

DWT is an algorithm for signal processing based on frequency decomposition. Compared with conventional Fourier transform, DWT has attractive characteristics of time-frequency localization and multiresolution analyses. In DWT, mother wavelet $\psi_{j,k}(t)$ and father wavelet $\phi_{j,k}(t)$ are dilated and translated to

$$\psi_{j,k}(t) = 2^{-j/2} \psi(2^{-j}t - k) \quad (\text{S1})$$

$$\phi_{j,k}(t) = 2^{-j/2} \phi(2^{-j}t - k) \quad (\text{S2})$$

j represents the scale and frequency; k represents the translation (wavelength in spectral data). It is assumed that spectra are consisted of noise (high frequency), spectral lines (medium frequency), and background (low frequency). $\psi_{j,k}(t)$ and $\phi_{j,k}(t)$ are respectively considered as a high and low pass filter for LIBS spectral data. In this work, the Daubechies wavelet family was adopted with the wavelet function db5, db6, db7, and db8 according to spectral characteristics in FL-LIBS. The $\psi_{j,k}(t)$ and $\phi_{j,k}(t)$ function graphs were shown in Fig. S1. Any spectrum can be decomposed as:

$$f(t) = \sum_{k \in Z} a_{J,k} \phi_{J,k}(t) + \sum_{j \leq J} \sum_{k \in Z} d_{j,k} \psi_{j,k}(t) \quad (\text{S3})$$

$\sum_{k \in Z} a_{J,k} \phi_{J,k}(t)$ and $\sum_{j \leq J} \sum_{k \in Z} d_{j,k} \psi_{j,k}(t)$ represent components of high frequency and low frequency in the spectral data, respectively; $a_{J,k}$ and $d_{j,k}$ correspond to detail and approximation coefficient. Noise often exists in high-frequency coefficients $d_{j,k}$ because of the irregular point of signal caused by it. Therefore, threshold processing for wavelet's high-frequency coefficients is the core of denoising. The algorithm was programmed using Matlab 2018b.

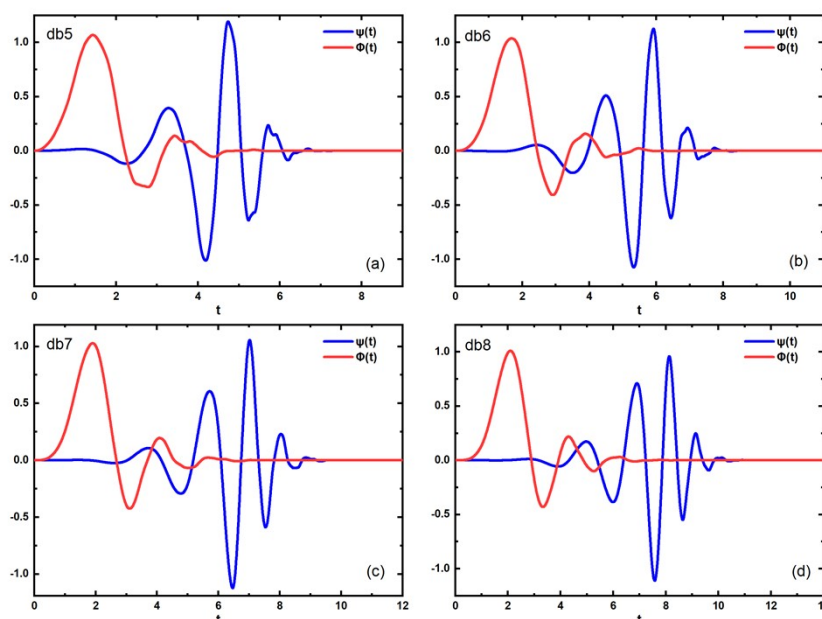


Fig. S1. Mother wavelet $\psi_{j,k}(t)$ function (blue line) and father wavelet $\phi_{j,k}(t)$ (red line). (a)db5; (b)db6; (c)db7; (d)db8.