

# Theoretical exploration of the origin of AXAFS by full-potential multiple scattering approach

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Fourier transform of the EXAFS signal yields a peak corresponding to the distance  $R$  of the nearest neighbor atoms; however, another peak sometimes appears at about  $R/2$ , where there are no atoms. The EXAFS signal contributing to this peak is called Atomic XAFS (AXAFS) [1]. Previous studies have argued that "AXAFS occurs due to the effects of anisotropic potential difference between atoms in solid and free atoms [2], and photoelectron scattering by the interatomic charge density [3]", but the origin of AXAFS is not clearly understood.

The EXAFS signal is defined by  $\chi = (\sigma_{\text{tot}} - \sigma_{\text{at}})/\sigma_{\text{at}}$ , where  $\sigma_{\text{tot}}$  and  $\sigma_{\text{at}}$  are the total and atomic absorption cross-section, respectively. In the Muffin-tin (MT) approximation,  $\sigma_{\text{at}}$  is calculated for the spherically symmetric absorbing atom, which has a potential step at its boundary. On the other hand, for the analysis of experimentally measured EXAFS or those calculated by the full-potential multiple scattering (FPMS) approach [4], we treat  $\sigma_{\text{at}}$  as a smooth function represented by a polynomial curve.

In this study, we theoretically derived  $\sigma_{\text{tot}}$  and  $\sigma_{\text{at}}$  using the Coulomb potential model and 3d-Square well potential model. We showed that the Fourier transform of  $\sigma_{\text{at}}$  has a prominent peak at the position corresponding to the atomic radius ( $a \sim R/2$ ), namely the half-distance peak is due to the phase shifts caused by the potential truncation in the MT approximation. Indeed, the AXAFS peak appear when a smooth polynomial background is used to extract "atomic background" from  $\sigma_{\text{tot}}$ , while the peak does not appear when  $\sigma_{\text{at}}$  is calculated by the MT approximation. The reason for this is that the AXAFS oscillation in  $\sigma_{\text{tot}}$  which is caused by MT approximation and the polynomial background  $\sigma_{\text{at}}$  do not perfectly match; in the FPMS calculation, there are no potential truncation, thus AXAFS does not appear even with a polynomial background. Furthermore, we confirmed that the whole peaks are not affected by the charge density modulation, thus AXAFS are not affected by the interatomic charge density, contrary to previous studies.

## References

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