Extending WiMDA for the data analysis of μ^-SR experiments

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Extending WiMDA for the data analysis of μ^-SR experiments

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Abstract. A software extension to the Windows Muon Data Analysis software package WiMDA has been developed for the analysis of μ^-SR data, which has been dubbed Negative-WiMDA. In designing Negative-WiMDA, some key features were considered: it should be easily accessed from the main analysis window of WiMDA; it should be able to account for multiple elements in a sample; it should be able to subtract signals treated as unwanted background, allowing the user to focus on a particular element of interest; it should be able to handle transverse-field (TF) data, and perhaps most importantly, it should be intuitive to use. The main features of Negative-WiMDA are presented here with a few examples of their use.

1. Introduction

The negative muon is often overlooked compared to its positive counterpart, partly due to the loss of around $\frac{5}{6}$ of the μ^- spin polarisation when a μ^- cascades down to the $1s$ muonic ground state after being captured by a nucleus. One needs to count for around 36 times as long to get statistics comparable to those of a μ^+SR experiment. This is one of the main reasons why μ^-SR has been exploited much less intensively than μ^+SR. However, due to the intense pulsed muon sources at ISIS and J-PARC and the development of a multi-detector counting system [1] there has been a recent revival of μ^-SR experiments, particularly in the study of hydrogen storage and battery materials [2, 3]. When stopped in a material of atomic number Z, μ^- forms a muonic atom and cascades down to its ground state. The muon Bohr radius is around 200 times smaller than the electron Bohr radius, and so this probe behaves like an ultra-dilute atom of apparent nuclear charge $Z-1$. The μ^- will be strongly hyperfine coupled to any nuclear spin on the capture atom, but if that nuclear spin is zero, as occurs for example with oxygen in MnO or carbon in graphite, the only coupling will be to the nuclear dipolar fields in a region very close to that capture nucleus. Another difficulty faced when performing μ^-SR experiments is that the average lifetime of a muonic atom depends on Z due to differing rates of nuclear capture. This means that the electron yield can be small compared to the positron yield in experiments with positive muons. This naturally leads to difficulties performing measurements on samples with $Z > 20$. Figure 1 shows how the average lifetime of muons is influenced by nuclear capture in each of the first 20 elements.

Despite these experimental difficulties, there has been a recent resurgence of μ^-SR experiments. Since there has been a lack of suitable fitting programs for the analysis of μ^-SR

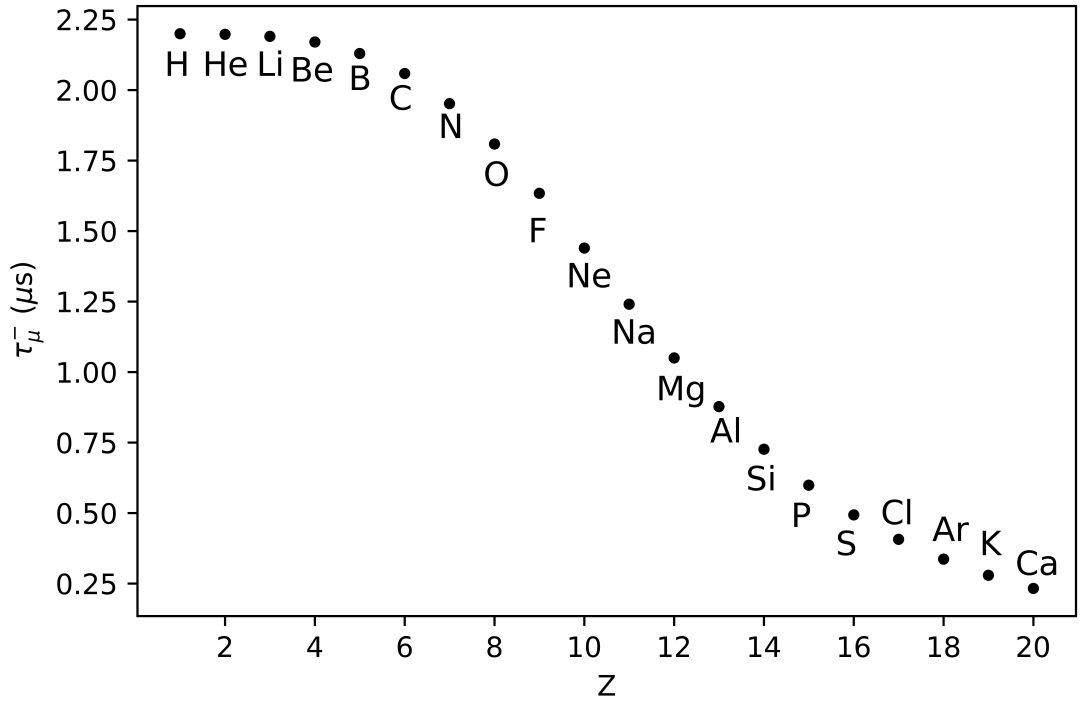

Figure 1. The average lifetime of negative muons captured in each of the first 20 elements.

data, new techniques have needed to be developed for this purpose, which have now been implemented in the Windows Muon Data Analysis software package WiMDA [4]. More detailed introductions to μ^-SR can be found in [5, 6]. In this paper, we describe the analysis software that has been developed and demonstrate its use in two example studies: MnO and graphite.

2. Negative-WiMDA

Figure 2(a) shows the main analysis window in WiMDA where the new polarity feature is illustrated (red box Figure 2(a)). If the muon data is available in the Nexus version 2 data format, then the file can contain information about the muon polarity. However most muon data collected to date does not contain this information. WiMDA therefore recognises whether an experiment was performed at a facility where negative muons could have been used and in this case it makes available a polarity selection button in the main analysis window. This button is hidden when only positive muons are available, i.e. for the EMU, HiFi and MUSR instruments at ISIS. The Negative-WiMDA window becomes visible and active on switching the polarity button to negative. This new window is shown in Figure 2(b). It allows for up to 5 elements to be included in the fit, plus a background component with a long-lived decay. Check boxes select which of these terms to include in the fitting (red box Figure 2(b)). The elements are selected in the tau lifetime box (blue box Figure 2(b)) where there is a drop-down

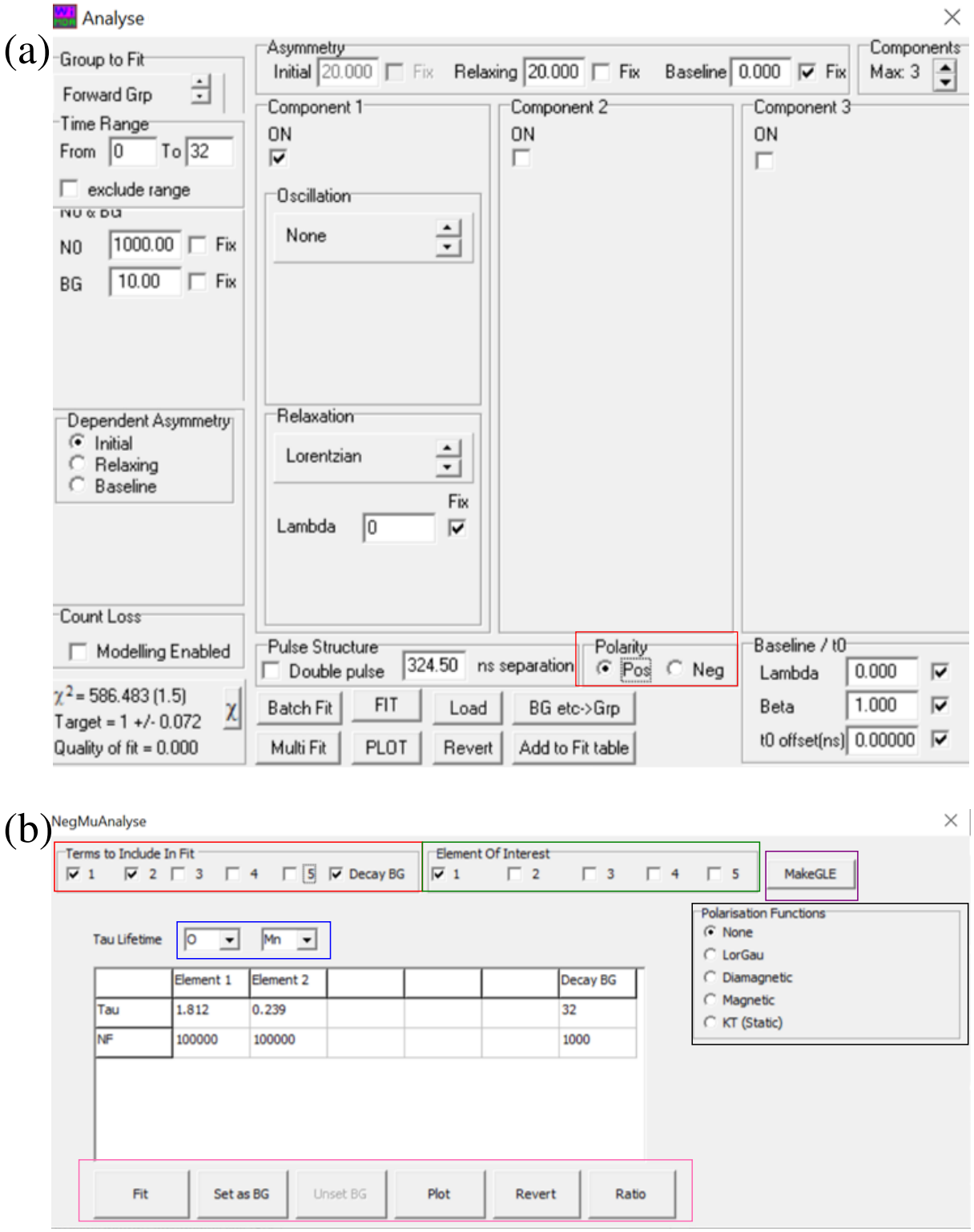

Figure 2. (a) The main analysis window in WiMDA with the new polarity button feature which allows users to open up (b) Negative-WiMDA, which has the main features surrounded by coloured boxes to make them easier to reference in the text.

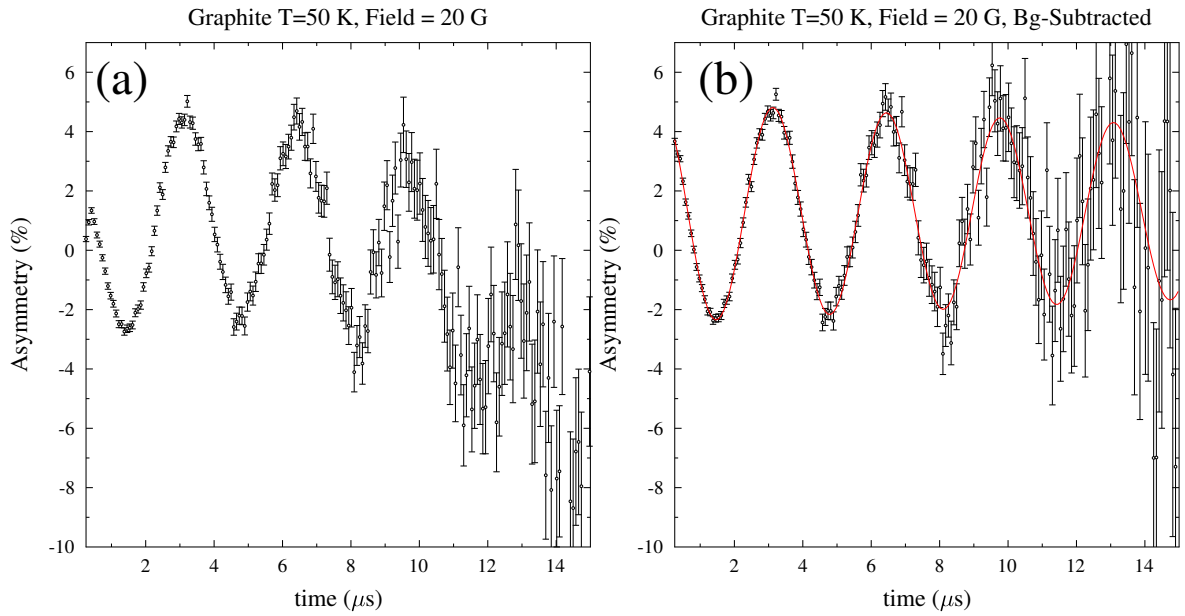

Figure 3. (a) The unsubtracted graphite signal and (b) the background subtracted asymmetry signal for graphite from a μ^-SR experiment with an applied 20 G TF.

menu of elements from hydrogen to lead. The average lifetimes of muons captured by these elements are then automatically initialised ready for fitting. Because the muon lifetime depends on the nucleus in which it is captured, it leads to a multi-component signal that complicates the analysis. However, this problem can be circumvented by subtracting the signals from the unwanted elements as a background signal. This works particularly well in the case where the signal of interest is from long lifetime light elements such as oxygen and carbon and the unwanted signals come from elements that have high Z and short lifetimes as well as from the long lifetime background. The subtraction can be done in Negative-WiMDA by first selecting the element of interest (i.e. the signal you wish to keep). In Figure 2(b) (green box), the element of interest has been selected as oxygen. Clicking the set as background button (pink box Figure 2(b)) after completing a successful fit using the fit button will subtract the fitted parameters from the total signal, leaving the user with just their desired signal of interest. Background subtraction is demonstrated in Figure 3 for a sample of graphite. The normalised count data was fit using the equation

$$N_{F,B}(t) = \sum_{i=1}^{4} N_{i,F,B}(t)\left(e^{-\frac{t_1}{\tau_i}} + e^{-\frac{t_2}{\tau_i}}\right)\left[1 + A_i e^{-\lambda_i t}\cos(\nu_i t + \phi_i)\right], \quad (1)$$

where the sum runs over the three elements included in the fit plus a long-lived decay background which is attributed to particles other than decay electrons from muons. In eq (1), t_1 and t_2 are used in the exponential terms involving the muon lifetime because the ARGUS instrument at ISIS operates with a double pulse structure at 40 Hz. Copper and zinc were also included in the fit because the graphite was contained in a brass sample holder. N_i is the normalisation constant at $t = 0$ for the ith decay process, τ_i is the average muon lifetime for the ith decay process, A_i is the muon decay asymmetry, which is non-zero only for the carbon contribution, ν_i is the frequency of muons precessing in the applied TF, and ϕ_i is the phase. This data was taken with an applied field of 20 G, and hence a polarisation function was added to the fit to

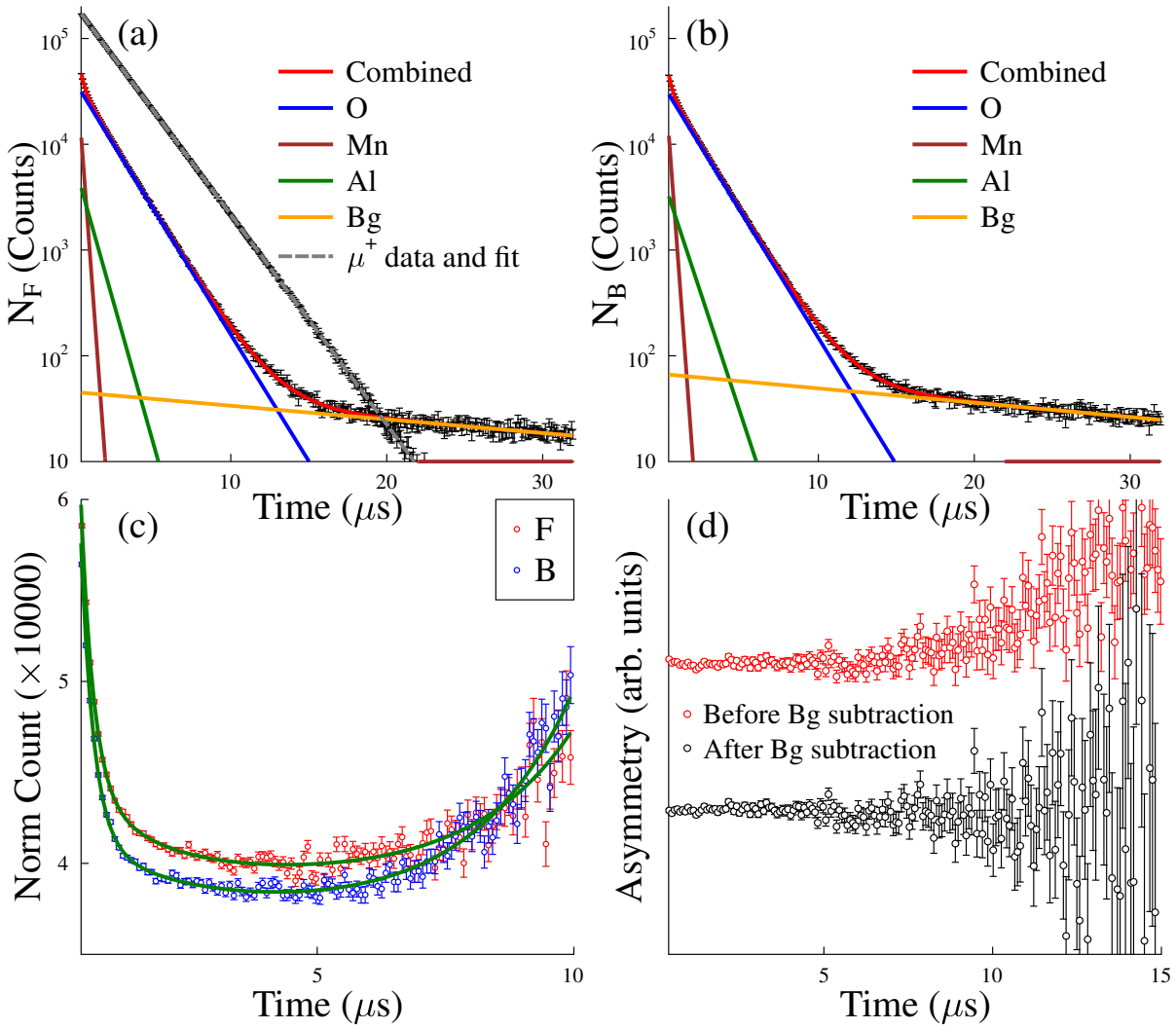

Figure 4. The time histograms for the ZF-μ^-SR spectrum in MnO for (a) the forward (F) detector and (b) the backward (B) detector. For comparison, the μ^+SR data and fit for MnO are shown in (a) where one can see just a single component in the decay signal, that being the free decay time of the muon. (c) The fitted F,B groups for MnO showing the count normalised to a decay with half-life $\tau_O = 1.8097\ \mu s$, reflecting the element of interest. (d) Asymmetry shown before and after background subtraction.

account for this (black box Figure 2(b)). After fitting, the background is removed and the new asymmetry is recalculated using

$$A(t) = \frac{N_{\mathrm{F,graphite}} - \alpha N_{\mathrm{B,graphite}}}{N_{\mathrm{F,graphite}} + \alpha N_{\mathrm{B,graphite}}}, \tag{2}$$

where α is included as a balancing factor to compensate for the difference in efficiency between the forward and backward detectors. Notice in Figure 3(a) that the unsubtracted data has a strange blip in the asymmetry at very short times because the copper and zinc contributions dominate in this region. At longer times, where the long-lived decay background dominates, the

asymmetry drops drastically after 10 μs. When the background has been removed, we see the signal from the carbon contribution only, and there is minimal relaxation taking place, which has been shown to agree with [7]. The errors in the data increase significantly after around 10 μs which is a residual effect of having the long-lived background in the original data.

When analysing data from μ^-SR experiments, one often wants to show the individual contributions of the elements making up the data. The analysis software is capable of producing such figures at the click of a button (purple box in Figure 2(b)). It recognises which elements are included in the fit, and saves their individual contribution to the overall spectra. The software then writes the data to a file which can be exported as a PDF. This can be seen in the example of MnO shown in Figure 4. The data from a matching μ^+SR experiment have also been included in Figure 4(a) to highlight the major differences in spectra arising from $\mu^\pm$SR experiments, and why we need these new analysis techniques.

3. Conclusion

Owing to the increase in popularity of μ^-SR experiments, data analysis software has been developed and implemented into WiMDA to aid users with making real time decisions about their experiment and subsequent analysis. The use of its main features have been demonstrated on samples of MnO and graphite. The new capabilities in WiMDA for μ^-SR data analysis will be made available in the forthcoming release of the WiMDA package [4]. The latest version of WiMDA is available to download at http://shadow.nd.rl.ac.uk/wimda/, along with detailed instructions on installation.

4. Acknowledgments

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