A Density Functional Theory and Magnetic Resonance Study of Radiation Damage in Plastic Scintillators

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Introduction

Energetic particles are detected in particle detectors as they pass through plastic scintillators. This interaction damages the plastics breaking C-H bonds within the polyvinyl-toluene (PVT) based polymers [1, 2]. In this study we aim to characterise the damage in the plastics caused by radiation damage using electron paramagnetic resonance (EPR) and we attempt to simulate the EPR spectra using a post density functional theory (DFT) method.

Theory

EPR is used to study the unpaired electrons and ions formed when bonds break in the plastics. This is done when samples are placed in a homogeneous magnetic field. When a resonant frequency is applied, an energy absorption peak is measured experimentally as a result of a transition between spin states. We can write down the Hamiltonian that shows the electron spin coupling $\vec{S}$ with the magnetic field, $\vec{B}$, and nuclear spin $\vec{I}$.

$$\mathcal{H} = \beta\vec{B}\cdot\mathbf{g}\cdot\vec{S} + \sum_l \vec{S}\cdot\mathbf{A}_l\cdot\vec{I}_l. \qquad (1)$$

We obtain information about the electronic structure of the system experimentally and computationally by analysing the g-tensor, **g**, and hyperfine-tensor, **A**.

Samples

- Two Eljen PVT plastics, EJ208 and EJ260, were cut and polished to a width of 250 μm.
- Samples are irradiated at iThemba Labs, Gauteng, using the tandem accelerator with 6 MeV protons to ensure ionisation.
- Samples are irradiated with five different doses and compared to an un-irradiated sample

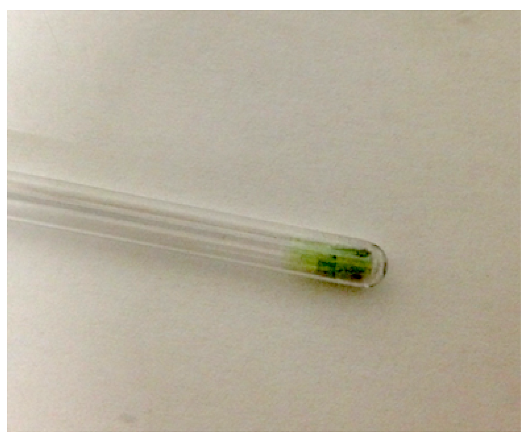

Figure 1: EJ260 irradiated to 80 MGy and placed inside a test tube

EPR Set Up

- Samples were tested using the Bruker ESP380e spectrometer
- A powder average signal is seen resulting in one EPR signal
- The spectra is integrated and analysed

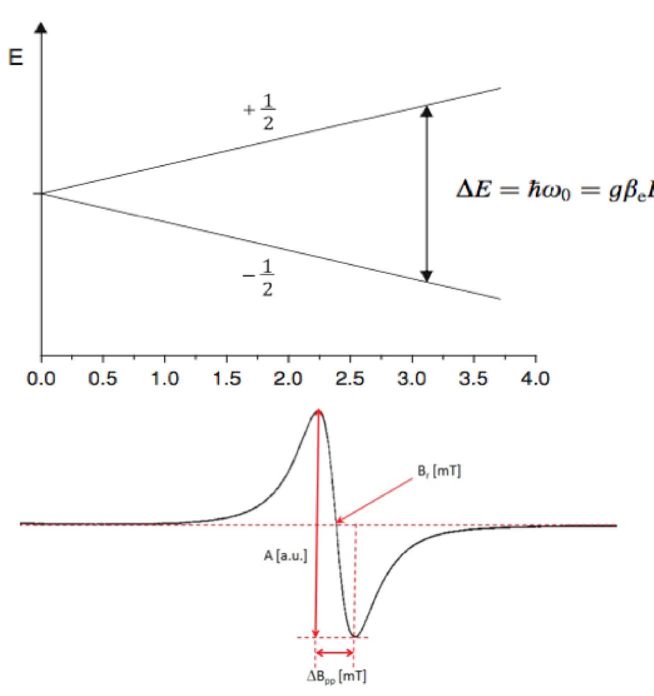

Figure 2: Resonance condition and spectrum

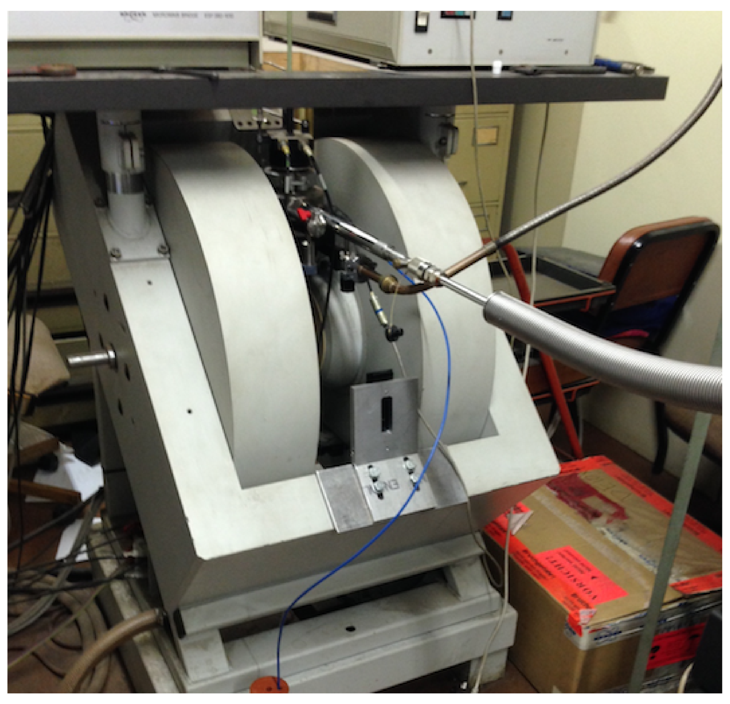

Figure 3: EPR set up at University of Witwatersrand

DFT Theory

We were able to calculate the g-tensor and hyperfine tensor for isomers of the PVT molecule by computing a linear magnetic and nuclear response to all the electrons, respectively, using a gauge including projector augmented wave (GIPAW) method [3, 4]. We can see changes in the g-tensor by removing hydrogen atoms using

$$\mathbf{g} = \mathbf{g}_e + \Delta\mathbf{g}, \qquad (2)$$

where $\mathbf{g}_e$ is the g-tensor of the free electrons.

Experimental EPR Results

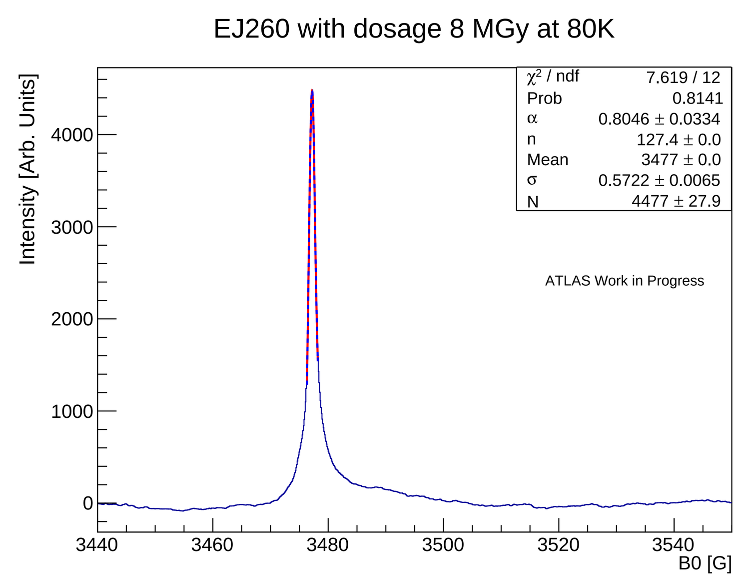

Figure 4: Integrated EPR spectrum for EJ260

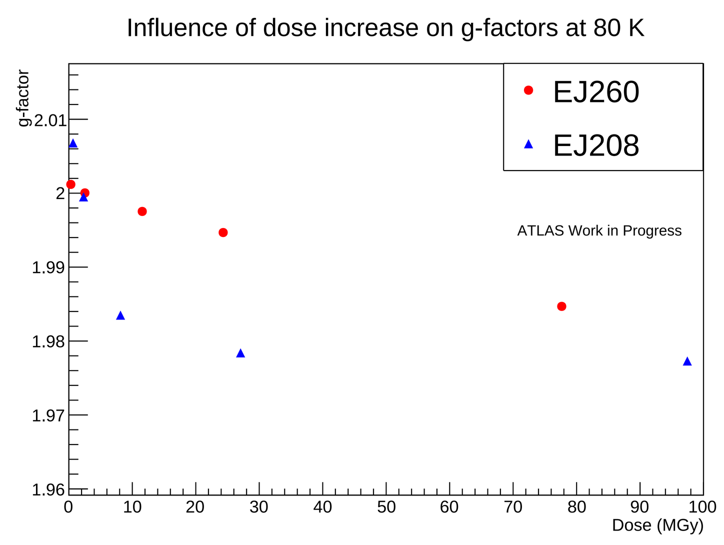

Figure 5: Effect of dose on g-factors of EJ208 and EJ260

Computational DFT Results

Analysis of 1-ethenyl-2methylbezene: an isomer of the PVT molecule

Hydrogens removed	Δg (ppm)			Total Energy (Ry)
	g_{xx}	g_{yy}	g_{zz}	
0	**-0.031**	**0.010**	**0.010**	**-114.167**
1	1065.91	174.41	-1179.69	-113.816
2	1185.23	138.51	-923.10	-113.815
3	-1282.97	-249.87	923.28	-113.811
4	67.25	-657.46	-679.41	-113.813
5	**-0.17**	**0.052**	**0.052**	**-114.064**
6	71.83	-651.25	-677.79	-113.884
7	71.83	-651.25	-677.7996	-113.884
8	**-0.11**	**-0.052**	**0.033**	**-114.171**

Table 1: Shift in g-tensor components and total energy of damaged and undamaged PVT isomer.

- 'Low' total energy values show smaller shift in g-tensor components
- Hyperfine tensor principle components change as samples are damaged effecting principle components of the g-tensor

Conclusion

- Increase in irradiation changes Δg and shows decrease in g-factor experimentally
  - Proton damage disorders plastic structure changing electron environment
- Peak is broadened by increase in number of unpaired electrons and ions
  - Hyperfine tensor changes and newer peaks form in EPR spectra

Future Work

- Four other plastics to be tested: two PVT based and two polystyrene bases
- EPR spectrum to be simulated using DFT calculations

References

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[3] Pickard C J and Mauri F 2002 *Physical review letters* **88** 086403 ISSN 0031-9007 (*Preprint* 0110092)

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Acknowledgments

CHPC Centre for High Performance Computing
South African Institute of Physics
NRF National Research Foundation
iThemba LABS Laboratory for Accelerator Based Sciences

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