Characterization of plastic scintillators using magnetic resonance techniques for the upgrade of the Tile Calorimeter in the ATLAS detector

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Abstract. In this study we look at radiation damage and its adverse effects on plastic scintillators housed within the Tile Calorimeter (TileCal) of the ATLAS detector. The study focuses on determining how the interaction of ionizing radiation with plastic scintillators effects their efficacy and desired properties such as high light output and fast decay time. Plastic scintillators form an integral part of the ATLAS trigger system and their optimal functionality is paramount to the success of ATLAS. Electron paramagnetic resonance (EPR) provides insight into the electronic structure of the plastics and can characterize the damage caused by ionizing radiation. Density functional theory (DFT) calculations will be performed in order to simulate the EPR signal. Preliminary EPR results investigate four different types of plastic scintillators. These include three polyvinyl-toluene based Eljen technologies: EJ200, EJ208 and EJ260, and one polystyrene based Dubna sample. It has been observed that the Dubna sample, identical on the current scintillator used in the ATLAS detector, undergoes more structural damage when compared to the Eljen samples.

Introduction
The increase in luminosity to $\sqrt{s} = 13$ TeV at the start of Run 2 in April 2015 will require that the Large Hadron Collider (LHC), its four detectors, and various components be upgraded in the phase one upgrade in 2018 [1].

The minimum bias trigger scintillator (MBTS) plastics are situated around the beam pipe and have a pseudo-rapidity, $\eta$ of $2.07 \leq |\eta| \leq 3.84$ [2]. There are, 16, 2 centimetre thick, polystyrene based plastics on each side of the ATLAS detector. The plastics are manufactured in Dubna and doped with 2% organic dopants optimize their functionality. Their main purpose, before nominal operation of the LHC, was to veto background from the beam and, since an effective mean was needed for proton-proton collisions, they provided a vital role in providing this. When the MBTS plastics interact with energetic particles, they produce light that is passed down to photo-multiplier tubes (PMTs) via wavelength shifting fibres where they are converted into a digital signal and analysed. However, these plastics are susceptible to radiation damage induced by the energetic diffractive particles that interact with them and it has been found that this interaction causes bonds to break in the benzene ring which is found in the molecule and is responsible for the scintillation mechanism in the plastics [3].
This study investigates the effect ionizing radiation has when it interacts with the various types of plastic scintillators. Electron paramagnetic resonance (EPR) investigates unpaired electrons and ions that are formed due to structural damage [4]. In addition to this, an ab initio computational approach will be used in order to replicate the EPR spectra seen by isolating the benzene derivative molecules responsible for scintillation the plastic scintillators.

Electron Paramagnetic Resonance

EPR spectroscopy is a powerful technique for studying unpaired electrons and ions in samples. Experimental results have shown that, as the energetic particles ionize the plastics, C-H bonds in the benzene derivative molecules break [5]. Therefore, employing EPR will allow us to gain vital information about the electronic structure of the samples. When a sample is placed between a large, homogeneous magnetic field, the magnetic moments of the unpaired electrons and ions couple to the magnetic fields. A resonance frequency, $\omega$, is then applied and corresponds to a transition between the two spin states. An absorption energy can be seen described by the resonant condition:

$$\Delta E = \hbar \omega = g \mu_B B_0,$$

where $\mu_B$ is the Bohr magnetron, $B_0$ is the external magnetic field intensity, and $g$ is called the g-factor.

Materials

Replicating the harsh environment the scintillators experience within the ATLAS detector is a non-trivial task. Two types of scintillators were considered for this study: one polyvinyl-toluene based sample with three candidates of Eljen technology and one polyester based sample. The three Eljen samples are named EJ200, EJ208 and EJ260. The Dubna sample is identical to the MBTS plastic used in the ATLAS detector. Each of these samples contain their respective dopants that aid the scintillation mechanism.

The tandem accelerator at iThemba Laboratory for Accelerator-Based Sciences (LABS) provided energetic proton beams that irradiated the samples. The 3 MV tandem accelerator is capable of energizing protons to around 6 MeV. This is sufficient to replicate the radiation environment seen by the MBTS plastics in the ATLAS detector. The particle interaction with the material was modelled using SRIM (Stopping and Range of Ions in Matter) which predicted that the stopping range in the two types of scintillators which occurred around 470 $\mu$m for the 6 MeV protons[6]. TRIM (Transport of Ions in Matter), an extension of SRIM, was used to calculated the average energy of each impinging proton at around 2.07 MeV. This value was needed to calculate the total absorbed dose that the scintillator experiences by the protons. Before this could be done, each sample needed to be machined to a size that would fit onto a carousel placed into the tandem accelerator and a width less than the stopping range. A volume of $1 \text{ cm} \times 1 \text{ cm} \times 250 \mu\text{m}$ was chosen and each sample was cut and polished to match this volume. Each plastic type was irradiated to two doses: 0.164 MGy and 1.46 MGy where Gy is the absorption of a joule of radiation energy per kilogram [7]. The absorbed dose was calculated using

$$D = \frac{I_b A E_{\text{ave}} \Delta t}{q m_{\text{ir}}} \text{Gy},$$

where $I_b$ is the beam current, $A$ is the area of the irradiated spot, $E_{\text{ave}}$ is the average energy per proton, $\Delta t$ is the time spent irradiating the sample, $q$ is the charge of the proton, and $m_{\text{ir}}$ is the mass of the irradiated spot. After each sample has been irradiated they (and the un-irradiated samples) can undergo EPR testing. EPR experiments were performed at the University of Witwatersrand and have verified this assumption as a signal from both un-irradiated and irradiated samples were seen.
**EPR Results**

The following results show the peak intensities of different samples. The peak heights are in arbitrary units as because they depend on sample size. However, since each sample has the same density and volume we do not need to apply a mass normalization. The resonant frequency is kept constant and the magnetic field is swept. Absorption peaks form at different magnetic field intensities depending on the which type ion is being detected.

Un-irradiated samples seen on the left of figure 1 (a) show that unpaired electrons and ions exist in the sample before irradiation. This is indicated by the absorption observed around 3488 Gauss which corresponds to the intensity of unpaired electrons in a sample.

Figure 1 (b) clearly indicates secondary peaks begin to form as samples are irradiated. The interaction with the ionizing radiation causes a formation of new unpaired electrons and ions ultimately damaging the scintillation mechanism as it alters the structure of the scintillator.

Un-irradiated samples at different doses

**Figure 2:** Comparison of polyvinyl-toluene sample EJ208 (a) and polystyrene sample Dubna (b) at various doses as magnetic field is swept for a constant resonant frequency.
Figure 2 (a) indicates the change is spectra of a polyvinyl-toluene sample, EJ208 and polystyrene Dubna sample (figure 2(b)) as dose is increased inducing more damage. It is evident that, initially, there is a larger intensity of unpaired electrons in EJ208. As the samples are bombarded by protons this intensity decreases. This is could be due to the C-H bonds breaking, releasing electrons and unpaired hydrogen atoms in the sample.

**Future Work**

**Computation Replication of Results**

EPR spectroscopy is a characterization technique and give a qualitative view of the scintillators and how damage alters their structure. A quantitative approach is needed in order to fully understand the problem. Thus, we look to model the system using a computational ab-initio approach. This will be done using density function theory (DFT) which is a theory for a correlated many-body systems that views any property of the system as a functional ground state energy, $E_0(\vec{r})$ [8]. From the ground state functional properties about the electronic structure of the system can be derived.

By isolating the optically active molecule (the benzene ring and its functional groups responsible for the scintillation mechanism) for both polyvinyl toluene and polystyrene, we can use DFT methods to simulate the EPR [9]. The goal would then be to correlate the two spectra sets with properties from the DFT predictions. These include, but are not limited to, number of unpaired electrons and ions in the system, ground and excited states of the system, and identification of functional groups and ions in un-irradiated and irradiated samples.

**Conclusion**

This project, accompanied with various other studies done on the plastic scintillators aims to find a suitable candidate for the replacement of the MBTS plastics as well as the plastic scintillators housed inside the gap region of the TileCal once they have lost their efficacy. We would also have a deeper understanding of radiation damage in plastic scintillators as a whole and hopefully this knowledge would aid in the design and manufacture of a plastic scintillator that is less susceptible to radiation damage than the technology currently available.

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