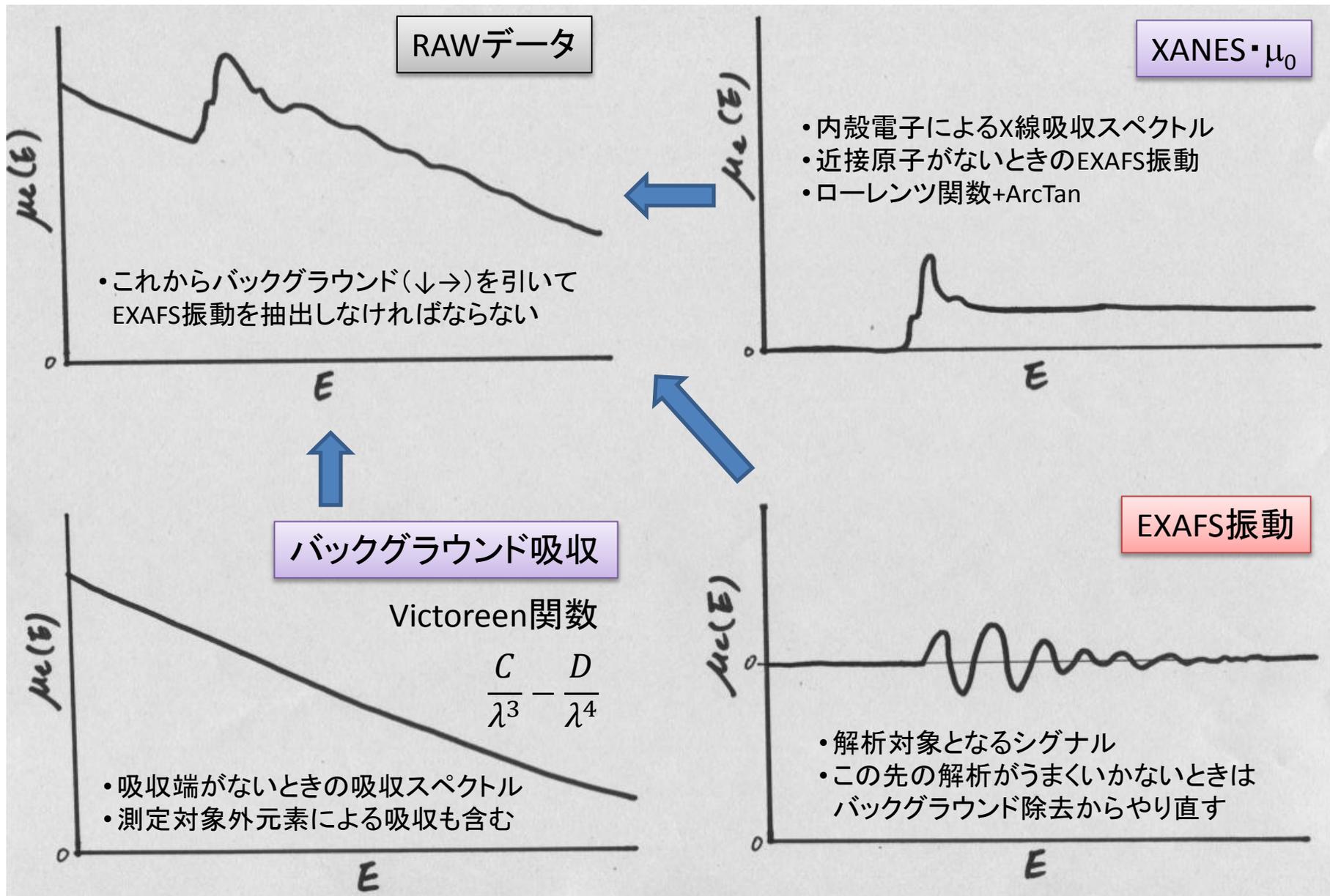


EXAFS解析 補足資料

2012.3 KEK-PF 仁谷浩明

XAFSスペクトルの構成要素



EXAFS振動の構成要素

単振動のEXAFS振動

$$\chi(k) = S_0^2 \frac{NF(k)}{kr^2} \exp(-2k^2\sigma^2) \sin(2kr + \phi(k))$$

S_0^2 : 減衰因子

N : 配位数

F : 散乱振幅

σ : デバイワラー因子

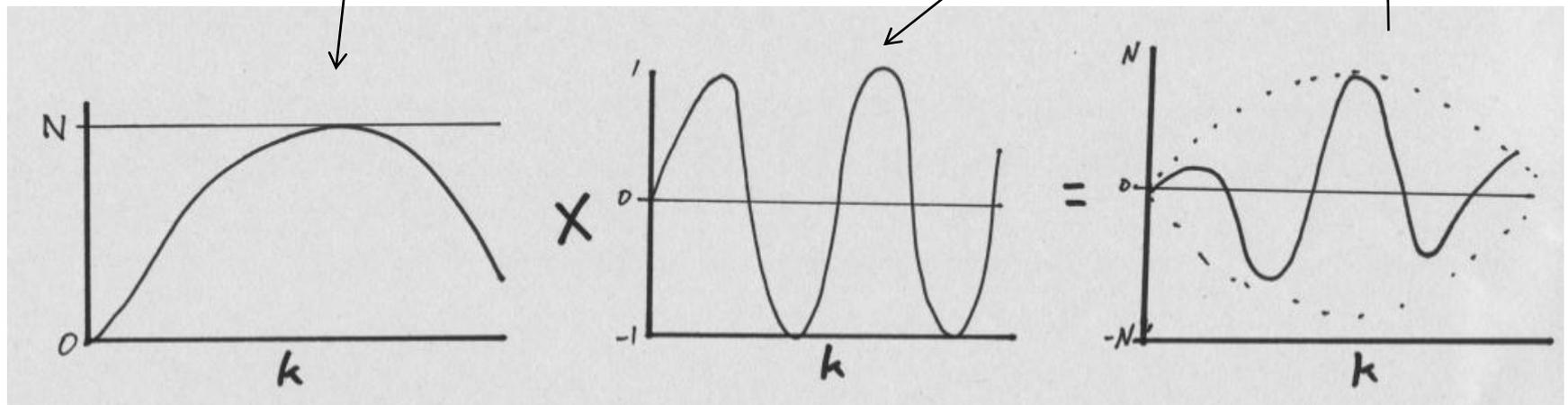
r : 原子間距離

ϕ : 位相シフト

ΔE_0 : EXAFS振動の原点補正

Sin波の振幅に影響

Sin波の振動数に影響

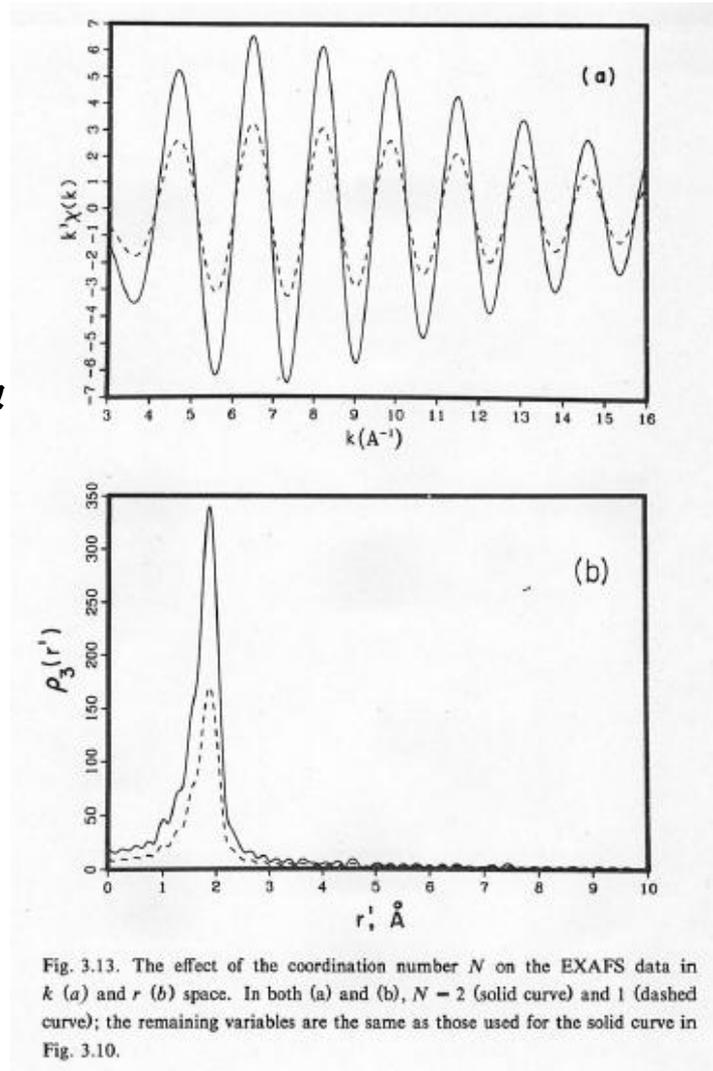


EXAFS振動の構成要素

S_0^2 と N どちらも k 依存性のない定数→両者は区別できない！

配位数が2倍になれば
振動振幅も2倍

S_0^2 は
標準試料の解析データ
から算出するか、
0.8~1.0の値を用いる

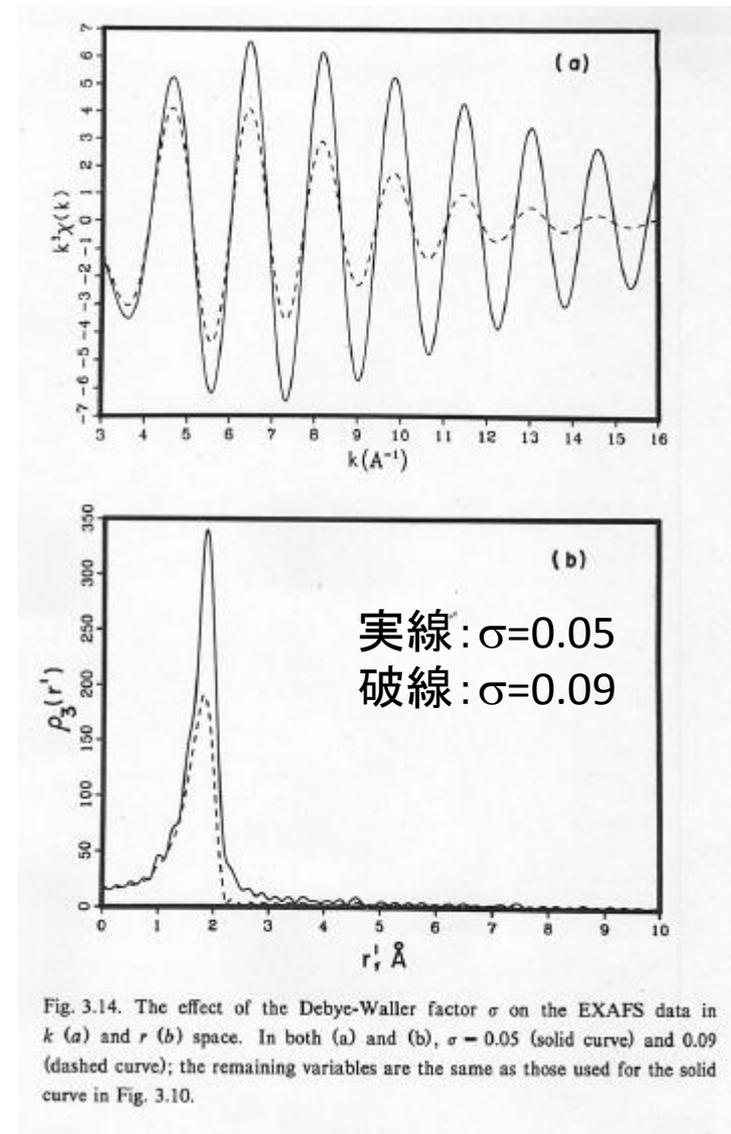
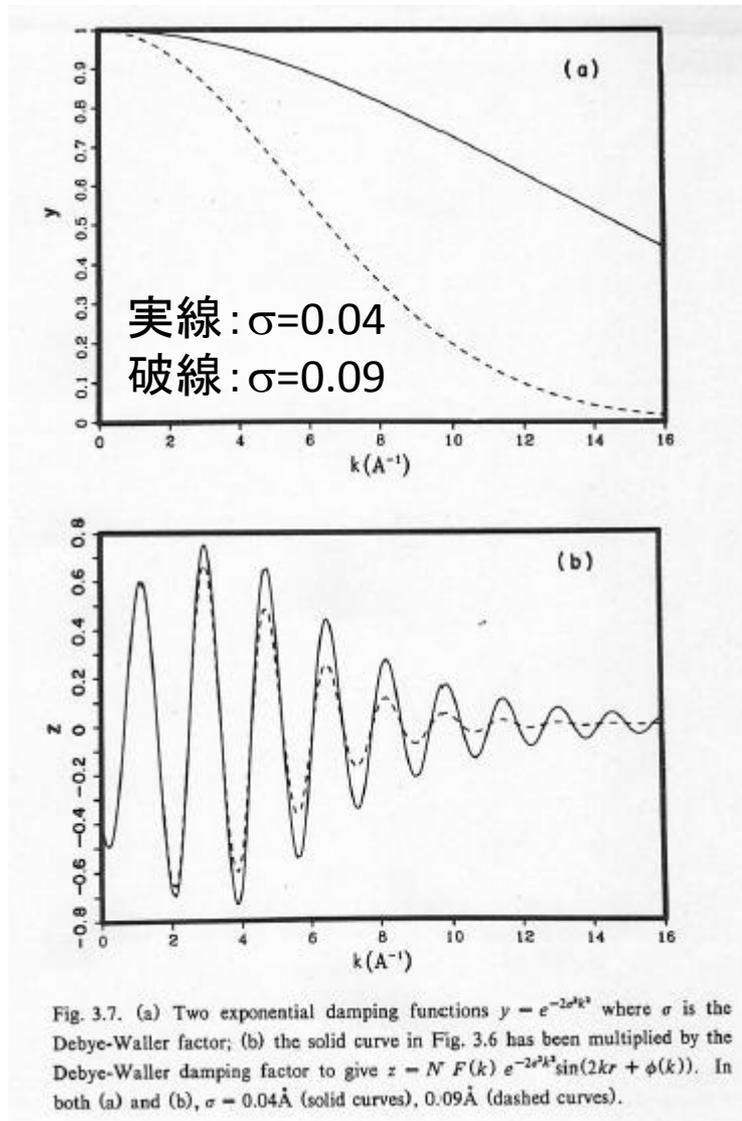


実線: $N=2$
破線: $N=1$

Fig. 3.13. The effect of the coordination number N on the EXAFS data in k (a) and r (b) space. In both (a) and (b), $N = 2$ (solid curve) and 1 (dashed curve); the remaining variables are the same as those used for the solid curve in Fig. 3.10.

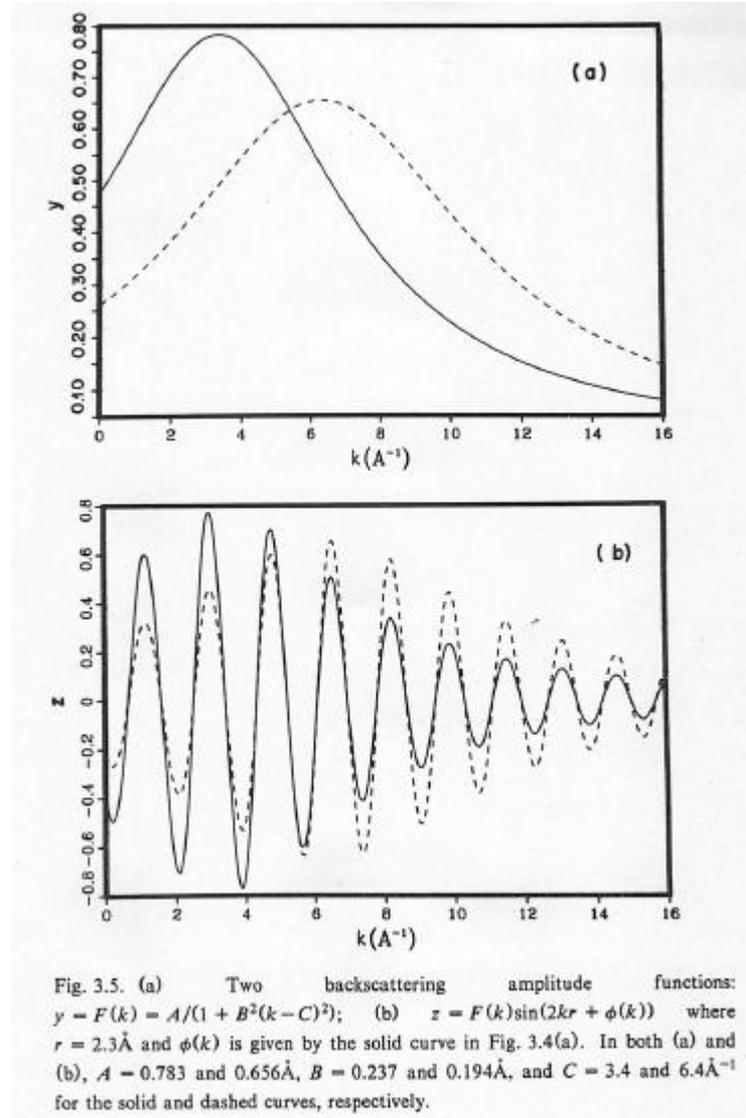
EXAFS振動の構成要素

$\sigma^2(k)$ 原子座標のぶれ(静的&動的)。大きいほど高k領域での減衰が大きくなる



EXAFS振動の構成要素

F(k) 散乱元素によって異なる[通常FEFFで計算]



重元素：高k領域にピーク
軽元素：低k領域にピーク

EXAFS振動の構成要素

R 原子間距離のフィッティング精度は0.001nm程度

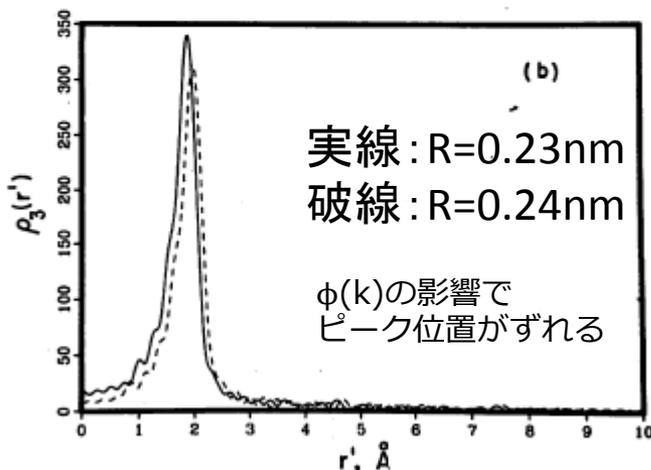
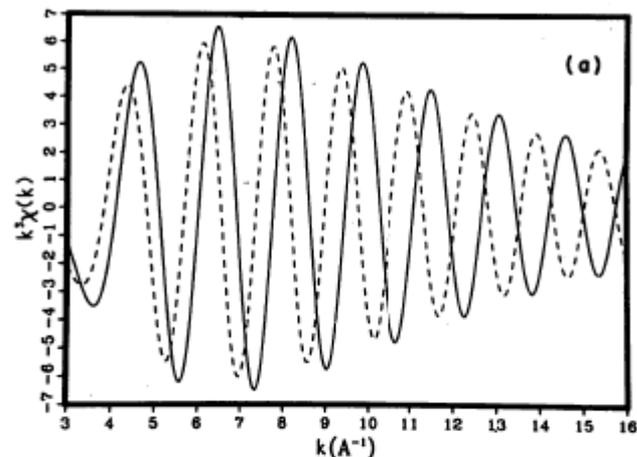
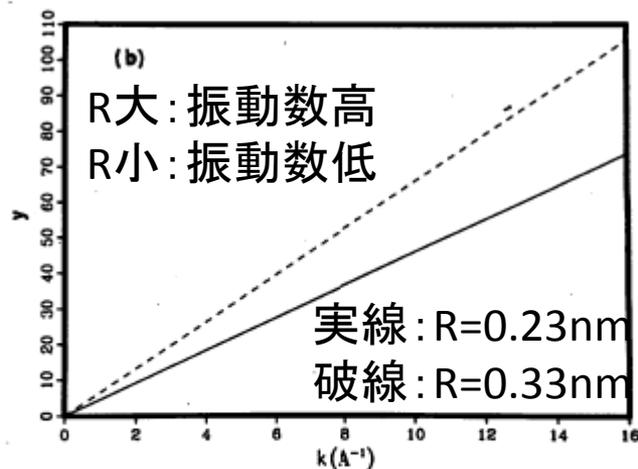
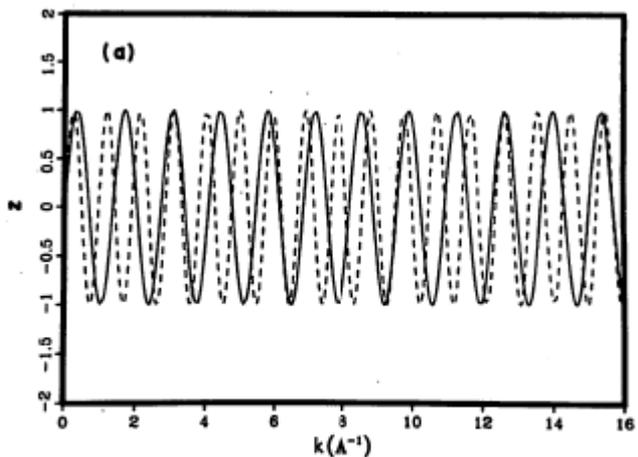
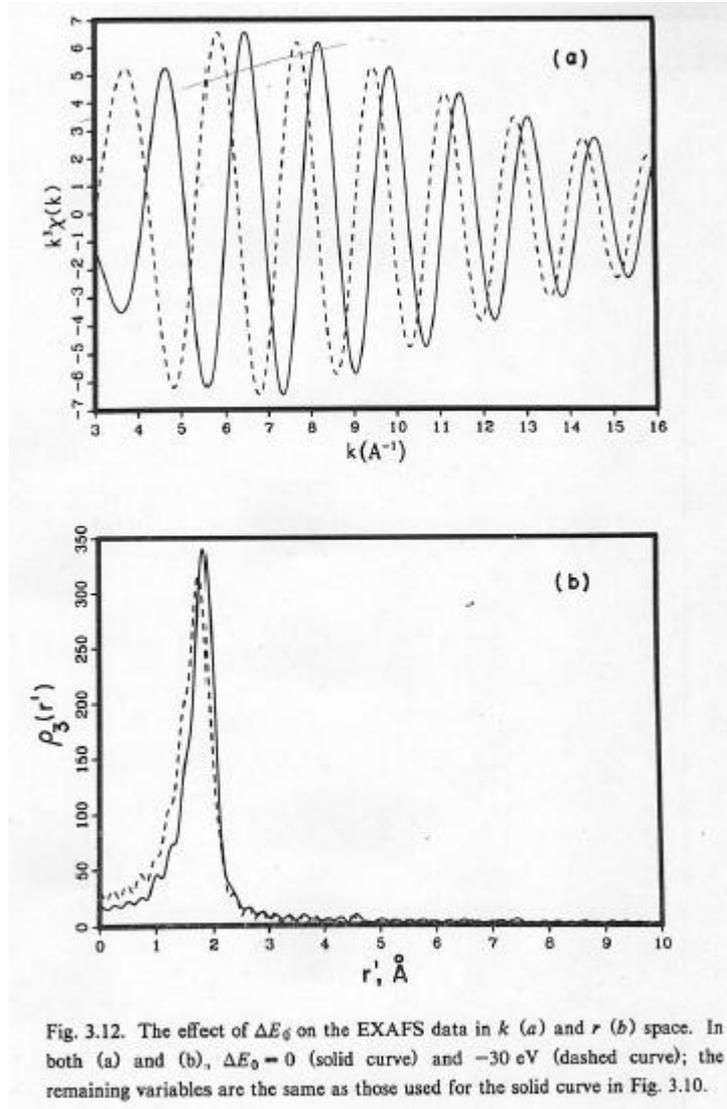


Fig. 3.1. (a) Two sine waves of different frequencies: $z = \sin(2kr)$; (b) the arguments: $y = 2kr$. In (a) and (b), $r = 2.3\text{\AA}$ (solid curves) and 3.3\AA (dashed curves).

Fig. 3.11. The effect of the distance r on the EXAFS data in k (a) and r (b) space. In both (a) and (b), $r = 2.3\text{\AA}$ (solid curve) and 2.4\AA (dashed curves); the remaining variables are the same as those used for the solid curve in Fig. 3.10.

EXAFS振動の構成要素

ΔE_0 低k領域で大きく影響する



実線: 0 eV
破線: -30 eV

ΔE_0 が30eV変化すると
Rが0.01nm程度異なるように
見える

Fig. 3.12. The effect of ΔE_0 on the EXAFS data in k (a) and r (b) space. In both (a) and (b), $\Delta E_0 = 0$ eV (solid curve) and -30 eV (dashed curve); the remaining variables are the same as those used for the solid curve in Fig. 3.10.