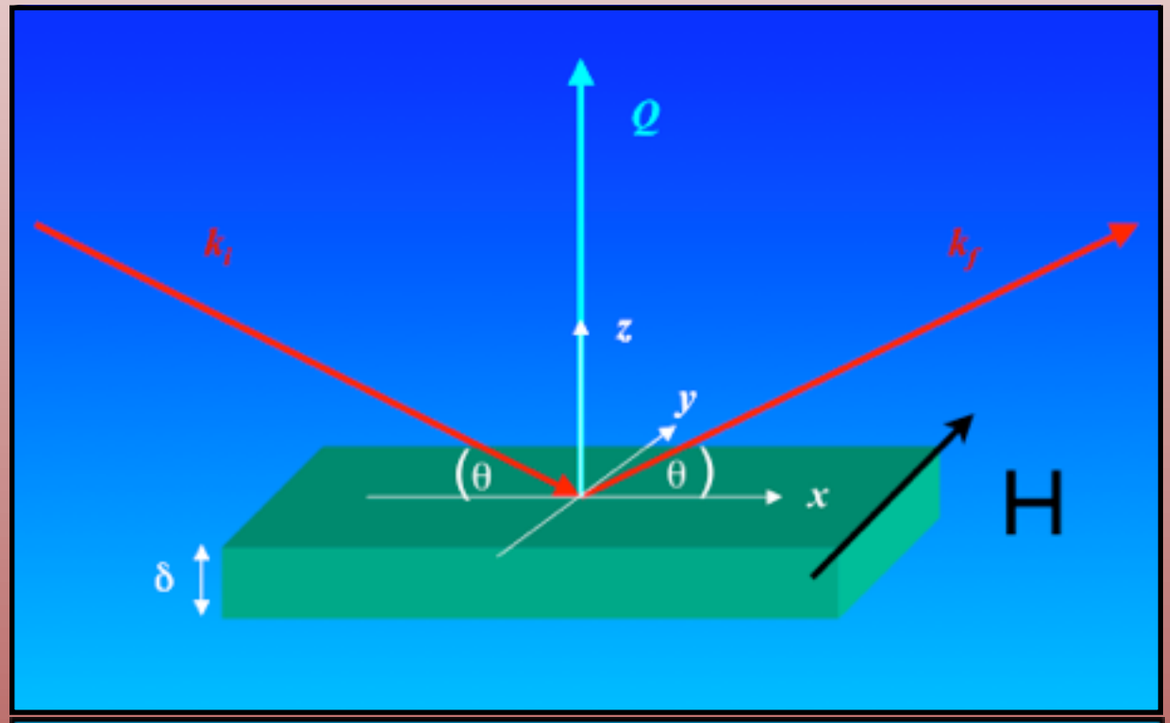
polarization analysis of specular neutron reflectivity

2009 NIST Center for Neutron Research Tutorial on Neutron Reflectometry

National Institute of Standards and Technology

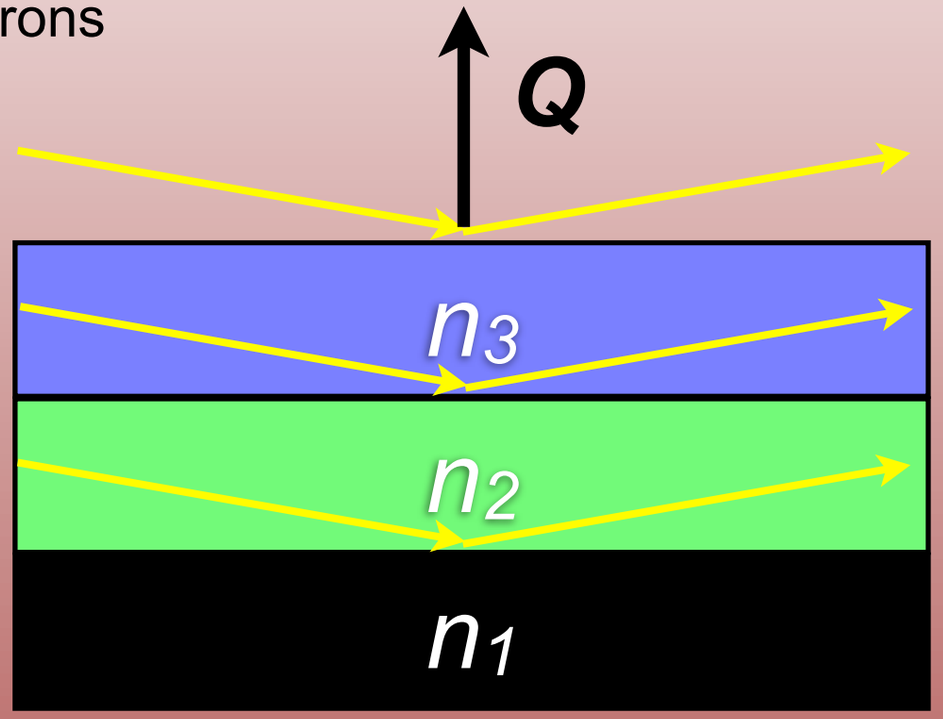
specular neutron reflectivity

- thin film or multilayer samples (flat slabs)
- polarize neutrons relative to guide field *H*
- measure intensity of neutron beam as a function of wavevector transfer
  - $Q = 4\pi \sin\theta/\lambda$
- specular: incident angle = exit angle
- *Q* along *z* - no in-plane momentum transfer
- special case
  - 1-D problem
  - Schrödinger equation for the neutron wavefunction is *exactly* solvable:
  - $[\partial^2/\partial z^2 + n(z)^2 k_0^2]\Psi = 0$
  - $R(Q_z)$ is a function *only* of $n(z)$
  - $n(z)^2 = 1 - 4\pi\rho(z) / k_0^2$



ρ: scattering length density

- $n(z)^2 = 1 - 4\pi\rho(z) / k_0^2$
  - ρ: scattering length density
  - interfaces between regions of differing n reflect neutrons
  - ***contrast*** in ρ produces features in R
  - $\rho_{total} = \rho_{nuclear} + \rho_{magnetic}$
- nuclear scattering length density
  - $\rho(z)_{nuc} = \sum_i N(z)_i * b(z)_i$
  - summation is over each constituent isotope
  - N is number density
  - b is nuclear scattering length
    - b is a measure of neutron-nuclei interaction
    - known values - just look 'em up
- magnetic scattering length density
  - $\rho(z)_{mag} = C*M(z)$
  - constant C
  - M is magnetization (magnetic moment per unit volume)
- ***$R(Q_z)$ sensitive to structural and magnetic depth profiles!***
- how does it all come together?



National Institute of Standards and Technology

spin-dependent reflectivities

•we consider polarized neutrons, spin-up (+) or spin-down (-) relative to in-plane ***H***

•we also have spin *analysis* such that we can choose to measure only + or only -

•angle Φ between vectors ***M*** and ***H*** (i.e. between ***M*** and neutron spin axis)

•two types of scattering processes

-non spin-flip

-consider in the Born Approximation

$$|R(Q_z)^{\pm\pm}|^2 \propto |b(z) \pm C^*M(z)\cos\Phi(z)|^2$$

-projection of ***M***(z) parallel to neutron spin axis causes R^{++} and R^{--} to be different

-spin-flip

-purely magnetic in origin

$$|R(Q_z)^{-+}|^2 = |R(Q_z)^{+-}|^2 \propto |C^*M(z)\sin\Phi(z)|^2$$

-projection of in-plane ***M***(z) perpendicular to neutron spin axis gives spin-flip reflectivity

•what about out of plane components of ***M***?

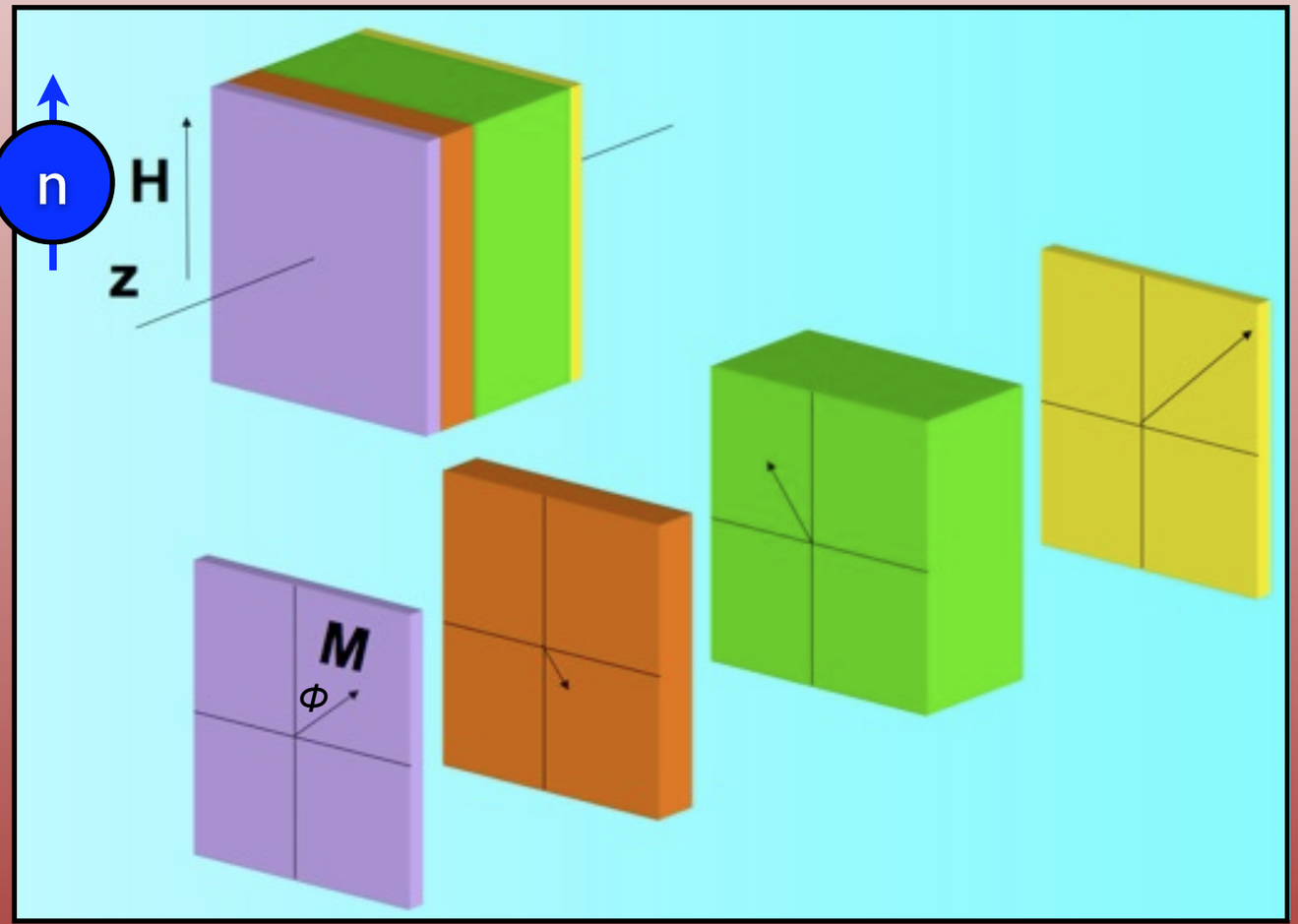
-neutrons do not scatter from ***M*** parallel to ***Q***!

•reflectometry with ***un***polarized neutrons also sensitive to magnetization

-incident and scattered beams have + and -

-magnetic profile is vague

-vector magnetic depth profiling is impossible



National Institute of Standards and Technology

spin-dependent reflectivities

•we consider polarized neutrons, spin-up (+) or spin-down (-) relative to in-plane ***H***

•we also have spin *analysis* such that we can choose to measure only + or only -

•angle Φ between vectors ***M*** and ***H*** (i.e. between ***M*** and neutron spin axis)

these are the pnr magnetic selection rules

•two types of scattering processes

-*non spin-flip*

-consider in the Born Approximation

$$|R(Q_z)^{\pm\pm}|^2 \propto |b(z) \pm C^*M(z)\cos\Phi(z)|^2$$

-projection of ***M***(z) parallel to neutron spin axis causes R^{++} and R^{--} to be different

-*spin-flip*

-*purely* magnetic in origin

$$|R(Q_z)^{-+}|^2 = |R(Q_z)^{+-}|^2 \propto |C^*M(z)\sin\Phi(z)|^2$$

-projection of in-plane ***M***(z) perpendicular to neutron spin axis gives spin-flip reflectivity

•what about out of plane components of ***M***?

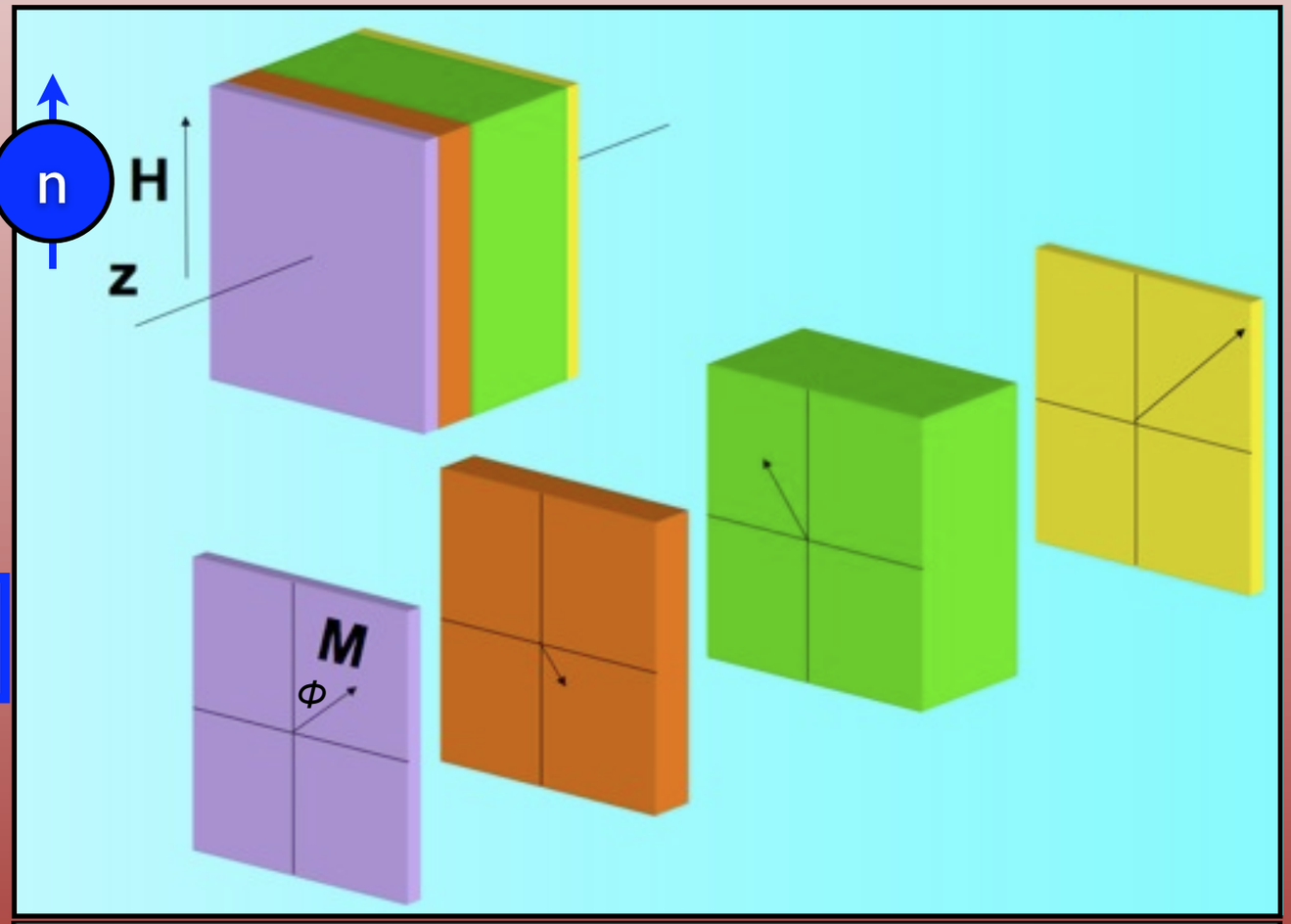
-neutrons do not scatter from ***M*** parallel to ***Q***!

•reflectometry with ***un***polarized neutrons also sensitive to magnetization

-incident and scattered beams have + and -

-magnetic profile is vague

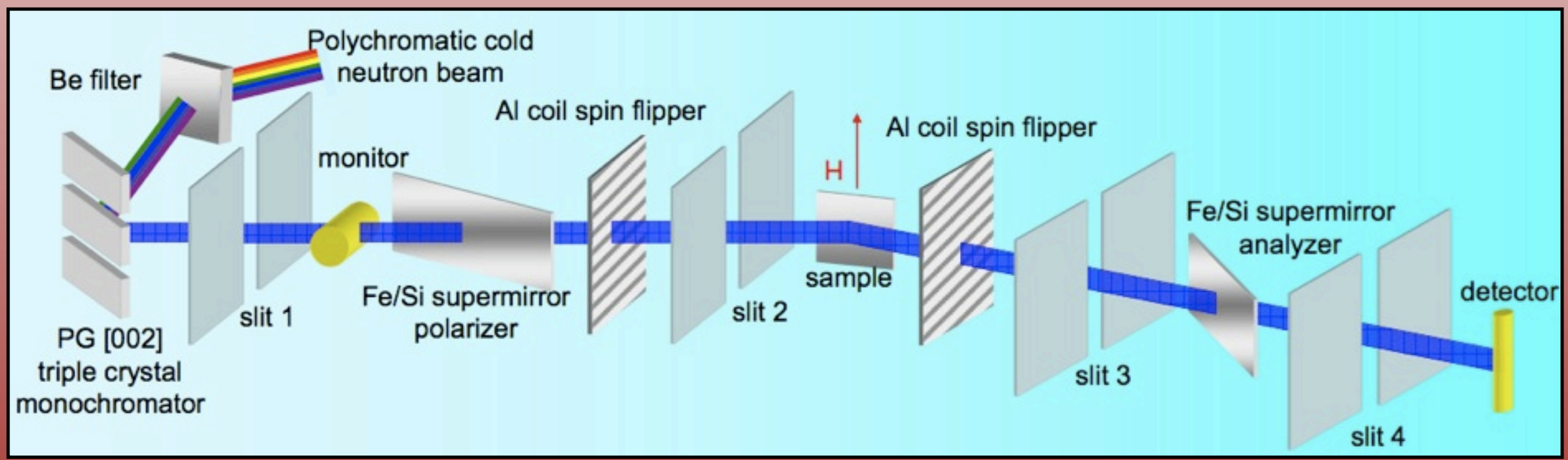
-vector magnetic depth profiling is impossible



National Institute of Standards and Technology

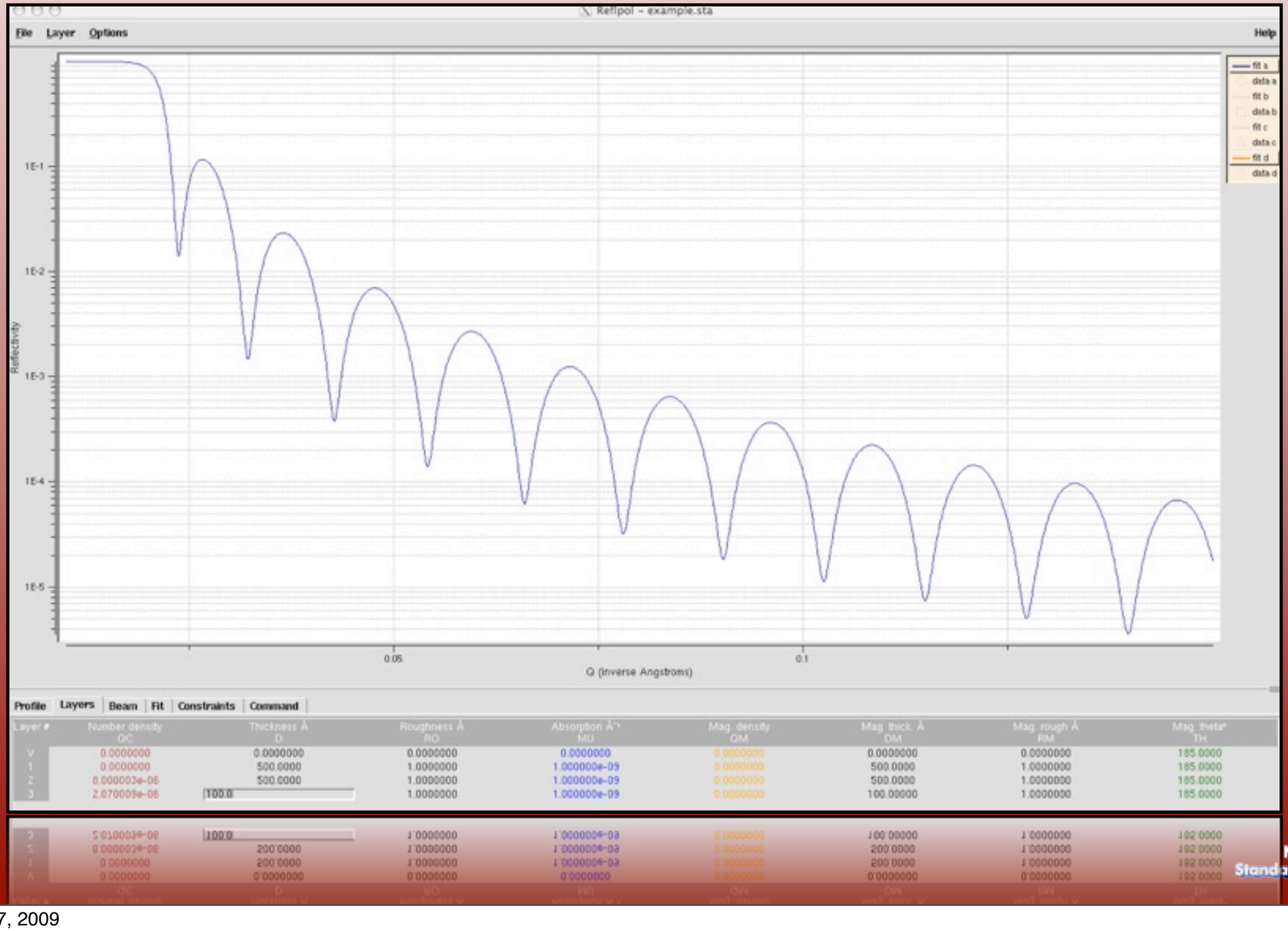
a neutron reflectometer

- NG1 polarized beam reflectometer
- like AND/R, without the PSD
  - optimized for high resolution specular measurements
- λ = 4.75 Å



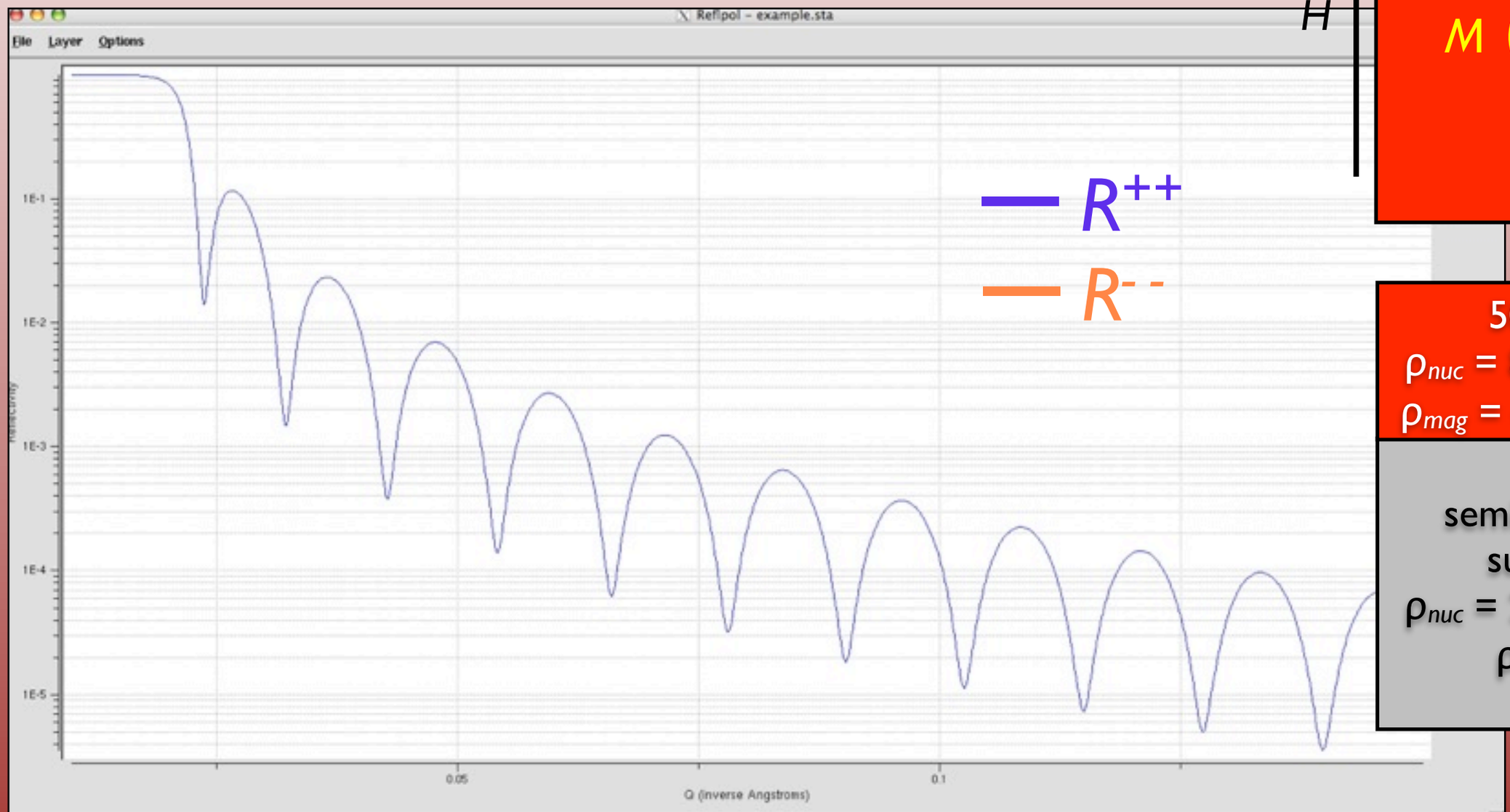
model fitting

- we typically rely on model fitting to extract information about samples
- physical properties are extracted from scattering length density profiles
- *Reflpol,* in-house software (*exact calculations*, not Born Approximation)



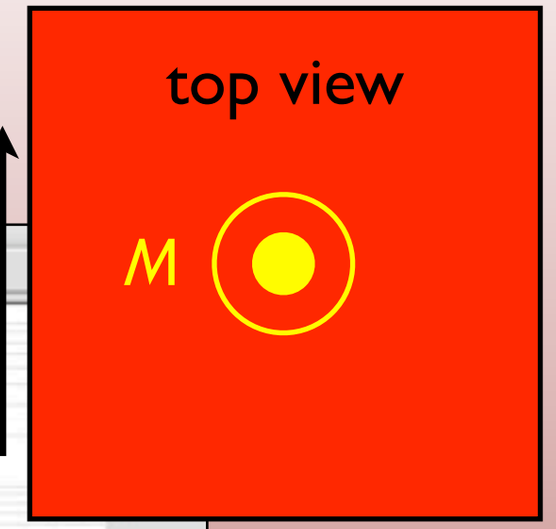
M out of plane

- Co on Si, ***M*** totally out of plane (invisible)
- critical edge comes from "net" sld
- $Q = 4\pi \sin\theta/\lambda$, R "automatically" falls off as Q^4
- $d \approx 2\pi / \Delta Q$
- amplitude comes from layer contrast
- roughness makes R falloff faster with Q
- R^{++} and R^{--} identical
- no spin flip, $R^{+-} = R^{-+} = 0$



R^{++}

R^{--}



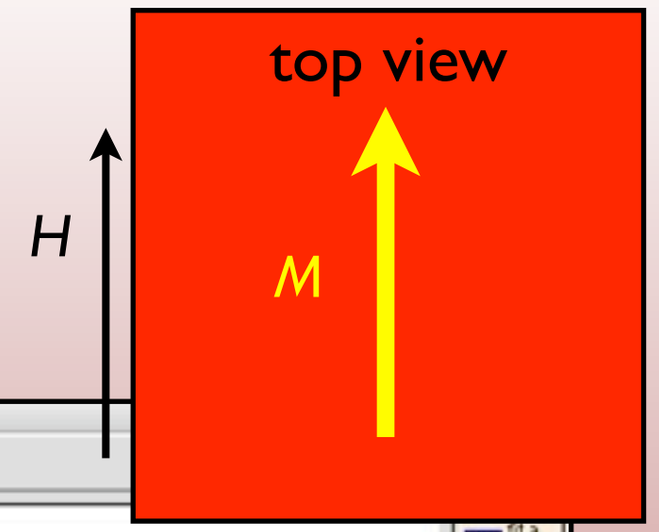
500 Å Fe
$\rho_{nuc} = 8.00 \times 10^{-6}$ Å^{-1}
$\rho_{mag} = 4.97 \times 10^{-6}$ Å^{-1}

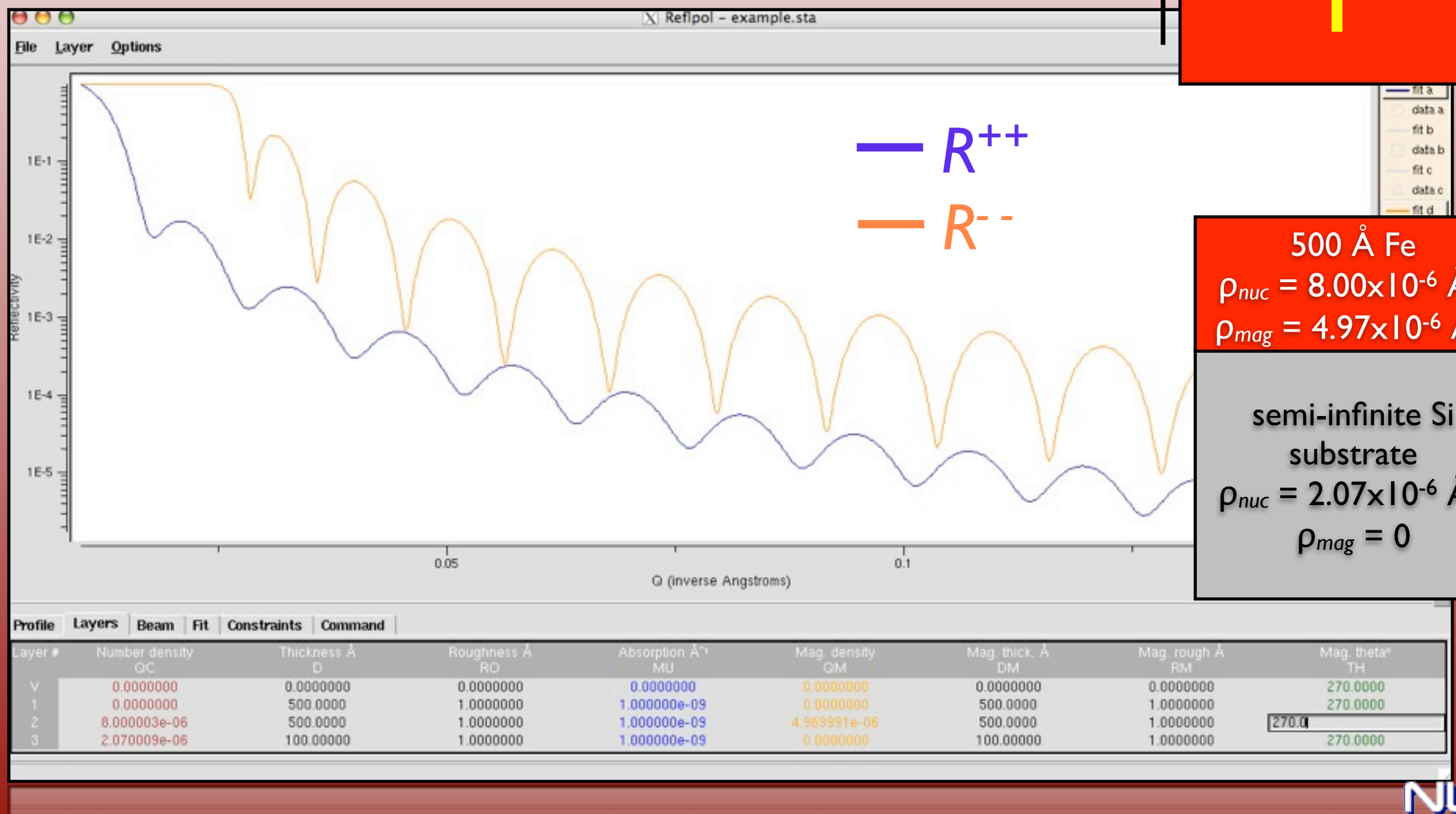
semi-infinite Si substrate
$\rho_{nuc} = 2.07 \times 10^{-6}$ Å^{-1}
$\rho_{mag} = 0$

NIST National Institute of Standards and Technology

M parallel to *H*

- R^{++} and R^{--} are split
- R^{++} and R^{--} have different critical edges
- no spin flip, $R^{+-} = R^{-+} = 0$





— R^{++}

— R^{--}

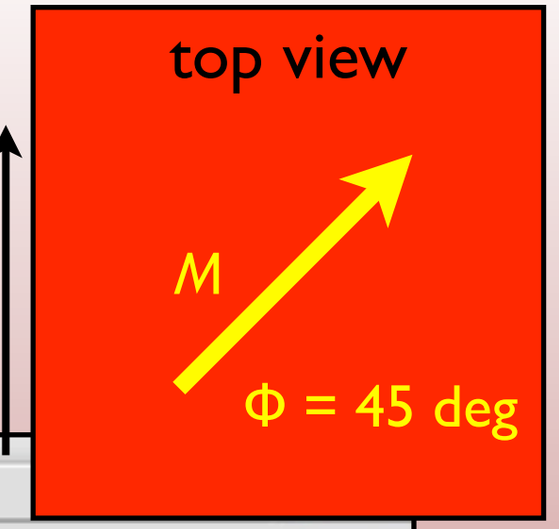
500 Å Fe
ρ_{nuc} = 8.00x10^{-6} Å^{-1}
ρ_{mag} = 4.97x10^{-6} Å^{-1}

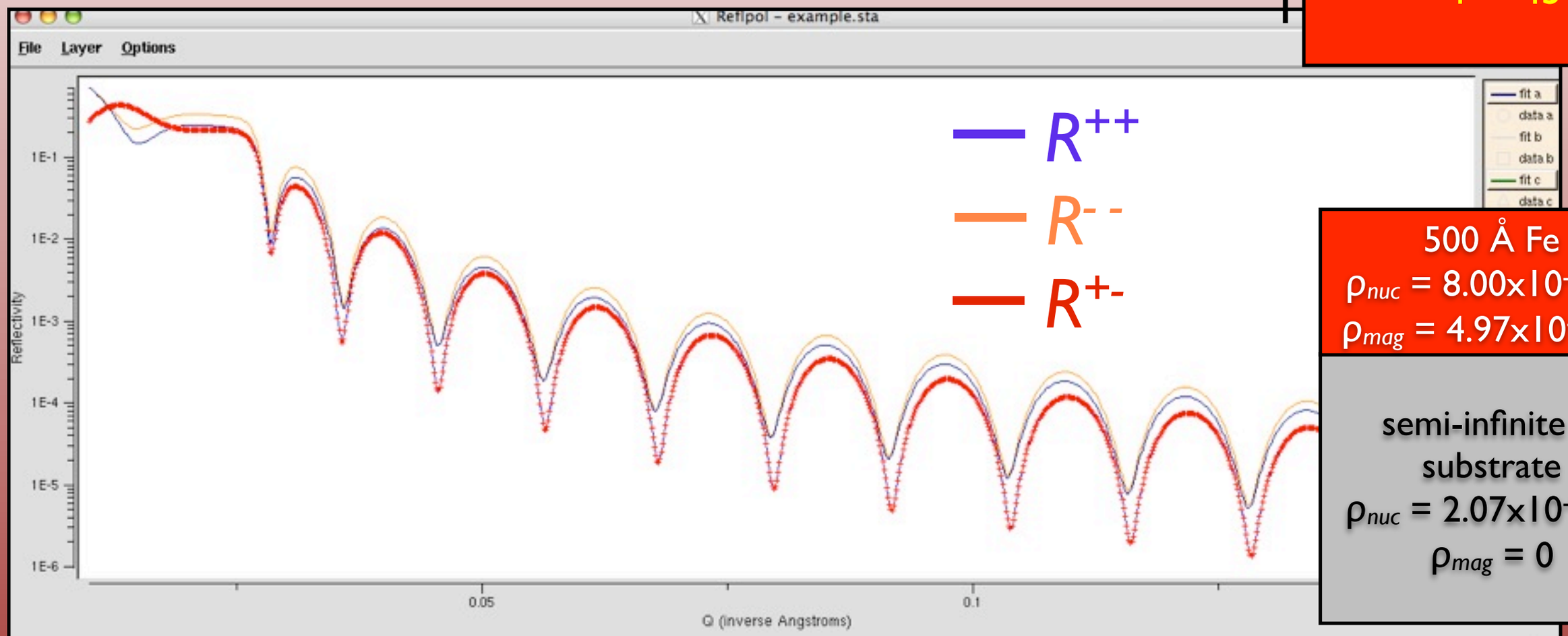
semi-infinite Si substrate
ρ_{nuc} = 2.07x10^{-6} Å^{-1}
ρ_{mag} = 0

NIST National Institute of Standards and Technology

M 45 deg from *H*

- R^{++} and R^{--} splitting is reduced
- $R^{+-} = R^{-+}$ has periodicity of Fe layer





500 Å Fe
ρ_{nuc} = 8.00x10^{-6} Å^{-1}
ρ_{mag} = 4.97x10^{-6} Å^{-1}

semi-infinite Si substrate
ρ_{nuc} = 2.07x10^{-6} Å^{-1}
ρ_{mag} = 0

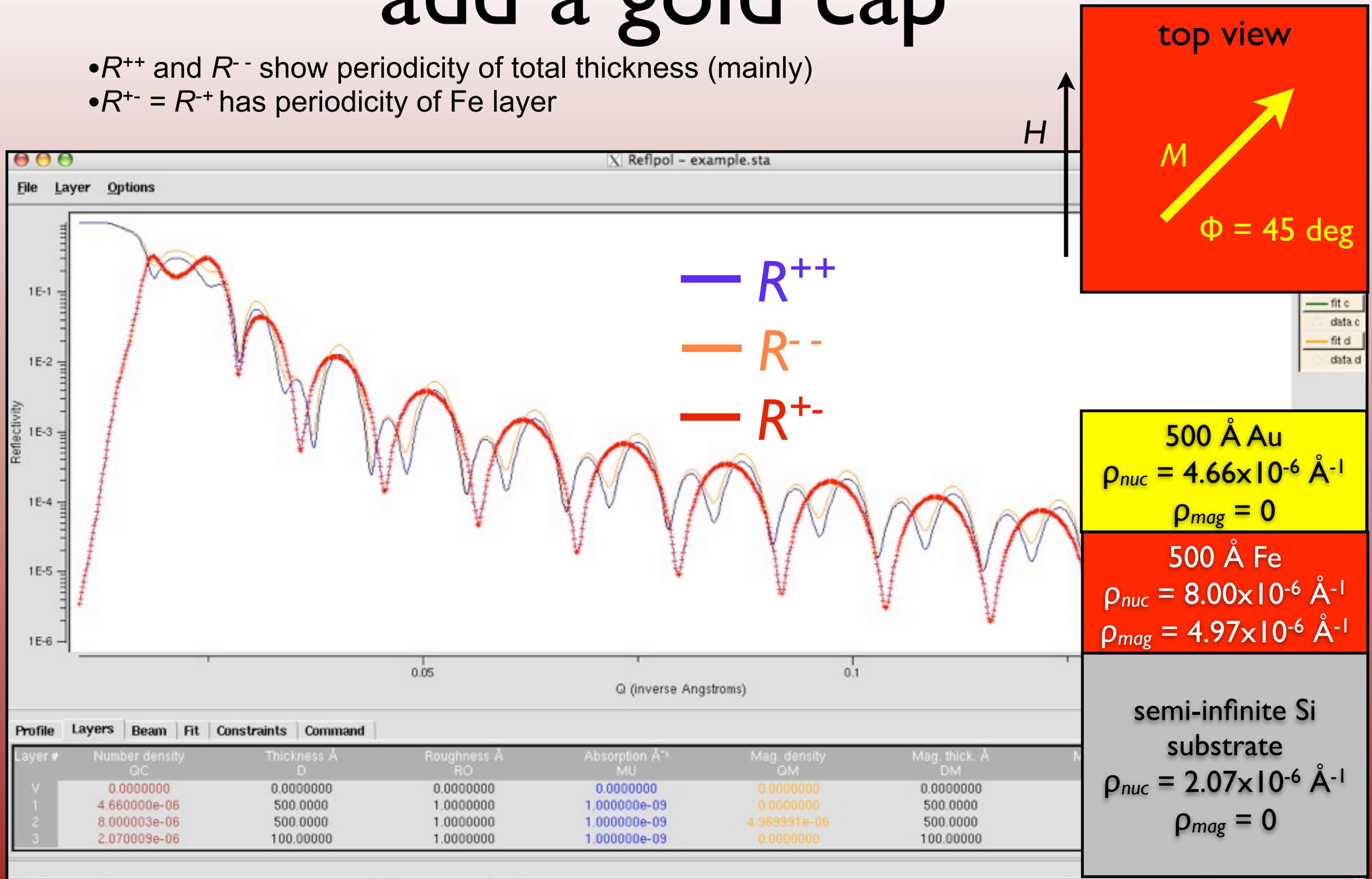
Profile | Layers | Beam | Fit | Constraints | Command

Layer #	Number density QC	Thickness Å D	Roughness Å RO	Absorption Å^{-1} MU	Mag. density QM	Mag. thick. Å DM	Mag. rough Å RM	Mag. theta° TH
V	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	185.0000
1	0.0000000	500.0	1.0000000	1.000000e-09	0.0000000	500.0000	1.0000000	185.0000
2	8.000003e-06	500.0000	1.0000000	1.000000e-09	4.969391e-06	500.0000	1.0000000	185.0000
3	2.070009e-06	100.00000	1.0000000	1.000000e-09	0.0000000	100.00000	1.0000000	185.0000

National Institute of Standards and Technology

add a gold cap

- R^{++} and R^{--} show periodicity of total thickness (mainly)
- $R^{+-} = R^{-+}$ has periodicity of Fe layer



500 Å Au
$\rho_{nuc} = 4.66 \times 10^{-6}$ Å^{-1}
$\rho_{mag} = 0$

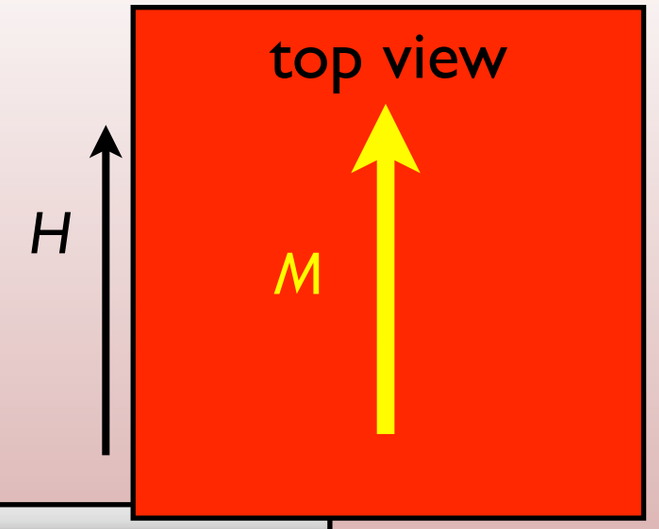
500 Å Fe
$\rho_{nuc} = 8.00 \times 10^{-6}$ Å^{-1}
$\rho_{mag} = 4.97 \times 10^{-6}$ Å^{-1}

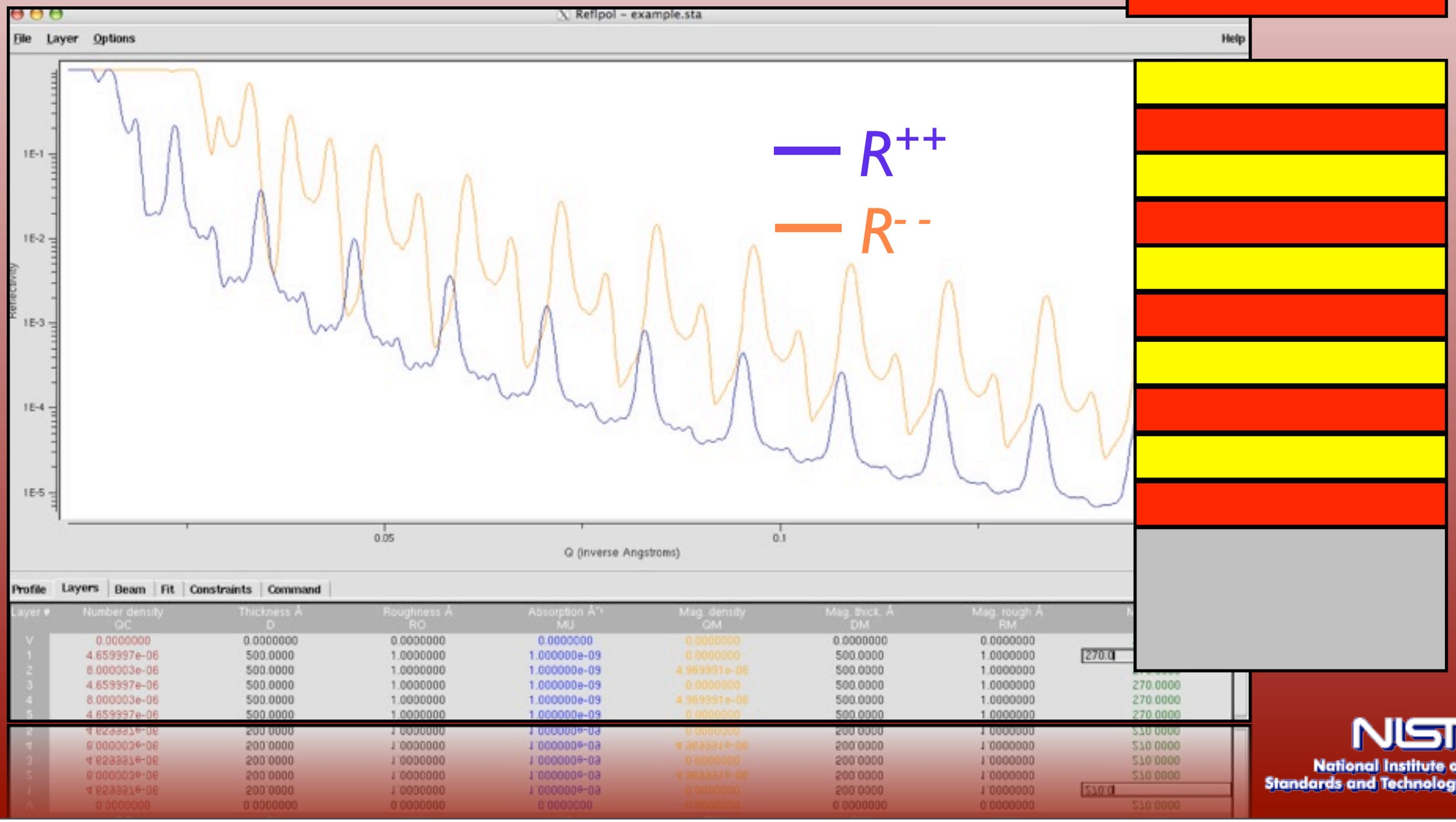
semi-infinite Si substrate
$\rho_{nuc} = 2.07 \times 10^{-6}$ Å^{-1}
$\rho_{mag} = 0$

National Institute of Standards and Technology

superlattice

- point *M* back along *H*
- [500 Å Fe / 500 Å Si] x 5
- Bragg peaks $Q = 2\pi/(d1 + d2)$
- signals corresponding to interfacial features are amplified

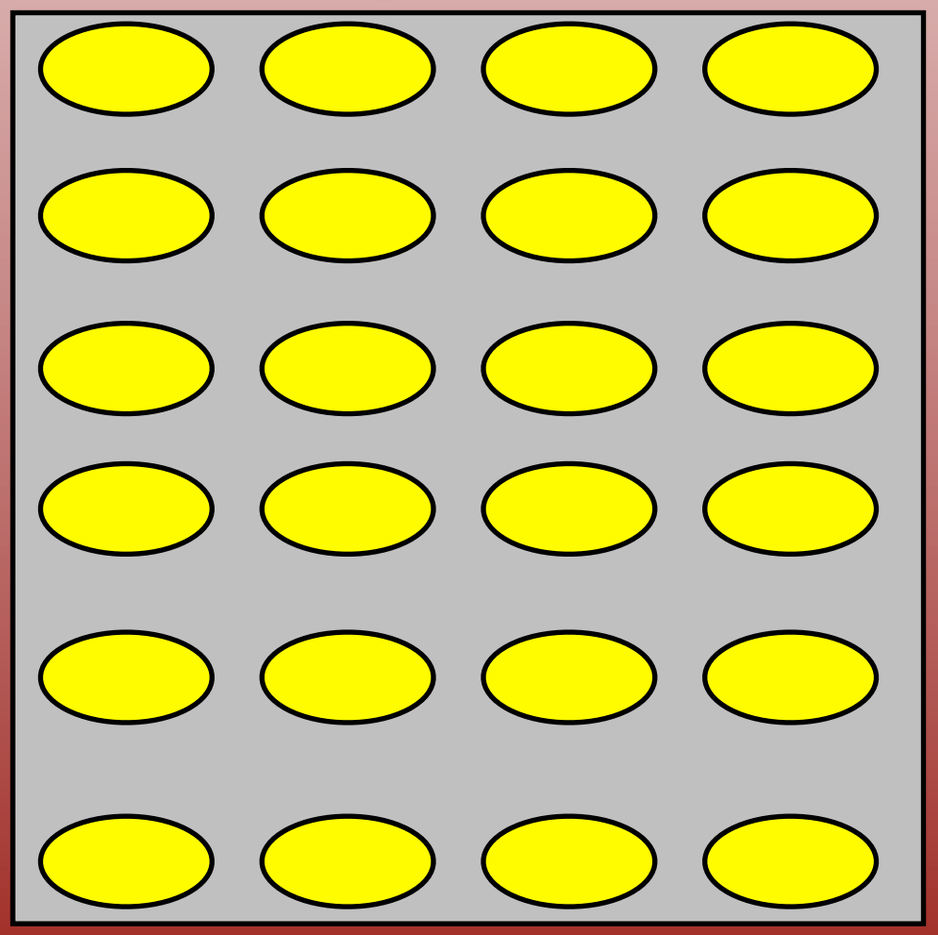




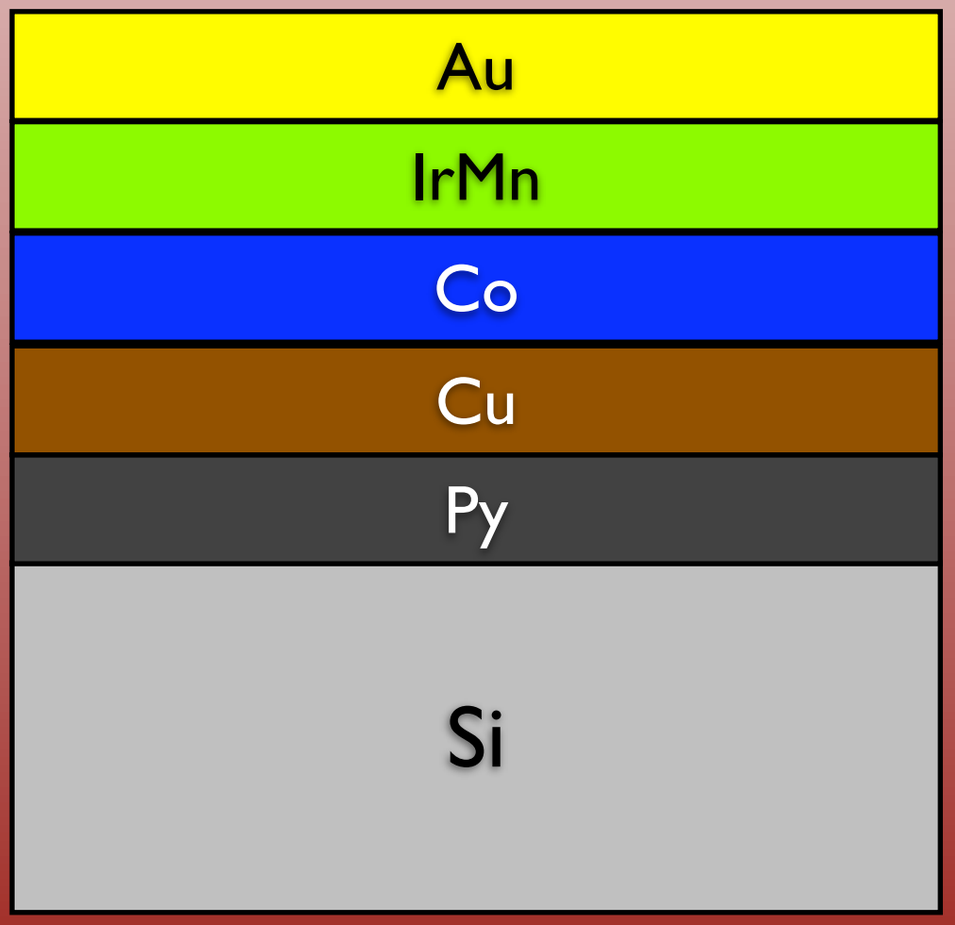
your sample

- patterened multilayer
- specular scattering will give us the structural and magnetic depth profiles
- elements and empty spaces are much smaller than neutron coherence length (~200 μm)
  - for the specular case, we can treat the sample as being uniform, but “dilute” in-plane

top view



side view



National Institute of Standards and Technology