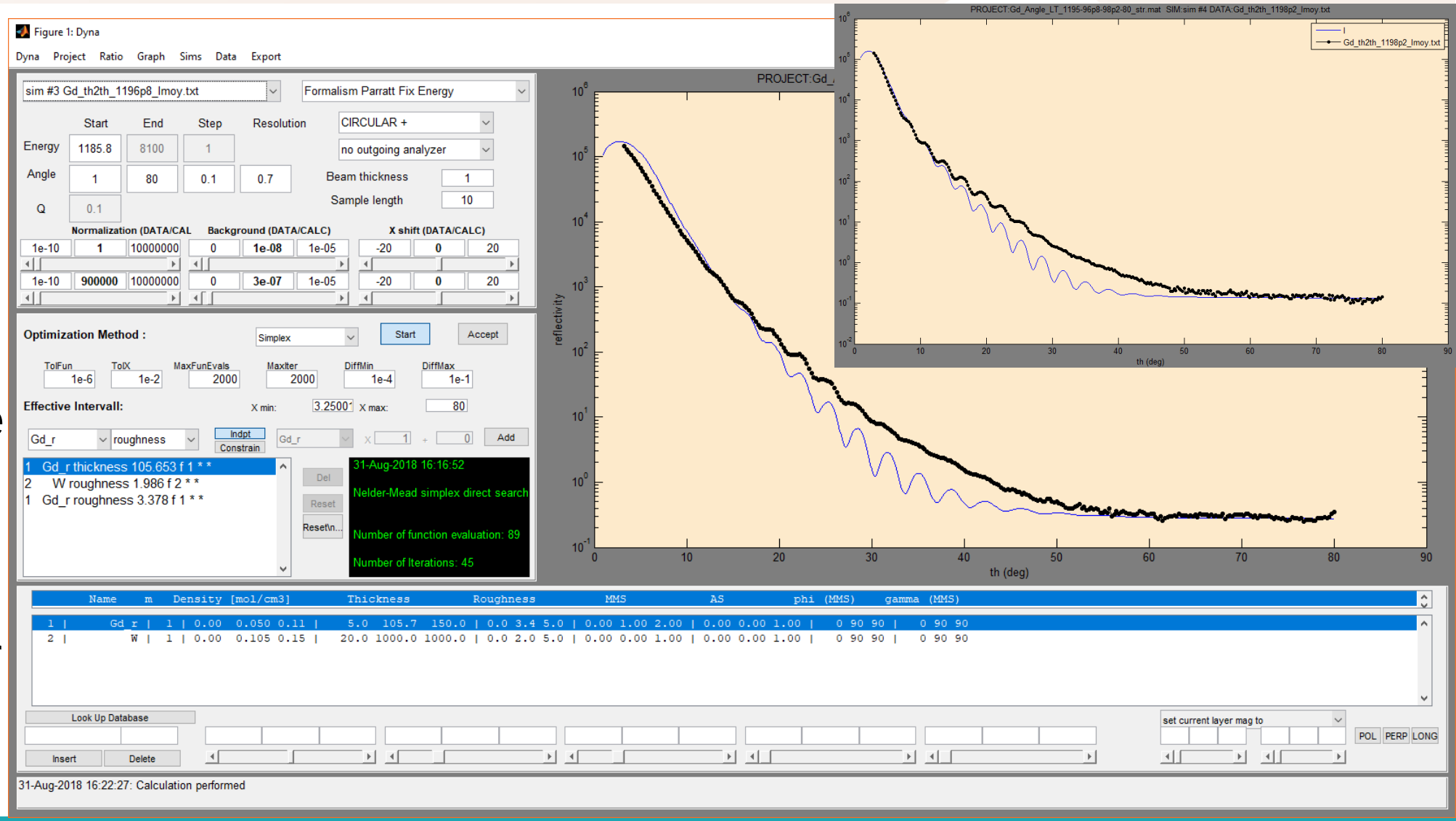
- 1195 eV (1183eV Dyna)
- Start fit only this energy (do not forget to save the previous energy!)
- Check 1180 eV => not so bad
- Check 1196,8 eV



III. How to use DYNA: Fit example Gd 10 nm on W: structure (1/3)

Add an energy at resonance

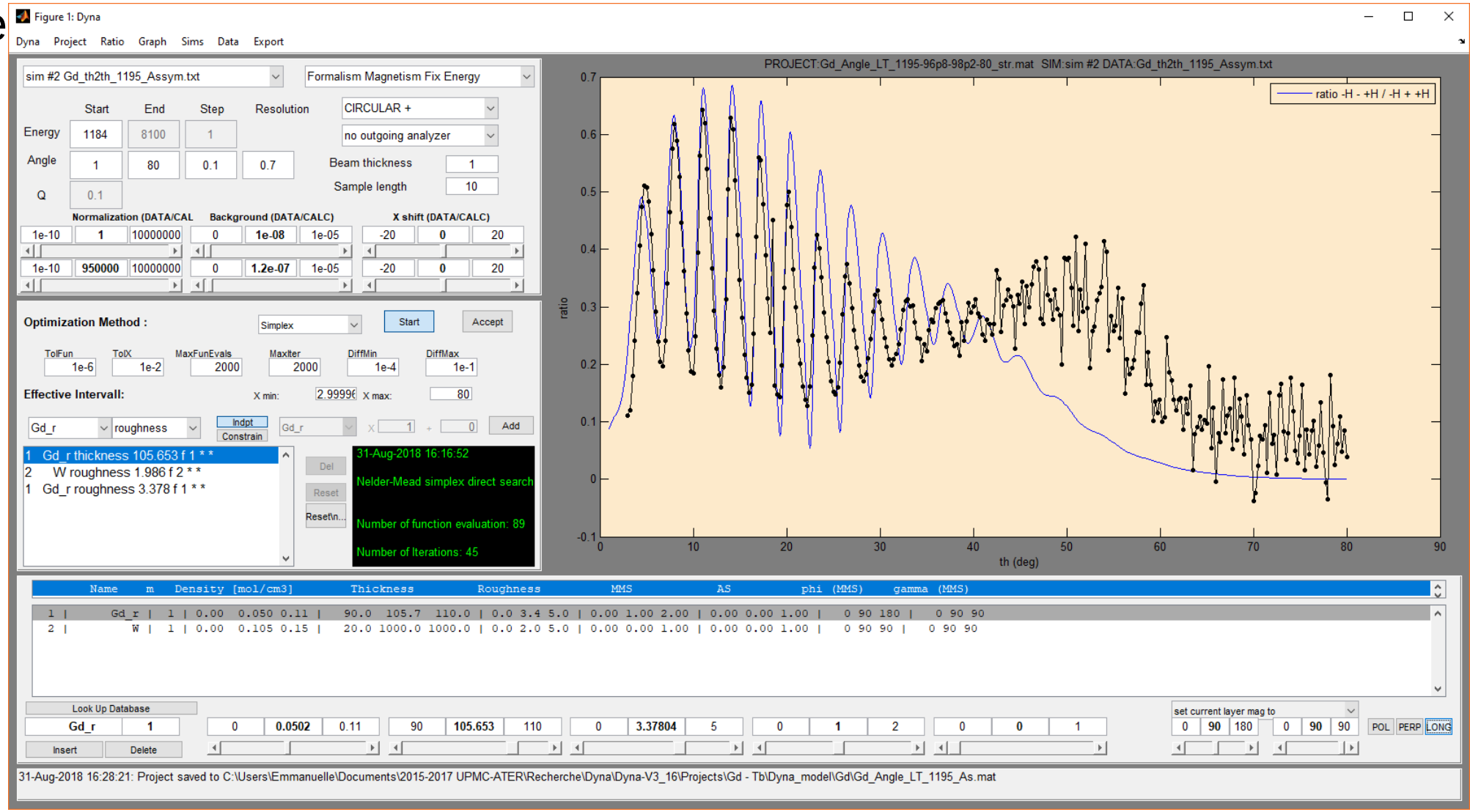
- 1195 eV (1183eV Dyna)
- Check 1196,8 eV and 1198,2
- Not perfect for both. Try to fit all the energy at the same time
- Need to fit each separately, the small difference should give error bars.



III. How to use DYNA: Fit example Gd 10 nm on W: Magnetism (1/3)

From the structure of 1195 eV look at the magnetism formalism and asymetry

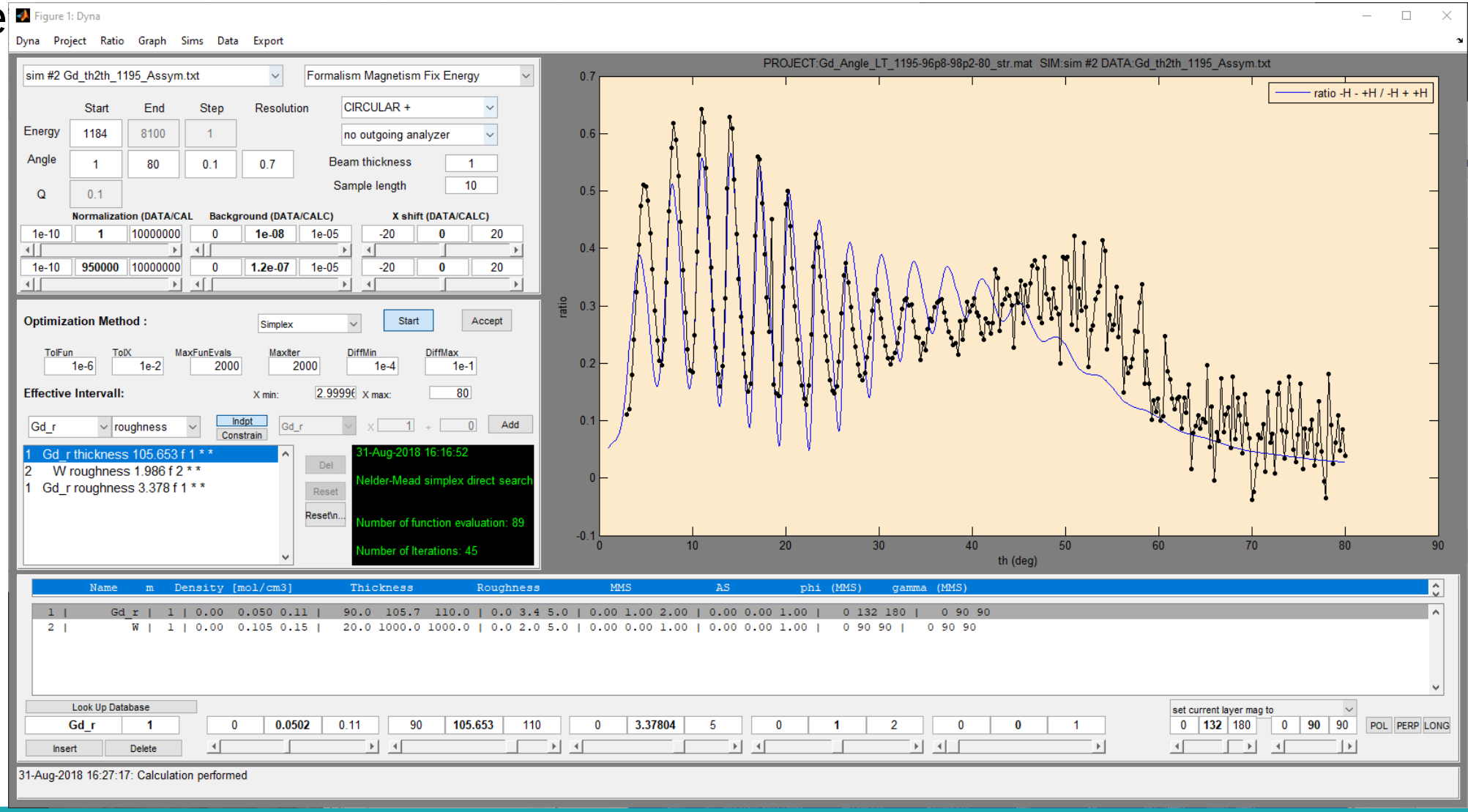
- Longitudinal geometry and mms = 1 => not good at high angle.



III. How to use DYNA: Fit example Gd 10 nm on W: Magnetism (1/3)

From the structure of 1195 eV look at the magnetism formalism and asymetry

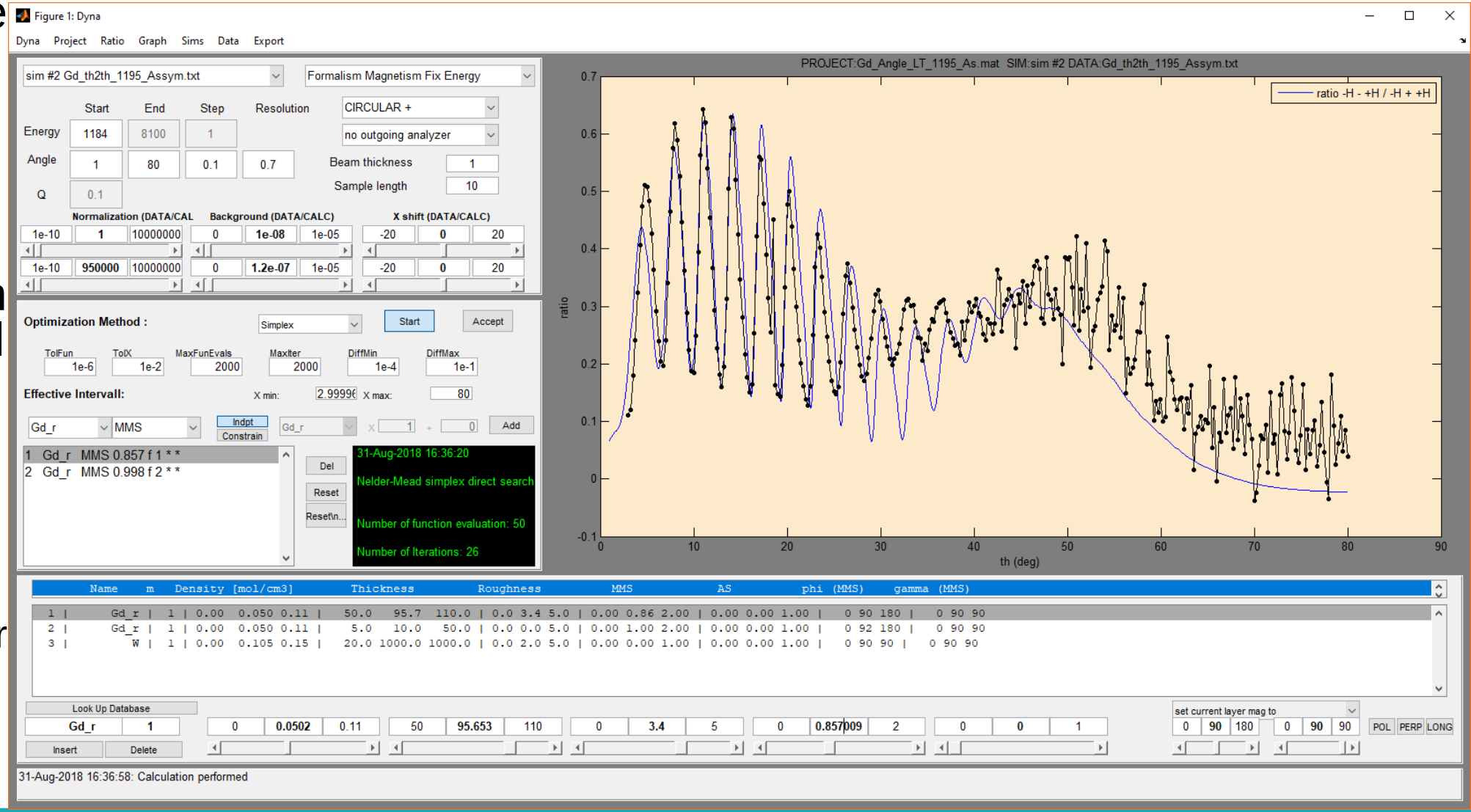
- Try to play with OP angle phi to fit large reflected angle => Better!
- Need to divide the magnetc layer



III. How to use DYNA: Fit example Gd 10 nm on W: Magnetism (1/3)

From the structure of 1195 eV look at the magnetism formalism and asymmetry

- Divide the magnetic layer in 2 (thickness total not changed) 95,7/10
- Fit the 2 mms
- To be continued
  - Check this model for other energy
  - Try 3mms
  - …



Outline

I. Principle of XRMR

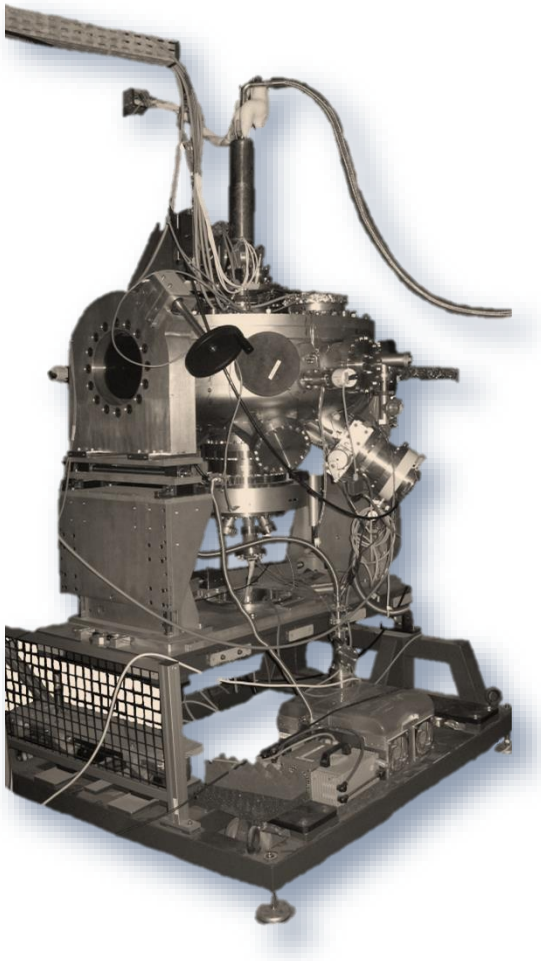
II. Formalism

1. Generality
2. Kinematic
3. Dynamic, what is Dyna doing

III. How to use DYNA a matricial dynamic formalism

1. Entry: Optical constant / Parameter
2. Starting: Build a layer / Set the configuration
3. Fitting: Add experimental data / play with the parameter

IV. Conclusions and Outlook



IV. Conclusion and Outlook

- Normally you have now all the basis to fit.

- It is important to go back and forth between different energy to be sure the model you found is unique and robust.

- The code is still evolving, so check from time to time if there is a new version on the website (http://neel.cnrs.fr/spip.php?article2575). If you have a suggestion, do not hesitate to contact us.

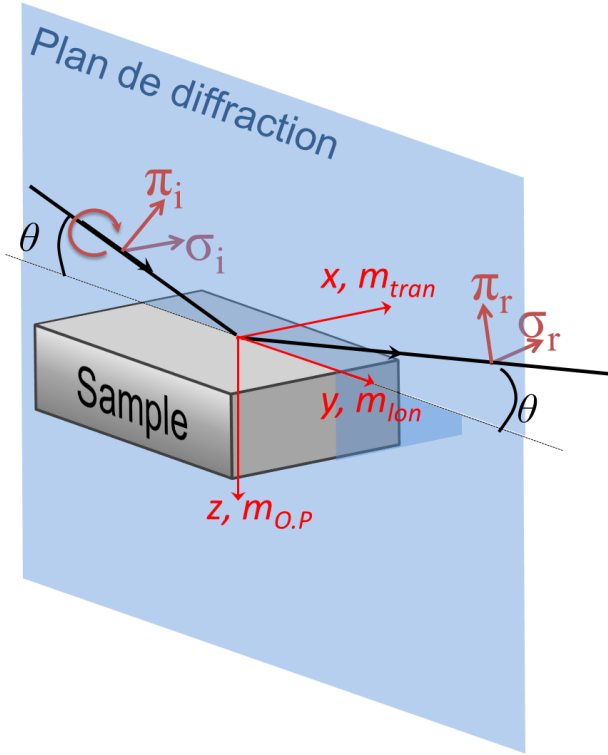
- Please cite this article if you are referring to DYNA in a paper.

  M. Elzo *et al.* JMMM **324**, 105-112 (2012),

Annex: Formalism: Deriving the equation

Resonant atomic scattering factor, f: Hannon *et al.* PRL **61**, 1245 (1989)

$$f(E) = (\mathbf{e}_r^* \cdot \mathbf{e}_i)\underbrace{(f_0 + F'(E) + iF''(E))}_{\text{Charge scattering} = F_c} - i(\mathbf{e}_r^* \times \mathbf{e}_i)\cdot \mathbf{m}\underbrace{(M'(E) + iM''(E))}_{\text{1st order magnetic scattering} = F_m}$$



Matrix expression based on the σ, π polarization states:

- $\boldsymbol{e_i} = \boldsymbol{\sigma}_i$ ou $\boldsymbol{\pi_i}$, et $\boldsymbol{e_r} = \boldsymbol{\sigma_r}$ ou $\boldsymbol{\pi_r}$
- $\hat{f}(E) = \begin{pmatrix} f_{\sigma_i,\sigma_r} & f_{\sigma_i,\pi_r} \\ f_{\pi_i,\sigma_r} & f_{\pi_i,\pi_r} \end{pmatrix}$
- Express $\boldsymbol{\sigma_i}$, $\boldsymbol{\pi_i}$, $\boldsymbol{\sigma_r}$, $\boldsymbol{\pi_r}$ and **m** in the (x,y,z base)
- f_{σ_i,σ_r} is $f(E)$ for $\boldsymbol{e_r} = \boldsymbol{\sigma_r}$ and $\boldsymbol{e_i} = \boldsymbol{\sigma_i}$
- f_{σ_i,π_r} is $f(E)$ for $\boldsymbol{e_r} = \boldsymbol{\pi_r}$ and $\boldsymbol{e_i} = \boldsymbol{\sigma_i}$
- etc. ...

Annex: Formalism: Deriving the equation

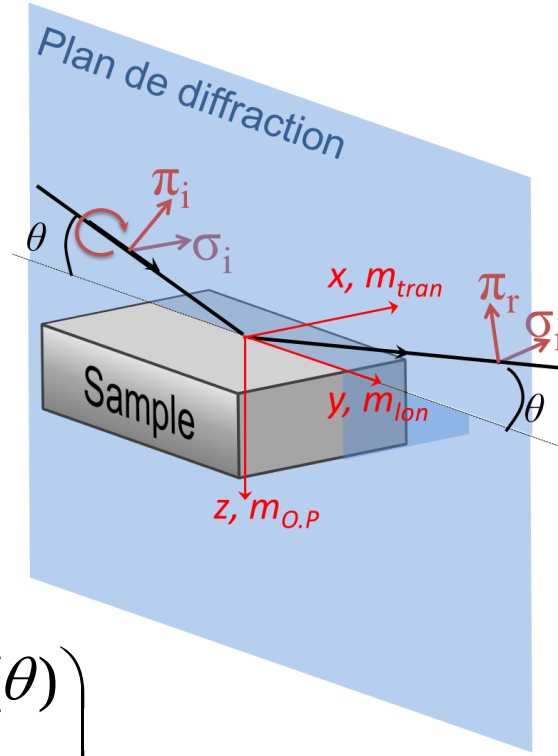
If $f_{e_i e_r} = F_c(\boldsymbol{e_r^*} \cdot \boldsymbol{e_i}) - iF_m(\boldsymbol{e_r^*} \times \boldsymbol{e_i}) \cdot \boldsymbol{m}$ and

$$\boldsymbol{\sigma}_i = \boldsymbol{\sigma}_r = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \boldsymbol{\pi}_i = \begin{pmatrix} 0 \\ \sin(\theta) \\ -\sin(\theta) \end{pmatrix}, \boldsymbol{\pi}_r = \begin{pmatrix} 0 \\ -\sin(\theta) \\ -\sin(\theta) \end{pmatrix}, et\ \boldsymbol{m} = \epsilon \begin{pmatrix} m_{tran} \\ m_{lon} \\ m_{O.P} \end{pmatrix} \text{ avec } \epsilon = \pm 1$$

Then

- $f_{\sigma_i,\sigma_r} = F_c$
- $f_{\sigma_i,\pi_r} = -i\epsilon F_m(m_{lon}\cos(\theta) + m_{O.P}\sin(\theta))$
- $f_{\pi_i,\sigma_r} = -i\epsilon F_m(m_{O.P}\sin(\theta) - m_{lon}\cos(\theta))$
- $f_{\pi_i,\pi_r} = F_c\cos(2\theta) + i\epsilon F_m\, m_{tran}\sin(2\theta)$

(A)



and

$$f(E) = F_c\begin{pmatrix} 1 & 0 \\ 0 & \cos(2\theta) \end{pmatrix} - iF_m\begin{pmatrix} 0 & m_{lon}\cos(\theta) + m_{O.P}\sin(\theta) \\ -m_{lon}\cos(\theta) + m_{O.P}\sin(\theta) & -m_{tran}\sin(2\theta) \end{pmatrix}$$

Annex: Formalism: Deriving the equation

From this resonant scattering factor, the reflected intensity can be calculated since $I \propto \left|\sum_j f_j e^{i\boldsymbol{Q}\boldsymbol{r}_j}\right|^2$. The reflected intensity can be decomposed in the σ_r, π_r basis and in the approximation that the scattering factor is independent of the atom, one find:

$$I = I_{\sigma_r} + I_{\pi_r} = \left|f_{\sigma_r}\right|^2 + \left|f_{\pi_r}\right|^2$$

For a general initial polarization, the resonant scattering factor can be written

$$\hat{f}_{\boldsymbol{e}} = \begin{pmatrix} f_{\sigma_i,\sigma_r} & f_{\sigma_i,\pi_r} \\ f_{\pi_i,\sigma_r} & f_{\pi_i,\pi_r} \end{pmatrix} \cdot \begin{pmatrix} \delta e_\sigma \\ -ie_\pi \end{pmatrix} = \begin{pmatrix} \delta e_\sigma f_{\sigma_i,\sigma_r} - ie_\pi f_{\sigma_i,\pi_r} \\ \delta e_\sigma f_{\pi_i,\sigma_r} - ie_\pi f_{\pi_i,\pi_r} \end{pmatrix} = \begin{pmatrix} f_{\sigma_r} \\ f_{\pi_r} \end{pmatrix}$$

Developing the equation and neglecting the magnetic term of order 2 or more one find the general expression of the reflected intensity with δ and ε = +/-1 and e_σ and e_π = 0 or 1

$$I_\delta^\epsilon = [e_\sigma^2 + e_\pi^2 \cos(2\theta)]|F_c|^2 + \epsilon\{e_\pi^2 m_{tran} \sin(4\theta)[F''M' -$$