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Continuous Cauchy wavelet transform analyses of EXAFS spectra: A qualitative approach

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ABSTRACT

To better understand the extended X-ray absorption fine structure (EXAFS) spectroscopic information obtained for complex materials such as those encountered in Earth materials, we propose to use the Continuous Cauchy Wavelet Transform (CCWT). Thanks to this method, EXAFS spectra can be visualized in three dimensions: the wavevector (k), the interatomic distance uncorrected for phase-shifts (R'), and the CCWT modulus (corresponding to the continuous decomposition of the EXAFS amplitude terms). Consequently, more straightforward qualitative interpretations of EXAFS spectra can be performed, even when spectral artifacts are present, such as multiple-scattering features, multi-electronic excitations, or noise. More particularly, this method provides important information concerning the k range of each EXAFS contribution, such as next nearest-neighbors identification. To illustrate the potential of CCWT analyses applied to EXAFS spectra, we present experimental and theoretical spectra obtained for thorite and zircon at the Th L_{II} and Zr K edges, respectively. Then, we present CCWT analyses of EXAFS spectra collected for amorphous materials of geochemical and environmental interest, including sodium trisilicate glass and an aqueous chloride solution, at the Mo K and Au L_{III} edges, respectively. Further studies based on CCWT phase terms are underway, in order to quantitatively characterize anharmonic information from EXAFS contributions.