**Fe foil**

12-05-2020 -Dmitry/.. 02-06-2021 – Bidyut/..

PETRA III Extension Beamline P65

XAS CONTINUOUS MODE

Chart, line chart

Description automatically generated

E0 = 7112 eV, Edge step = **2.6**, **2.3**, Pre-edge = -150 to -30 eV, Normalization = 50 to 900 eV

Chart

Description automatically generated

kw = 2

Chart, line chart

Description automatically generatedk range = 2.0 – 14.2 Å-1

Chart, line chart

Description automatically generated

Chart, histogram

Description automatically generated

Project title : Fitting Fe\_foil\_Fe\_K\_300\_00000\_xdi.chi This fit at : 16:37:39 on 20 April, 2022

Artemis 0.8.012 using Some Windows OS, perl 5.008008, Tk 804.027, and Ifeffit 1.2.11

Independent points = 30.612304688 Number of variables = 12.000000000

Chi-square = 5783.512946565 Reduced Chi-square = 310.735991253

R-factor = 0.000123087 Measurement uncertainty (k) = 0.000272022

Measurement uncertainty (R) = 0.099326177 Number of data sets = 1.000000000

Guess parameters +/- uncertainties (initial guess):

**amp = 0.7075040 +/- 0.0672380 (1.0000)**

enot = 7.7040360 +/- 0.8926530 (0.0000)

delr = -0.0032870 +/- 0.0037410 (0.0000)

ss = 0.0059200 +/- 0.0006520 (0.0030)

delr2 = -0.0201680 +/- 0.0106660 (0.0000)

ss2 = 0.0090420 +/- 0.0018610 (0.0030)

delr3 = 0.0026170 +/- 0.0199290 (0.0000)

ss3 = 0.0104260 +/- 0.0020800 (0.0030)

delr4 = 0.0223450 +/- 0.0080260 (0.0000)

ss4 = 0.0059640 +/- 0.0006530 (0.0030)

delr5 = 0.1981110 +/- 0.0522800 (0.0000)

ss5 = 0.0088180 +/- 0.0026670 (0.0030)

k-range = 2.029 - 14.215 dk = 1.000 k-window = hanning k-weight = 3

R-range = 1.000 - 5.000 dR = 0.000 R-window = hanning fitting space = R

FEFF0: Path 1: [Fe1\_1] .. id = reff= 2.4855, nlegs= 2, path= Fe<->Fe

r = 2.482213

degen = 8.000000

s02 = 0.707504

e0 = 7.704036

dr = -0.003287

ss2 = 0.005920

FEFF0: Path 2: [Fe1\_2] .. id = reff= 2.8700, nlegs= 2, path= Fe<->Fe

r = 2.849832

degen = 6.000000

s02 = 0.707504

e0 = 7.704036

dr = -0.020168

ss2 = 0.009042

FEFF0: Path 5: [Fe1\_3] .. id = reff= 4.0588, nlegs= 2, path= Fe<->Fe

r = 4.061417

degen = 12.000000

s02 = 0.707504

e0 = 7.704036

dr = 0.002617

ss2 = 0.010426

FEFF0: Path 8: [Fe1\_4] .. id = reff= 4.7594, nlegs= 2, path= Fe<->Fe

r = 4.781745

degen = 24.000000

s02 = 0.707504

e0 = 7.704036

dr = 0.022345

ss2 = 0.005964

FEFF0: Path 4: [Fe1\_2 Fe1\_1] .. id = reff= 3.9205, nlegs= 3, path= Fe->Fe->Fe->Fe

r = 3.897045

degen = 48.000000

s02 = 0.707504

e0 = 7.704036

dr = -0.023455

ss2 = 0.014962

FEFF0: Path 7: [Fe1\_3 Fe1\_1] .. id = reff= 4.5149, nlegs= 3, path= Fe->Fe->Fe->Fe

r = 4.514230

degen = 48.000000

s02 = 0.707504

e0 = 7.704036

dr = -0.000670

FEFF0: Path 10: [Fe1\_5] .. id = reff= 4.9710, nlegs= 2, path= Fe<->Fe

r = 5.169111

degen = 8.000000

s02 = 0.707504

e0 = 7.704036

dr = 0.198111

ss2 = 0.008818