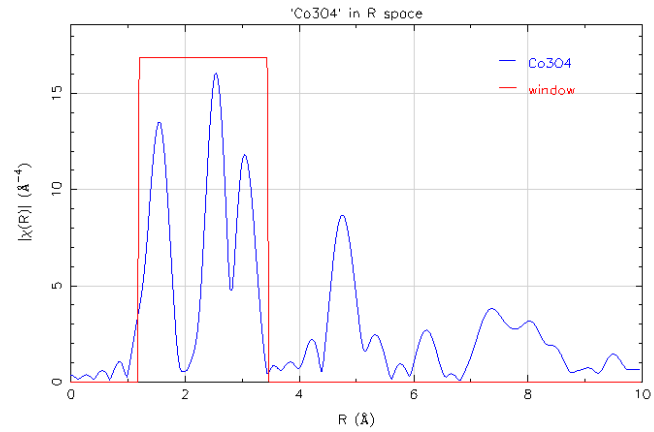
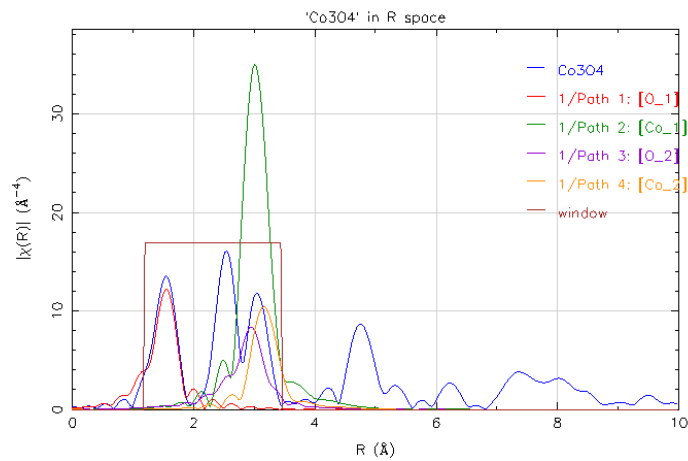


Experimental:



Model (Co3O4, space group: #227):



Atoms		feff.inp		Interpretation			
Titles							
Co3O4							
Co3 O4							
Llu, X.							
Space group	227	Core	EI	X	Y	Z	
A	8.12890	1	●	Co	0.12500	0.12500	0.12500
B	8.12890	2	●	Co	0.50000	0.50000	0.50000
C	8.12890	3	●	O	0.26300	0.26300	0.26300
Alpha	90.00000						
Beta	90.00000						
Gamma	90.00000						
Cluster size	8.94179						
Edge	K						
Shift vector	0						
	0						
	0						

"F d -3 m" appears in the International Tables with multiple choices of origin. If the atoms list seems wrong, you should use a shift vector of:  
-0.125, -0.125, -0.125

Questions:

- (1) Why the second peak (ca. 3 Å) in experimental data is missing in the Co<sub>3</sub>O<sub>4</sub> model?
- (2) Why need to add the “shift vector” suggested by Artemis? Actually, no action is required and the software change the Co core from 0.125, 0.125, 0.125 to 0.5 0.5 0.5, and keep the shift vector as 0 0 0.