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U.S. Department of ENERGY

Understanding the EXAFS equation

Dali Yang

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Wednesday, March 11, 2026

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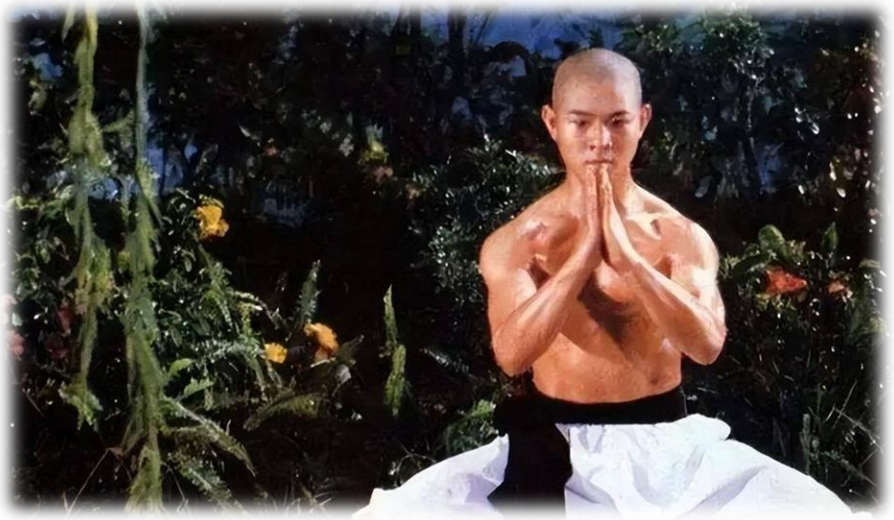
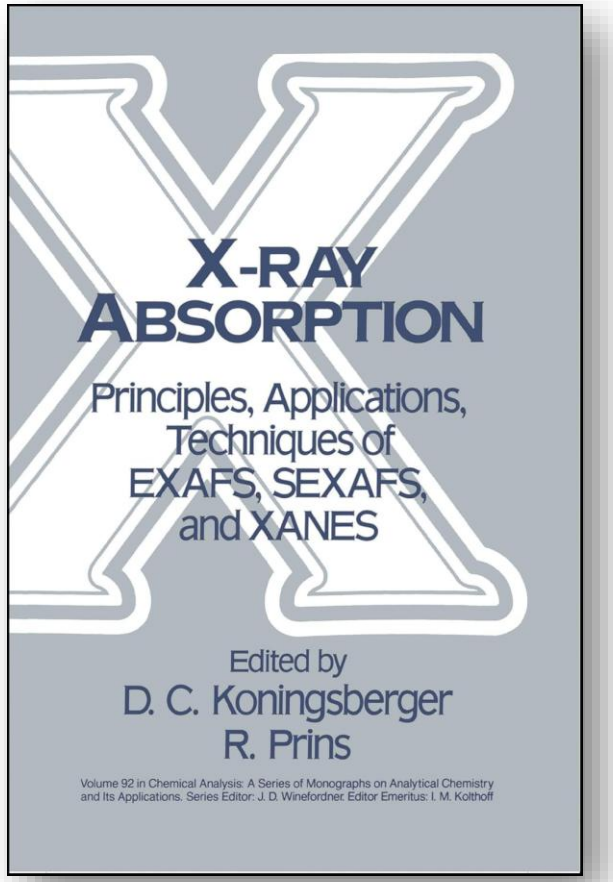
EXAFS analysis is Kong-Fu



Cultivating the **inner power (Qi)**

$$\chi(k) = \sum_j \frac{S_0{}^2 N_j}{k R_j{}^2} F_j(k) e^{-2k^2 \sigma_j{}^2} e^{-\frac{2R_j}{\lambda(k)}} \sin[2kR_j + \delta_{ij}(k)]$$

$$k = \frac{\sqrt{2\mathrm{m}(E - E_0)}}{\hbar}$$



Standing on the shoulder of Giants

ME 27, NUMBER 18 PHYSICAL REVIEW LETTERS 1 NOVEMB

New Technique for Investigating Noncrystalline Structures: Fourier Analysis of the Extended X-Ray–Absorption Fine Structure*

Dale E. Sayers† and Edward A. Stern†‡
Department of Physics, University of Washington, Seattle, Washington 98105
and
Farrel W. Lytle
Boeing Scientific Research Laboratories, Seattle, Washington 98124
(Received 16 July 1971)

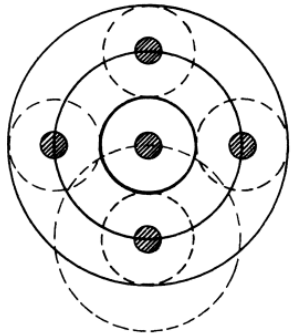
Ed Stern Dale Sayers Farrel Lytle

PHYSICAL REVIEW B VOLUME 10, NUMBER 8 15 OCTOBER 1974

Theory of the extended x-ray-absorption fine structure*

Edward A. Stern
Department of Physics, University of Washington, Seattle, Washington 98195
(Received 14 March 1974)

A general theory of the fine structure observed on the high-energy side of the K-absorption edge (EXAFS) is presented. The form of the theory presented is useful when the excited atom is not too



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Warren award 1979

$$\chi(k) = \sum_j \frac{{S_0}^2 N_j}{k{R_j}^2} F_j(k) e^{-2k^2 {\sigma_j}^2} e^{-\frac{2R_j}{\lambda(k)}} \sin[2kR_j + \delta_{ij}(k)]$$

$$k = \frac{\sqrt{2\mathrm{m}(E - E_0)}}{\hbar}$$

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$$\chi_j(k) = \frac{{S_0}^2 N_j}{k{R_j}^2} F_j(k) e^{-2k^2{\sigma_j}^2} e^{-\frac{2R_j}{\lambda(k)}} \sin[2kR_j + \delta_{ij}(k)]$$

$$k = \frac{\sqrt{2\mathrm{m}(E - E_0)}}{\hbar}$$

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$$\chi_j(k) = \frac{S_0^{\,2} N_j}{k R_j^{\,2}} F_j(k) e^{-2k^2\sigma_j^{\,2}} e^{-\frac{2R_j}{\lambda(k)}} \sin[2kR_j + \delta_{ij}(k)]$$

$$k = \frac{\sqrt{2\mathrm{m}(E - E_0)}}{\hbar}$$

$$\chi_j(k) = A_j(k)\frac{N_j}{kR_j^2}F_j(k)\sin[2kR_j + \delta_{ij}(k)]$$

$$k = \frac{\sqrt{2\mathrm{m}(E - E_0)}}{\hbar}$$

Origin of k

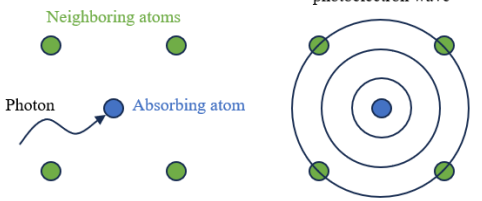
$$k = \frac{2\pi}{\lambda}$$

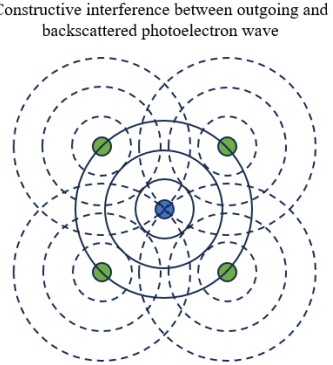
$$\lambda = \frac{h}{p}$$

$$\frac{p^2}{2m} = E - E_0$$

$$k = \frac{\sqrt{2\mathrm{m}(E - E_0)}}{\hbar}$$

Origin of phase $2kR_j$





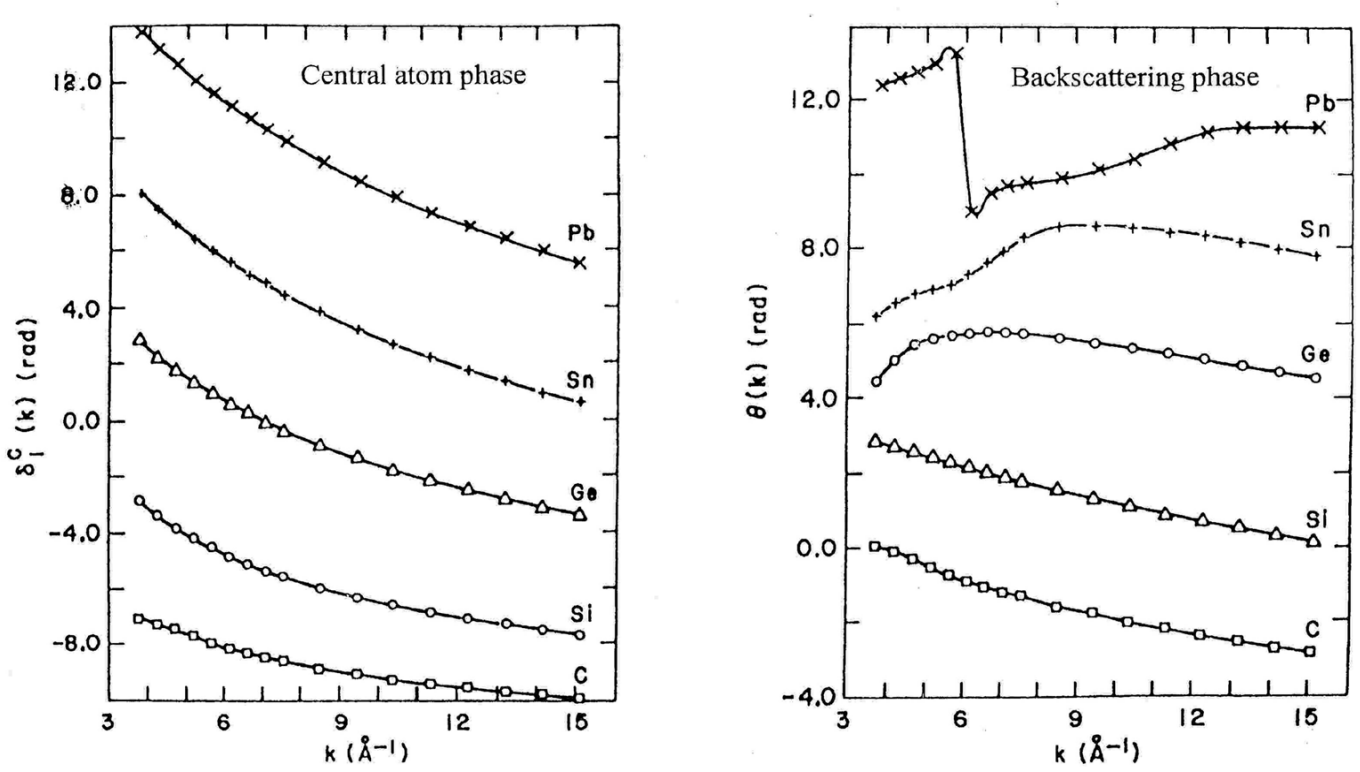
- Core hole lifetime ~ 10^{-15} s (1 fs, K-edge)
- Photoelectron wave interference (~ 10^{-16} s)
- Spherical out-going wave: $\Psi_o = \frac{e^{ikR}}{R}$ $(k = \frac{2\pi}{\lambda})$
- Back-scattered wave: $\Psi_{sc} = T_j(2k)\frac{e^{ik|R-R_j|}}{|R-R_j|}$ ($T_j(2k)$: amplitude of backscattering, depending on the character of the back-scatter)
- When r = 0, at the absorber, $\Psi_o\Psi_{sc} = T_j(2k)\frac{e^{i2kR_j}}{R_j^{\,2}}$

Origin of phase shift $\delta_{ij}(k)$

- Euler equation: $e^{ix} = cosx + isinx$
- Potentials add phase shift: $T_j(2k)\,\frac{e^{i[2kR_j+\delta_{ij}(k)-\frac{\pi}{2}]}}{R_j^{\,2}}$
- $I \propto |\Psi|^2$
- $\chi_j(k) = A\,\frac{T_j(2k)}{R_j^{\,2}}\sin[2kR_j + \delta_{ij}(k)]$
- $\delta_{ij}(k) = 2\delta_l(k) + \beta_j(k)$

Origin of phase shift $\delta_{ij}(k)$

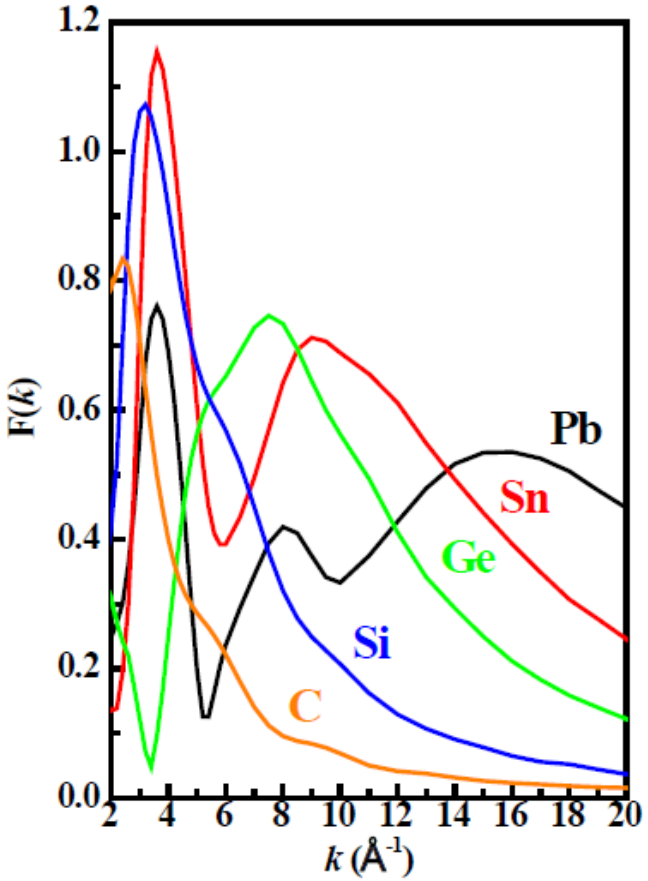
- $\delta_{ij}(k) = 2\delta_l(k) + \beta_j(k)$



Teo, B. K. & Lee, P. A. *Journal of the American Chemical Society* **1979**, *101*, 2815–2832.

Origin of backscattering amplitude $F_j(k)$

- $\chi_j(k) = A\frac{T_j(2k)}{R_j^{\,2}}\sin[2kR_j + \delta_{ij}(k)]$
- $\frac{F_j(k)}{k} = AT_j(2k)$
- $\chi_j(k) = \frac{F_j(k)}{kR_j^{\,2}}\sin[2kR_j + \delta_{ij}(k)]$



$$\chi_j(k) = \frac{{S_0}^2 N_j}{k{R_j}^2} F_j(k) e^{-2k^2{\sigma_j}^2} e^{-\frac{2R_j}{\lambda(k)}} \sin[2kR_j + \delta_{ij}(k)]$$

Debye-Waller factor $\sigma_j{}^2$

- Thermal vibrations (Gaussian disorder)
  - Two models can be used to minimize independent points when fitting:
    - Debye temperature model
    - Einstein approximation model

- Structural disorder
  - EXAFS analysis resolution: $\Delta R \geq \pi/2\Delta k$
  - When $\Delta k = 12$ (k-range: 3 – 15 Å^{-1}), $\Delta R > 0.13$ Å

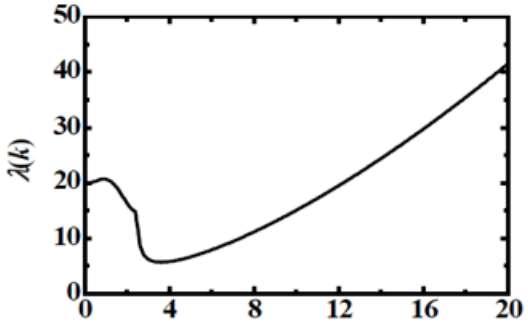
$$\chi_j(k) = \frac{{S_0}^2 N_j}{k{R_j}^2} F_j(k) e^{-2k^2{\sigma_j}^2} e^{-\frac{2R_j}{\lambda(k)}} \sin[2kR_j + \delta_{ij}(k)]$$

Mean free path $\lambda(k)$

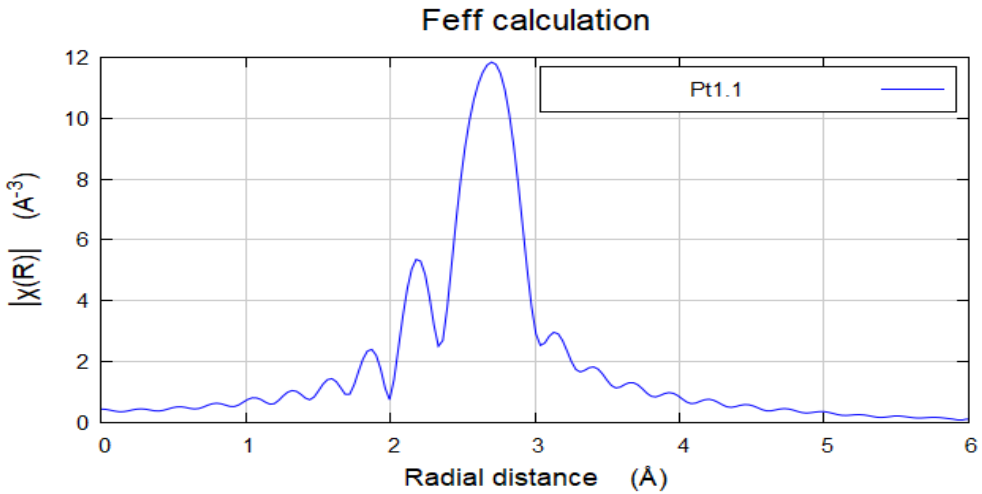
- Core hole lifetime ~ 10^{-15} s (1 fs, K-edge)
- Photoelectron wave interference (~ 10^{-16} s)
- $\lambda(k)$ is equivalent to a finite lifetime to the excited state

Pause and Quiz

- Why $\lambda(k)$ is a function of k?



- Which one caused a double peak in Ni-Pt single scattering path?
  - A. $F_j(k)$
  - B. $\delta_{ij}(k)$



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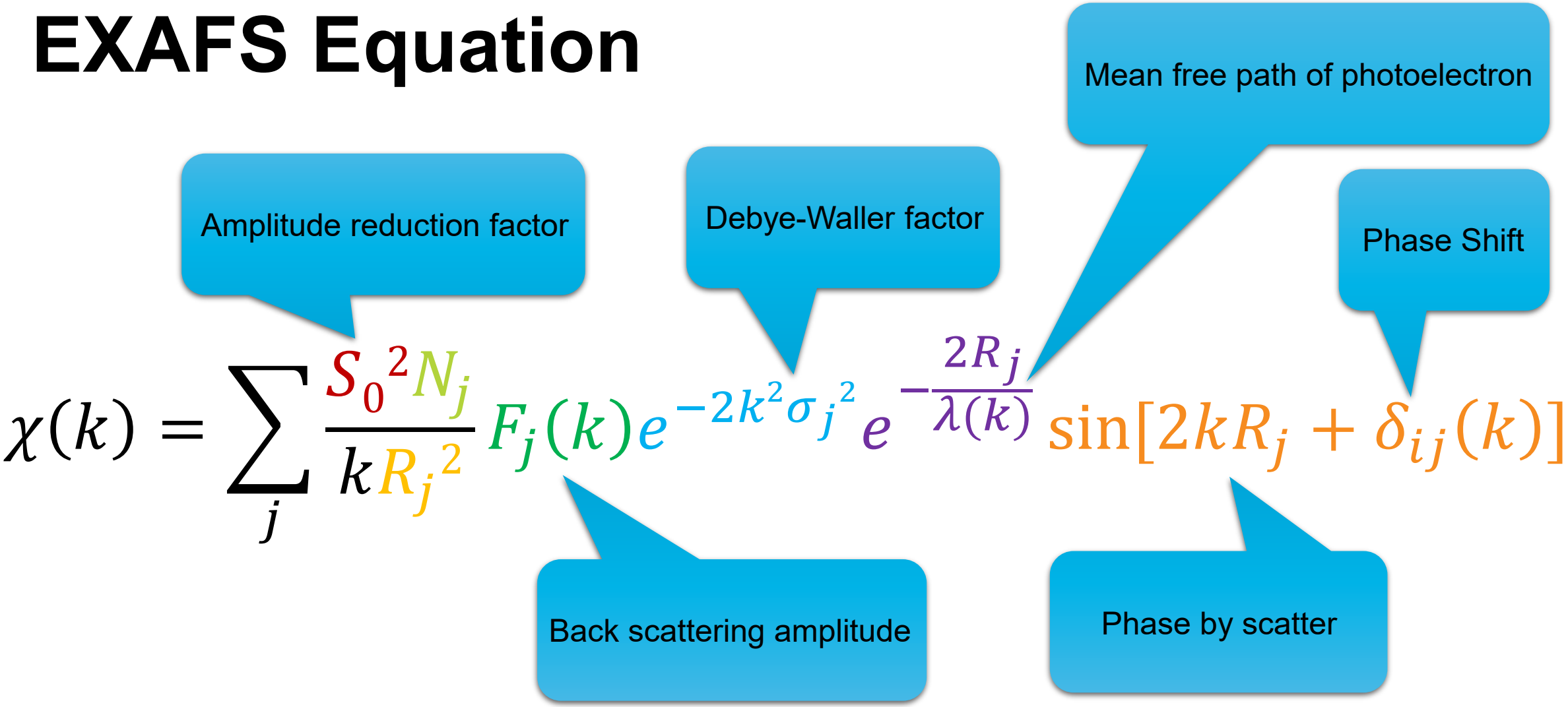
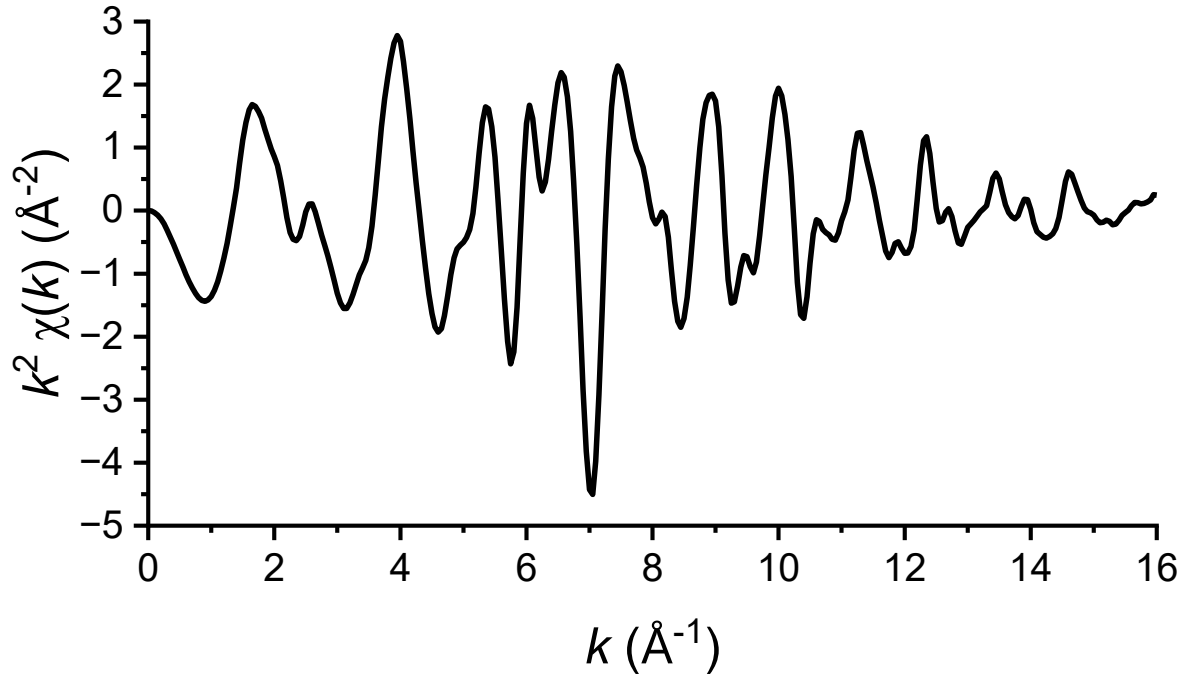
Two steps that appear to be underutilized in studying EXAFS are to plot any final curve based on analytically determined parameters to see if the results are consistent with the raw data. In particular, it is important to see whether small differences that may be indicated in the analysis can really be detected in the original data. The other approach is to use modeling programs to model the results and take their transforms. One must be able to adjust any parameter to see if it has a significant effect on the results when compared to the data, either visually or using some numerical criteria.

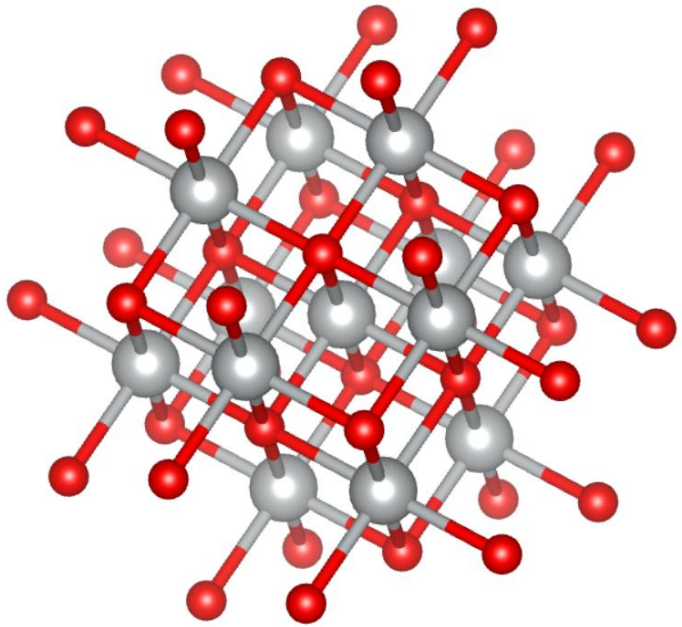
-----D. E. Sayer and B. A. Bunker

EXAFS Equation

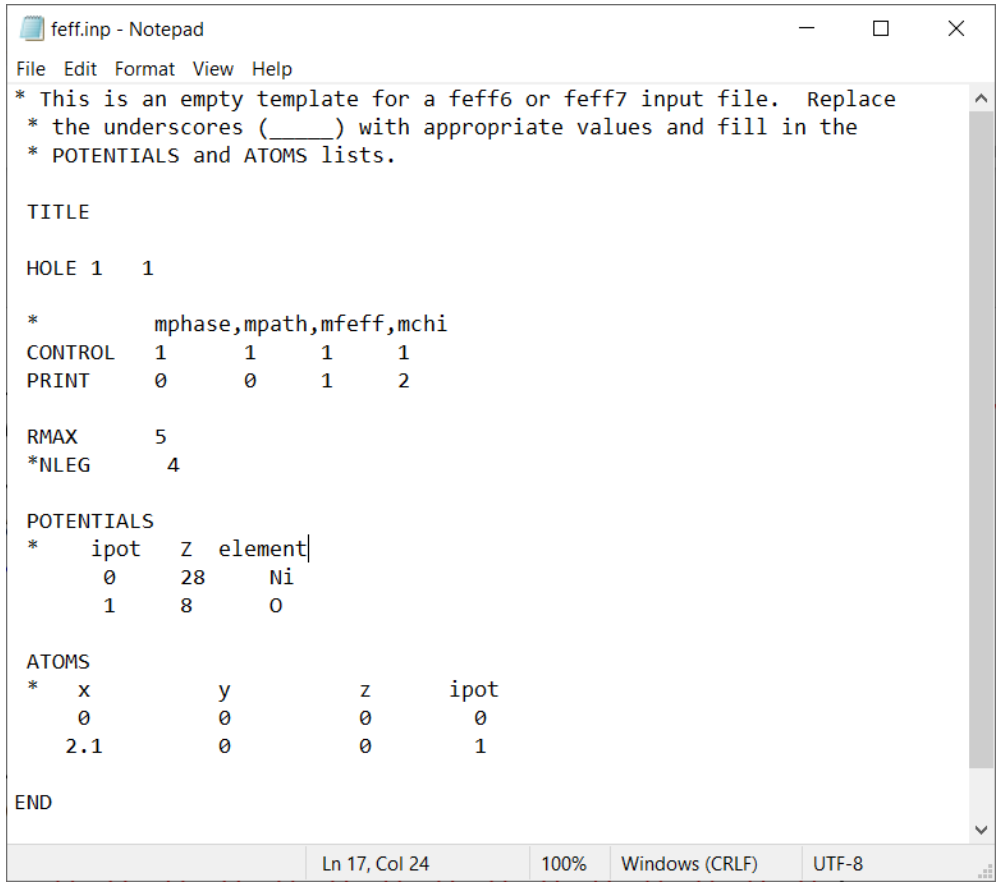


NiO EXAFS and crystal structure





Calculating $f(k), \delta(k), \lambda(k)$ from FEFF



feffNNNN.dat file contains:

- Path geometry
- Data for $f(k), \delta(k)$ ***and*** $\lambda(k)$

Visualizing these data will increase the understanding of EXAFS equation

Calculating $f(k), \delta(k), \lambda(k)$ from FEFF

feff0001.dat - Notepad

File Edit Format View Help

```
Nickel oxide                                              Feff 6.01l  potph 4.12
NI O
Cairns, R W
X-Ray Studies of the System Nickel-Oxygen-Water. I. Nickelous Oxide and
Hydroxide
Abs   Z=28 Rmt= 1.137 Rnm= 1.319 K shell
Pot 1 Z=28 Rmt= 1.154 Rnm= 1.363
Pot 2 Z= 8 Rmt= 0.932 Rnm= 1.098
Gam_ch=1.602E+00 H-L exch
Mu=-3.517E+00 kf=2.112E+00 Vint=-2.052E+01 Rs_int= 1.717
Path    1      icalc       2                              Feff 6.01l genfmt 1.44
---------------------------------------------------------------------------
  2   6.000    2.0842    2.3951   -3.51651 nleg, deg, reff, rnrmav(bohr), edge
        x         y         z   pot at#
    0.0000    0.0000    0.0000  0  28 Ni       absorbing atom
    0.0000    2.0842    0.0000  2   8 O
   k    real[2*phc]   mag[feff]  phase[feff] red factor   lambda      real[p]@#
 0.000  2.9235E+00  0.0000E+00 -3.1236E+00  0.1011E+01  2.0103E+01  2.1130E+00
 0.200  2.9215E+00  9.7575E-02 -3.9262E+00  0.1011E+01  2.0187E+01  2.1220E+00
 0.400  2.9155E+00  1.9122E-01 -4.6669E+00  0.1011E+01  2.0409E+01  2.1489E+00
 0.600  2.9055E+00  2.7774E-01 -5.3473E+00  0.1011E+01  2.0686E+01  2.1931E+00
 0.800  2.8914E+00  3.5513E-01 -5.9694E+00  0.1012E+01  2.0890E+01  2.2535E+00
 1.000  2.8729E+00  4.2252E-01 -6.5352E+00  0.1013E+01  2.0880E+01  2.3294E+00
 1.200  2.8498E+00  4.7996E-01 -7.0468E+00  0.1015E+01  2.0548E+01  2.4196E+00
 1.400  2.8212E+00  5.2797E-01 -7.5056E+00  0.1018E+01  1.9860E+01  2.5233E+00
 1.600  2.7859E+00  5.6716E-01 -7.9127E+00  0.1023E+01  1.8881E+01  2.6400E+00
 1.800  2.7423E+00  5.9797E-01 -8.2685E+00  0.1028E+01  1.7749E+01  2.7691E+00
 2.000  2.6882E+00  6.2045E-01 -8.5732E+00  0.1035E+01  1.6632E+01  2.9105E+00
 2.200  2.6211E+00  6.3417E-01 -8.8269E+00  0.1042E+01  1.5687E+01  3.0643E+00
 2.400  2.5381E+00  6.3824E-01 -9.0300E+00  0.1047E+01  1.5050E+01  3.2308E+00
 2.600  2.3811E+00  6.5294E-01 -9.1198E+00  0.1117E+01  1.0341E+01  3.4426E+00
 2.800  2.3942E+00  7.0904E-01 -9.3969E+00  0.1201E+01  7.3472E+00  3.5706E+00
 3.000  2.4023E+00  7.3244E-01 -9.6250E+00  0.1241E+01  6.3436E+00  3.7059E+00
```

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feffNNNN.dat file contains:

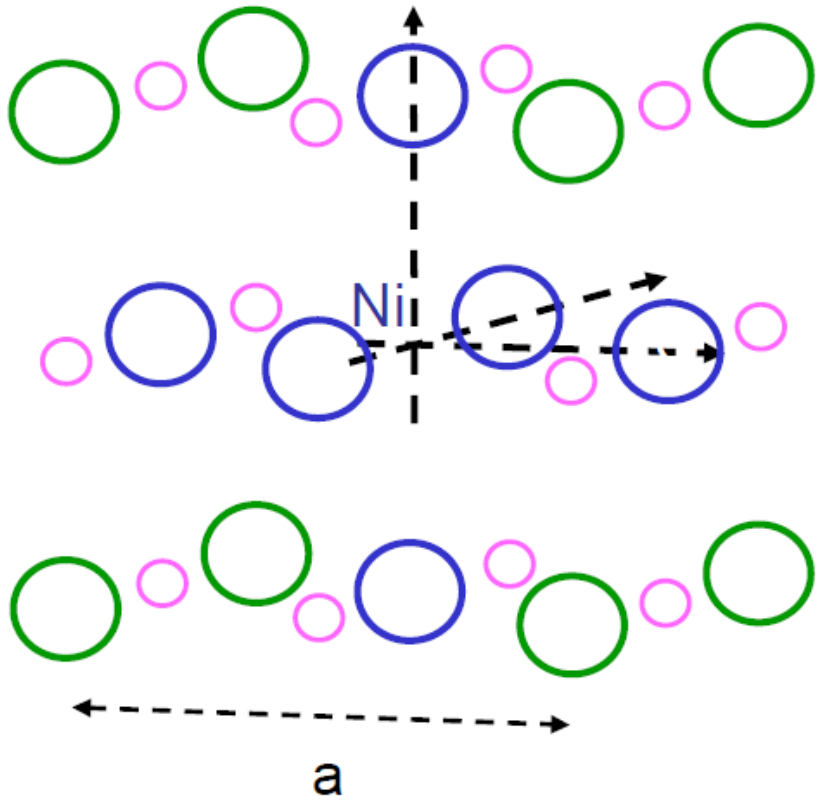
- Path geometry
- Data for $f(k), \delta(k)$ ***and*** $\lambda(k)$

Visualizing these data will increase the understanding of EXAFS equation

*You need to interpolate the data before making plots

Nickel Oxide

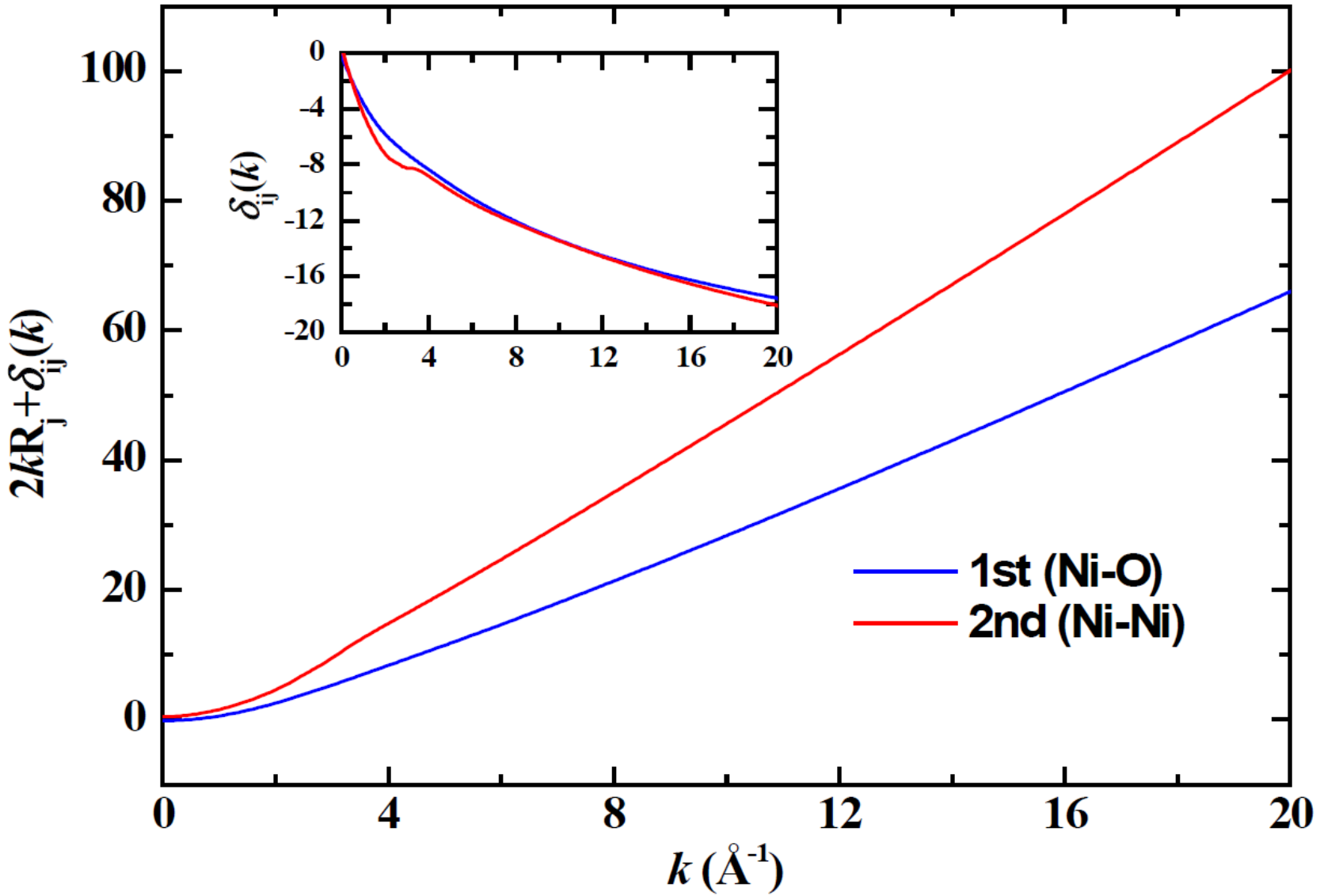
Crystal structure : face centered cubic (fcc)
Lattice constant a : 4.178 Å
Ni occupies corner site: (000)
O occupies body center site: (½½½)



absorbing atom: Ni

Shell	element	distance (Å)	coordination no.
1st	O	2.09	6
2nd	Ni	2.95	12
3rd	O	3.62	8

$$\chi(k) = \sum_j \frac{N_j}{kR_j^2} S_i(k) F_j(k) e^{-2k^2\sigma_j^2} e^{-2R_j/\lambda(k)} \sin[2kR_j + \delta_{ij}(k)]$$



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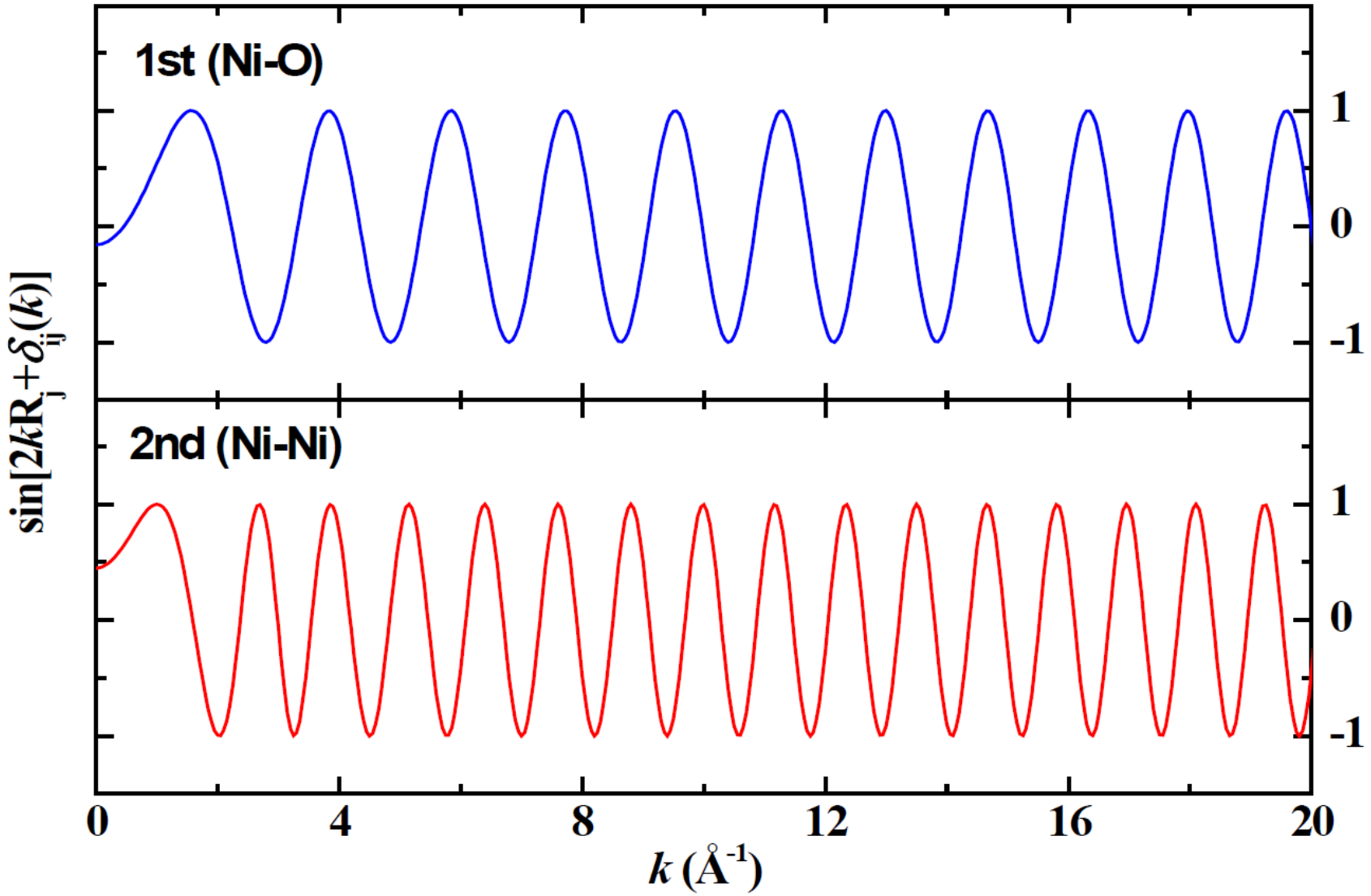

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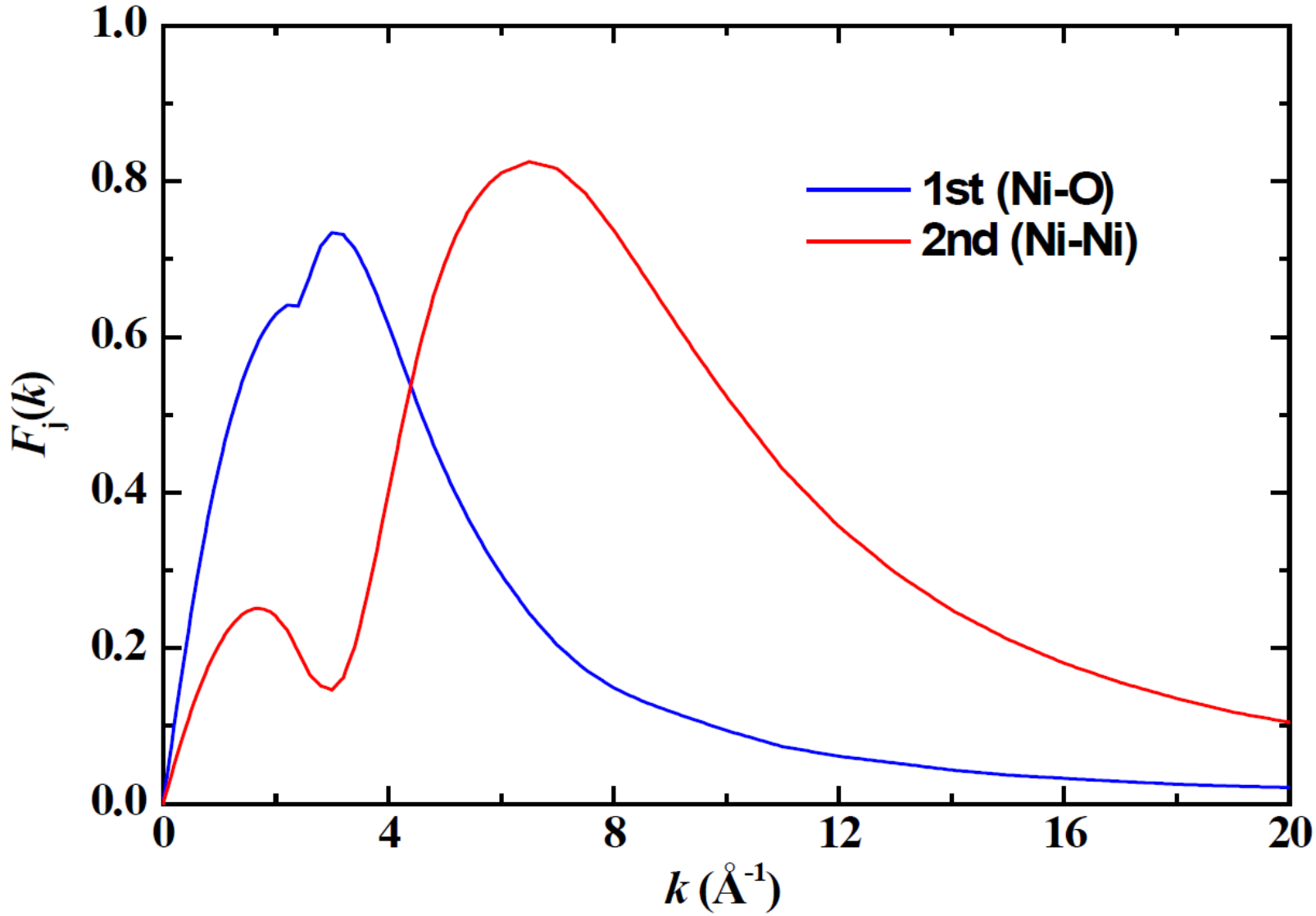

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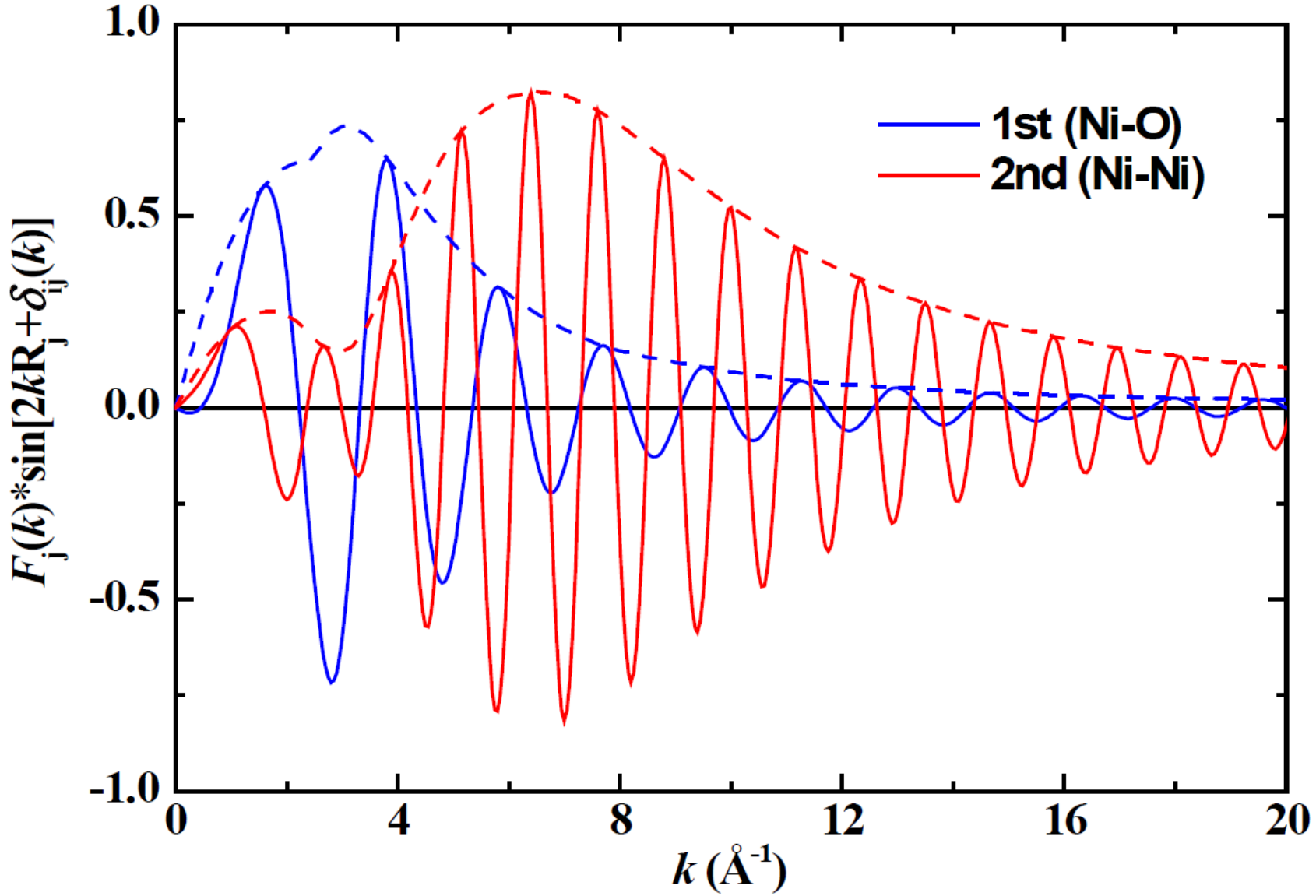
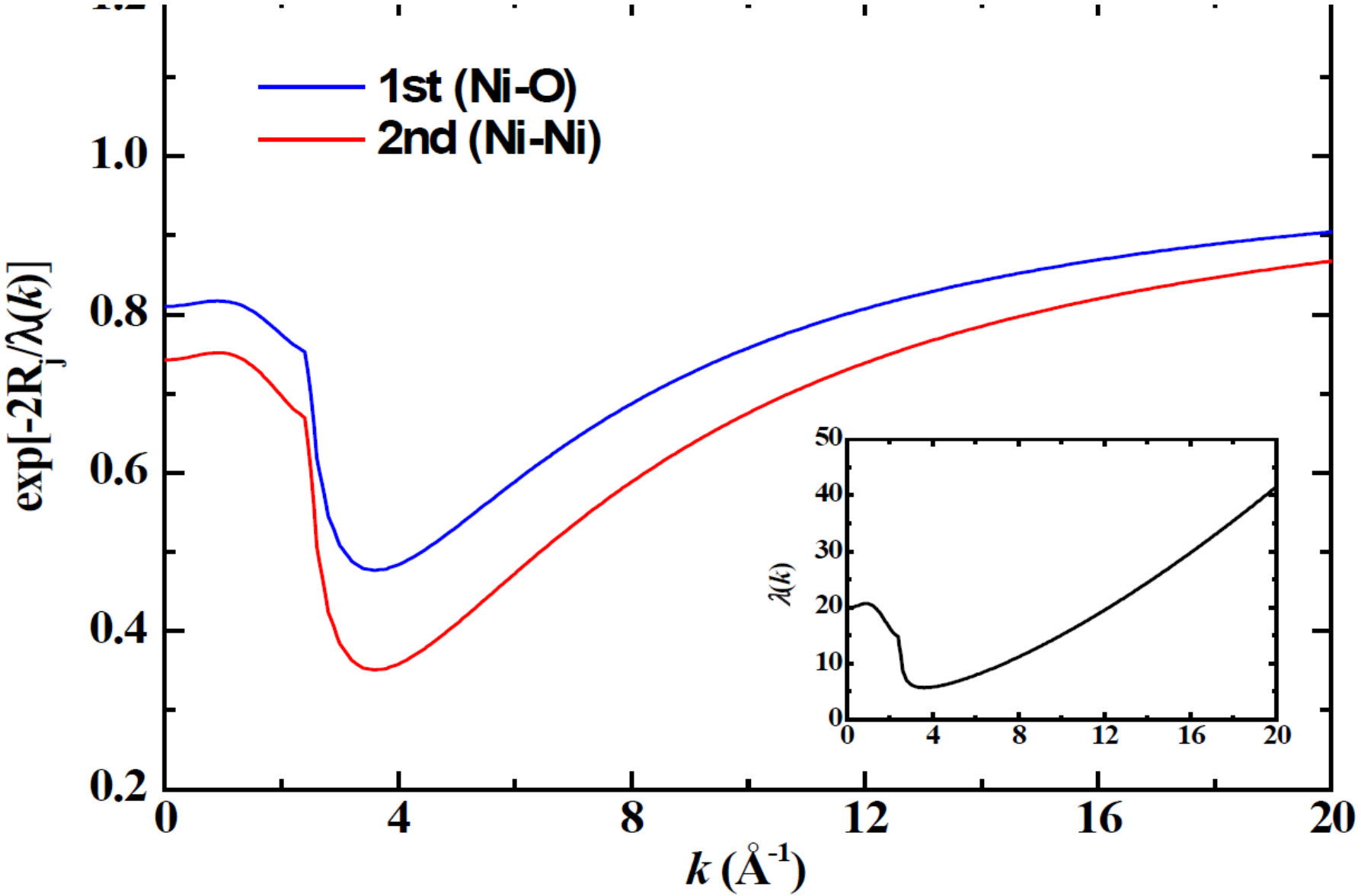
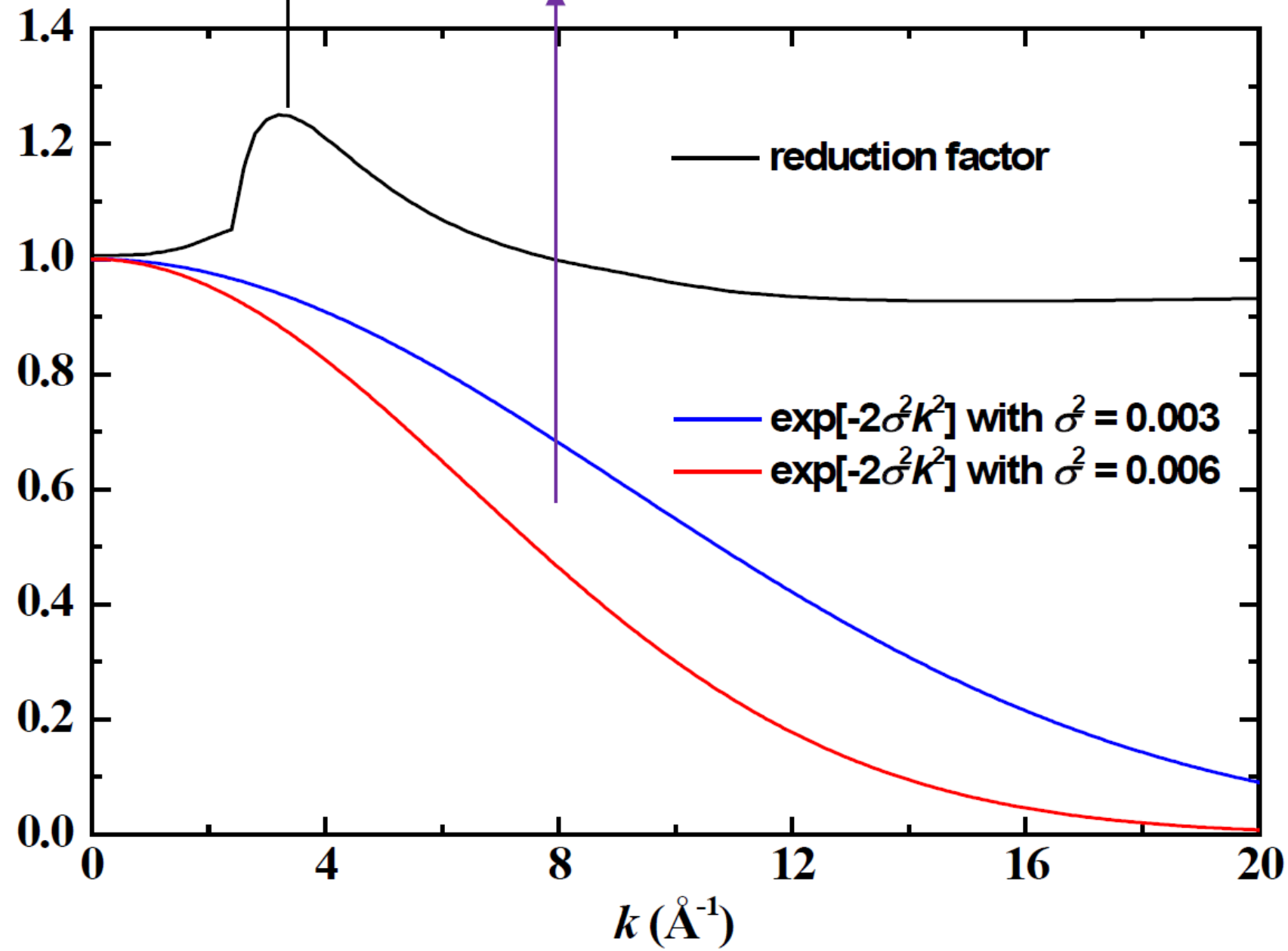


$$\chi(k) = \sum_j \frac{N_j}{kR_j^2} S_i(k) F_j(k) e^{-2k^2\sigma_j^2} e^{-2R_j/\lambda(k)} \sin[2kR_j + \delta_{ij}(k)]$$



$$\chi(k) = \sum_j \frac{N_j}{kR_j^2} S_i(k) F_j(k) \exp(-2\sigma_j^2 k^2) \exp\left[-2R_j/\lambda(k)\right] \sin\left[2kR_j + \delta_{ij}(k)\right]$$



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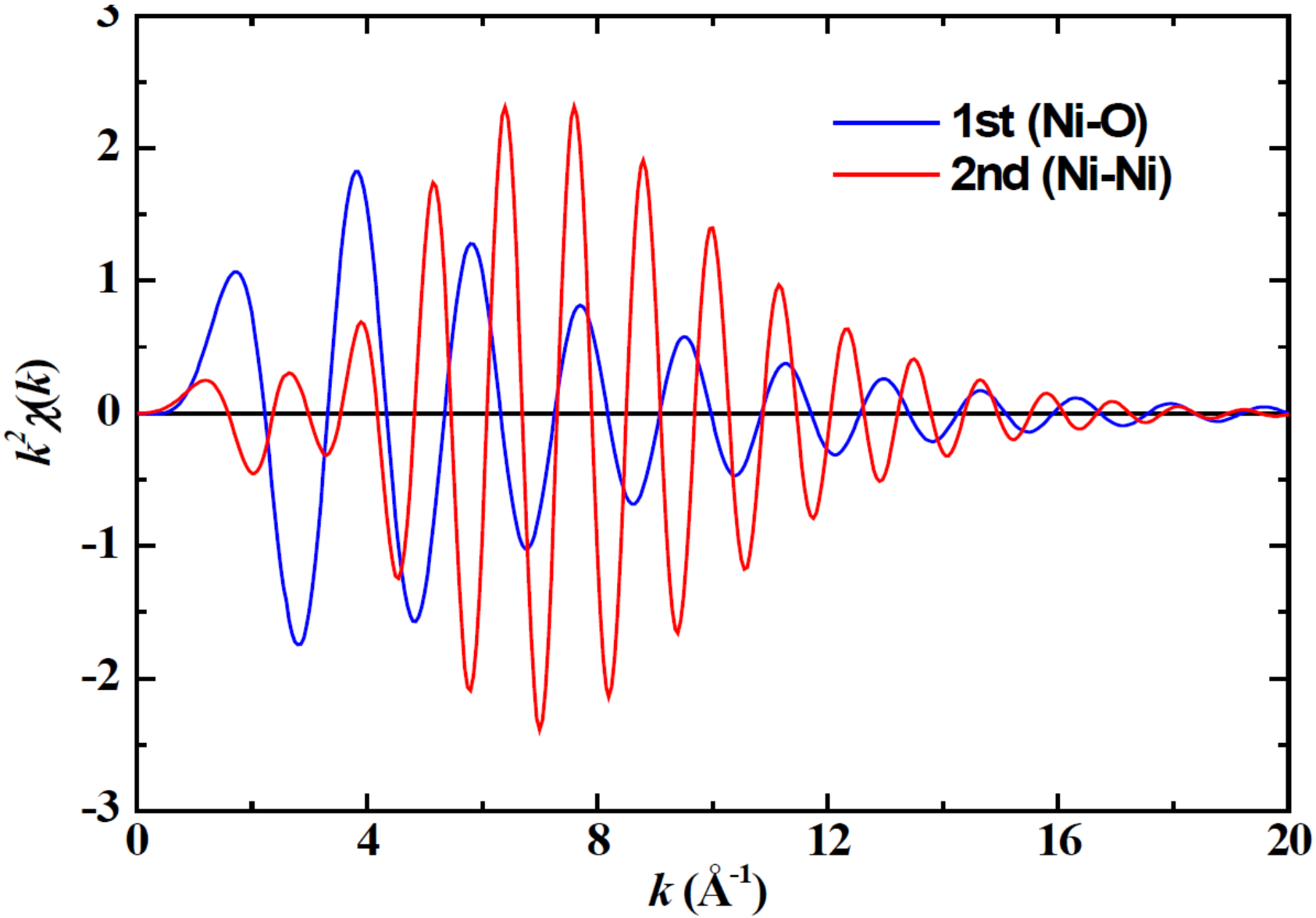

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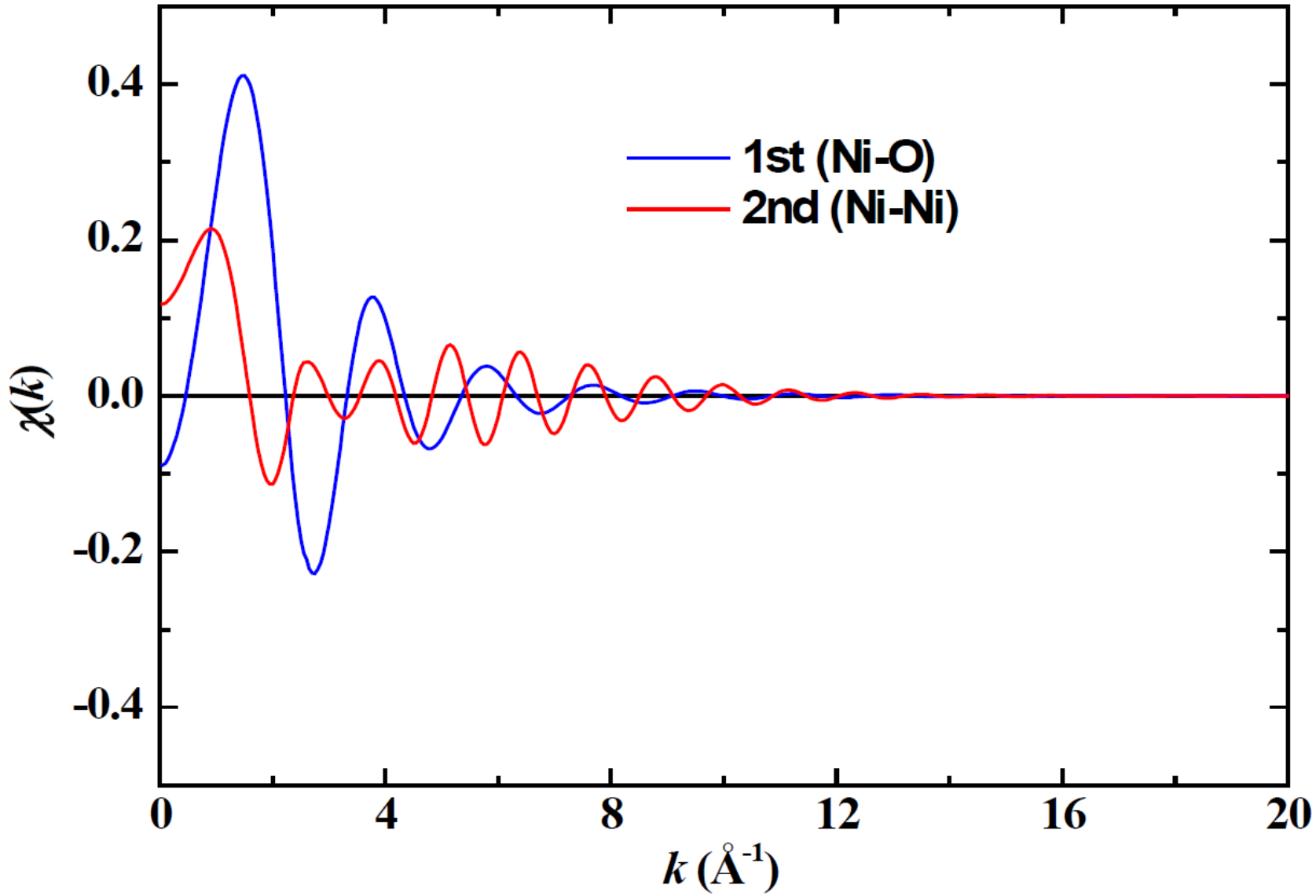

Thank you for your attention!