Monte Carlo simulation using GEANT 4 of the EMU μMSR facility at ISIS

JM Hartman SH Connell

University of Johannesburg, Johannesburg, South Africa

E-mail: `hartman.jonathan2@gmail.com`

Abstract. A Monte Carlo simulation has been performed for studying Muon Spin Rotation, Resonance and Relaxation (MSR) measurements on the EMU apparatus of the ISIS facility of the Rutherford Appleton Laboratory in the UK. In these measurements, implanted muons which are almost fully polarised act as local probes of their magnetic environment within a particular host material to be studied. The evolution of the polarization of the muon ensemble is monitored by observing the decay positrons. The purpose of the study was to understand that false asymmetry that can be observed for samples small compared to the beam lateral dimensions. In this case, a significant number of the muons stop and decay outside and downstream of the sample. The GEANT 4 toolkit was used for developing the Monte Carlo simulation. This is a set of C++ libraries developed by CERN to simulate particle physics experiments. However, GEANT 4 can be also be used for other applications that need not have anything to do with particle or high-energy physics. In the simulation, the effect of the external magnetic field on both the incident muon and decay positron trajectories is modeled. It is shown that this leads to a strong field dependence in both the stopping location of muons and the efficiency of the positron detection. The various contributing factors to the systematic field dependent false asymmetry could be quantified. The simulation has been performed in support of the interpretation of experiments on diamond samples where the behaviour of the hydrogen-analogue atom, muonium, is studied.

1. Introduction

The type of MSR measurement being simulated involves the observation of muon ensemble polarization as a function of the longitudinal external magnetic field (LF-μSR). This data can then be decomposed into separate relative contributions from the three states for the muon typically observed in semi-conductors and wide band gap materials. These are the bare muon, muonium, dimagnetic muon state. The EMU facility has no detector to veto the flypast muon, which are significant for small samples, and which therefore contribute to the data as a false field dependent asymmetry. The Monte Carlo simulation is required to quantify separately the contributions to the false asymmetry from both the field dependent changes to the muon and the position histories.

2. Simulation of MUSR

Using the Geant 4 library, the application first creates the geometry of the EMU Spectrometer at the ISIS facility. The geometry simulated by the application consists of a tube with the diamond sample in the center and detectors along the outside of the tube. In the centre and the source of the muons at one end and a stop at the other end. Added to the the setup is also a simulated magnetic field generated by two loops of current, the purpose of which is to create a focusing effect on the muon beams in order to focus them on the diamond. In order to calculate the resultant magnetic field, the field from each of the two loops are calculated separately and then added together vectorially at every point in space. The accuracy of the computed value of the magnetic field was checked by visually comparing the radius of the helical track made by a charged particle in the field to the calculated value made by a pen and paper calculation.

The starting position of the beam is varied randomly within a circular radius of 5 cm at the source of the muon beam. The application was run over a range of diamond sizes, and field strengths on the UJ cluster using a Swift script (although it could also be run on the SA Grid without swift) in order to determine the asymmetry as a function of diamond size and field strength. In order to parallelize each run across many processes, a single run consisting of many events is broken up into multiple runs each with a smaller number of events but each starting with a different random number seed so that there is still a different random distribution for each these separate runs. The An extra utility was added to be able to kill the secondary tracks depending on whether it originates from the diamond or not. In this way, one would be able to plot the true asymmetry of just the positrons resulting from muons that interacted with the diamond separately from the false asymmetry from the positrons that did not originate from the diamond. Each run on the cluster outputs a single line of data in a text file. When the application is finished running on the cluster, all the data from each of these output text files can be collected into a single file by the *cat* command. This data text file can be opened in a spreadsheet program, making sure to use a space separated option, in order to remove the unnecessary data and text before being read by a second ROOT application used to plot the data. The ROOT application scans the text file and takes the average of the asymmetry values corresponding to the same values for field strength and diamond size but have different random number seeds. The application then plots a 3D graph of the data using the histogram object in ROOT's library.

The calculations were then repeated except that it was done for a columnated beam of muons and with the number of muons hitting the diamond were counted instead of the asymmetry being calculated. The purpose of this was to check that the simulated magnetic field focuses the beam on the diamond sample as expected. The result of this calculation can then be compared with experimental data. In this case, each run of the application on the cluster still outputs a text file of a line of data like before when the asymmetry is being calculated, except that it outputs an extra variable which is a count of the number muons that interacted with the diamond in that run. This data can be collected into a single text file as before, although it's also read by a modified version of the ROOT application that was previously used to plot asymmetry with respect to the field strength and diamond size. The modifications to the ROOT application are to take into account the fact that the number of muon interactions with the diamond sample are to be plotted against the field strength and diamond size instead of the asymmetry and that the number of hits calculated with different random number must be added together instead of the average taken. This graph is created using a graph object instead of a histogram object in ROOT's library in order to be able to plot logarithmically spaced data.

3. Results from the Geant 4 simulation

The results are as follows. As shown in figure 1, the total asymmetry forms a slope with respect to the diamond size as well as a small slope that increases with an increase in field strength.

It would be expected that most of the slope with respect to field strength as shown in figure 1 must be due to the false asymmetry from the positrons that originate from the beamstop rather than the diamond sample since the field at the center is symmetrical. This is the case because

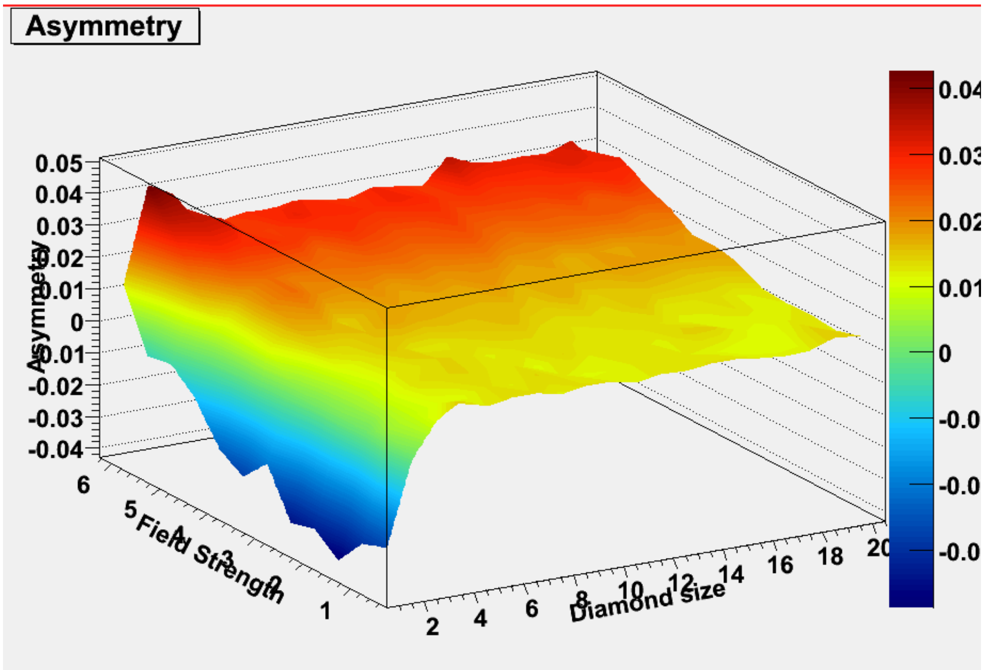

Figure 1. Total asymmetry calculated from the application. This figure is slightly noisy due to statistical fluctuations in the random number generation.

when only the asymmetry due to the positrons originating from the sample is plotted against diamond size and field strength, then the slope of the graph with respect to field strength is extremely small compared to that in figure 1 as shown in figure 2. A cross section of figure 2 at a diamond size of 5 mm is shown in figure 3.

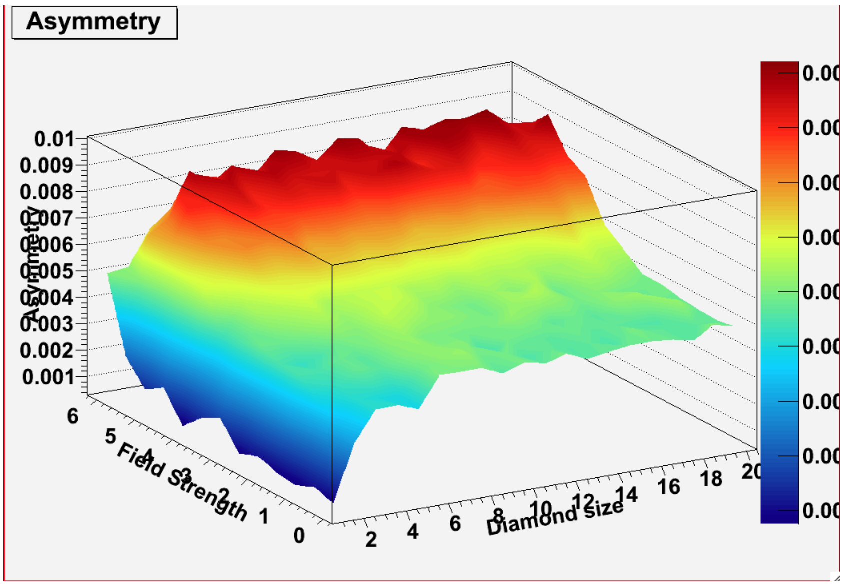

Figure 2. Asymmetry of the positrons originating from the diamond. Again, there are statistical fluctuations in the data.

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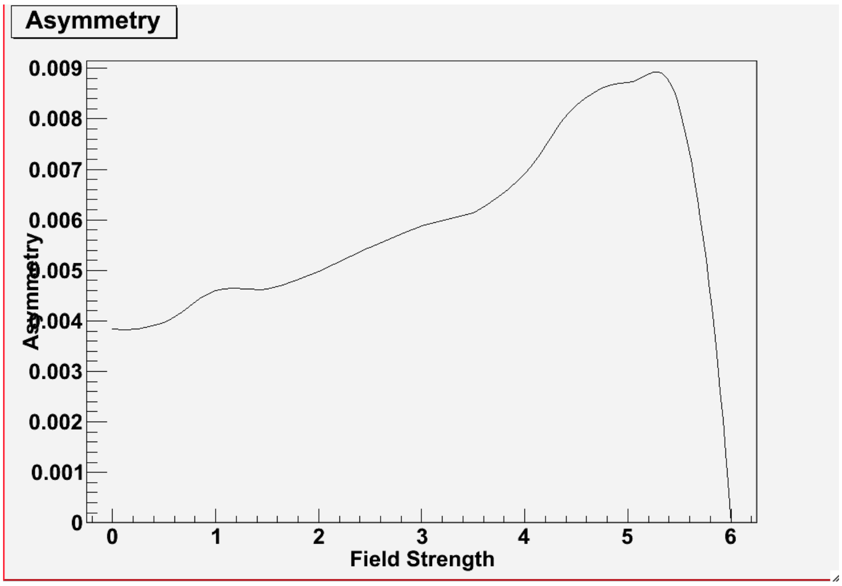

Figure 3. Asymmetry of the positrons originating from the diamond when the diamond size is 5 mm.

Figure 4 shows the false asymmetry due to positrons originating from the beam stop.

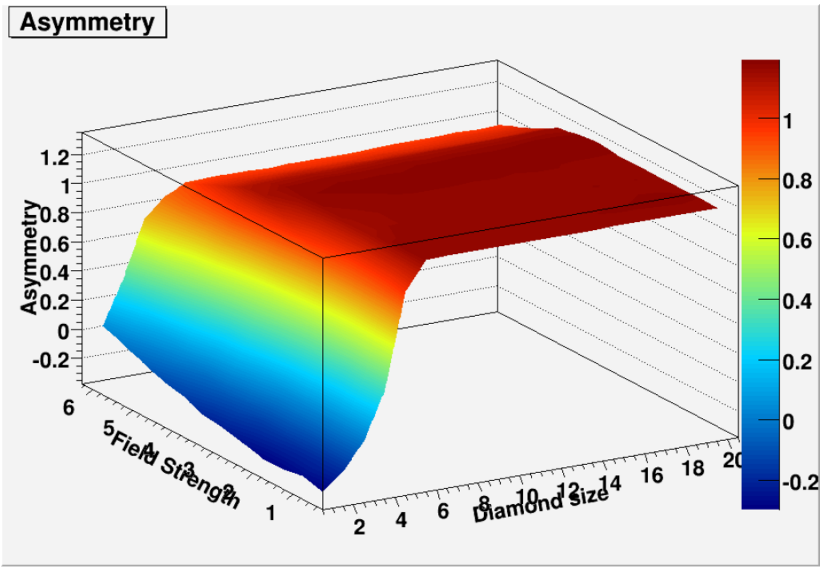

Figure 4. False asymmetry due to the positrons originating from the beam stop.

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Figure 5 shows the number hits or muon interactions with the diamond with respect to diamond size and field strength. Field strength is plotted on a logarithmic scale. The number of hits increase smoothly with respect to diamond size. The increase in the number of hits with respect to field strength is steeper.

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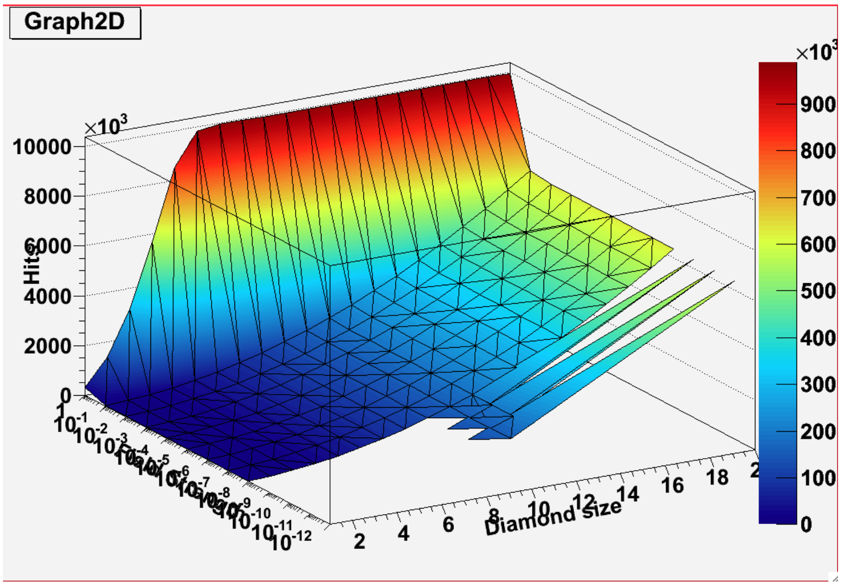

Figure 5. Number of muon interactions with respect to diamond size and field strength, calculated using a columnated muon beam. The triangle objects represent Delaunay triangles which is what ROOT used to render a 3D graph object, as apposed to histogram objects.

4. conclusions and further work

As expected, figures 2 and 4 indicate that most of the asymmetry with respect to field strength as shown in figure 1 is actually the false asymmetry due to positrons originating from the beam stop. One would expect that there would be no asymmetry in figure 2 at all due to the fact that the magnetic field should be completely symmetric about the center of the tube where the diamond sample is placed, however the muons might only interact when they hit the surface of the diamond. Since, in the simulation, the diamond was centered at the center of the tube, the surface where the muons would interact is slightly offset from the center and this is probably the reason for the small asymmetry as shown in figure 2.

The way the number of muon hits increase with field strength and diamond size for the columnated muon beam is exactly what is expected. It appears as though the application correctly simulates what the field in the experimental setup was designed to do.

In future work, the following goals will be persued:

1. Determine the field dependence of the detector efficiency for positrons originating from the sample.
2. Determine the field dependent distribution of impact positions of flypast muons.
3. Determine detector efficiency for positrons originating from flypast muons