MCMCBISA

Positron Annihilation Lifetime Spectroscopy

For the researchers or companies who want to extract the lifetimes and relative weigths of the components formig the PALS spectrum that characterize material defects and vacancies on an atomic scale we **offer** a new procedure **that overcomes** the inherent ambiguity involved in solving the inverse problem. **Unlike** other avaible methods **our solution** is to **combine** a Markov chain Monte Carlo Bayesan inference (**MCMCBI**) together with a simulated annealing algorithm (**SA**). **It provides** a robust tool for fitting **a parameter-dependent model** to the experimentally data and gives information on the reliability of the results. **We demonstrate** its high-resolution capability and usefulness for analyzing **multicomponent positron lifetime spectra** in polymers.

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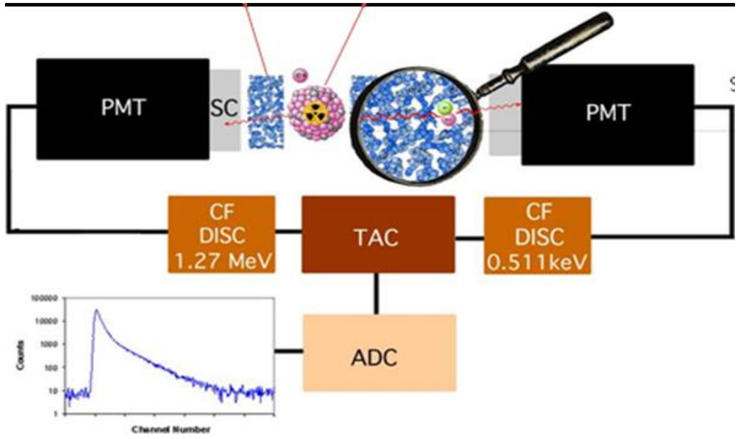
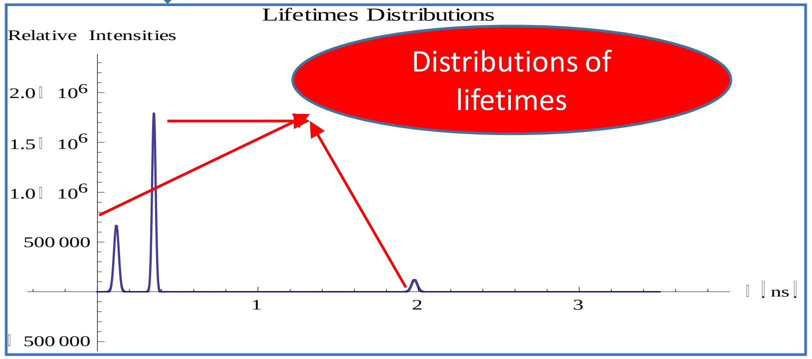
PALS spectrometers and electronics



The resulting PALS spectrum is a histogram of the number of counts with a particular lifetime



Features

- Bayesian analysis with variaty prior and proposal structures
- Random search
- MCMC and SA methods
- Coded in Mathematica

Benefits

- Allows user to specify the statistics for the data and to include any prior kowledge for the parameters
- Robust fitting tools
- Independent of the user's biase for the initial choice of the parameters
- Creating or modifying matherials for improved performances

- **The application of PALS <u>for interrogating defects and pores in metals, ceramics and polymers</u>** is well established.
- **PALS indicates characteristic of the physicochemical properties of the material.**