Hyperfine Spectroscopy and Characterization of Muonium Centers in ZnGeP$_2$

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Overview of MuSR

- MuSR = Muon Spin Research (Relaxation/Rotation/Resonance)
- App: Semiconductors – exp. analog for H defects
- Implant 100% Spin-polarized Muons
- Spin vector evolves in local magnetic environment
- e\(^+\) emitted preferentially along spin direction
- e\(^+\) count information then analyzed
Muonium

<table>
<thead>
<tr>
<th></th>
<th>Muon</th>
<th>Proton</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass ($m_p$)</td>
<td>0.1126 ≈ 1/9</td>
<td>1</td>
</tr>
<tr>
<td>Spin</td>
<td>$\frac{1}{2}$</td>
<td>$\frac{1}{2}$</td>
</tr>
<tr>
<td>Gyro. Ratio, $\gamma$ ($s^{-1} T^{-1}$)</td>
<td>8.51607 x 10^8 ≈3.2 x $\gamma_p$</td>
<td>2.67520 x 10^8</td>
</tr>
<tr>
<td>Lifetime, $\tau$ ($\mu s$)</td>
<td>2.19709</td>
<td>Stable</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Muonium</th>
<th>Hydrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reduced e$^-$ mass ($m_e$)</td>
<td>0.995187</td>
<td>0.999456</td>
</tr>
<tr>
<td>Ground-state Radius (Å)</td>
<td>0.531736</td>
<td>0.529465</td>
</tr>
<tr>
<td>Ground-state Energy (eV)</td>
<td>-13.5403</td>
<td>-13.5984</td>
</tr>
</tbody>
</table>


Brewer, http://musr.ca
Overview of MuSR: TF

Transverse Field (TF)-μSR

Field applied \( \perp \) to initial spin polarization
\( \rightarrow \) \( \mu^+ \) spin precession about applied field

\( \text{Mu}^0 = \mu^+ + e^- \)
\( \rightarrow \) spin-orbit coupling
\( \rightarrow \) affects local field of \( \mu^+ \)
\( \rightarrow \) diff prec. Freq for:
\( |\uparrow \mu> + |\uparrow e> \& |\uparrow \mu> + |\downarrow e> \)

Brewer, http://musr.ca
Hyperfine Spectroscopy of ZnGeP$_2$
(from TF-$\mu$SR)

- 431.55 MHz (+/- 0.004)
- 1534.07 MHz (+/- 0.06)

$A_1 = \nu_{34} - \nu_{12} = 1965.6$ MHz

$\nu_{12}$
$\mu^+$
$\nu_{34}$

542.16 MHz

Mu$^0$ in ZnGeP$_2$
4.0 Tesla

Overview of MuSR: LF

B applied $\parallel$ to $\mu^+$ spin pol. → breaks HF interaction

$\Rightarrow$ Change in Spin P(t) from:
1) local environment (nearby nuclear moments)
2) muonium motion ($e^-$ spin-flip w/ each site change, transferring back to $\mu^+$ contributing to $\Delta P(t)$)

**HF info from $T_1^{-1}$ depolarization curves (field dep. of Amp.)**

**Current analysis suggests axially symmetric anisotropic HF interaction with:**

$\rightarrow A_2 = 3185 \text{ MHz} \ & D = 374 \text{ MHz}$


Note: TF vs LF results for HF term(s)

TF data:

\[ A_1 = 1961.8 \pm 2.3 \text{ MHz} \]
(isotropic – experimental determination)

LF data:

\[ A_2 = 3185 \text{ MHz} \]
\[ D = 374 \text{ MHz} \]

Why the different HF?

ZnGeP$_2$: Structure

- Chalcopyrite structured II-IV-V$_2$ material
- Zincblende structure (c.f. III-V), doubled unit-cell
- III-Sublattice replaced by II-IV atoms, 1:1
- V replaced by V$_2$
- 2 T-sites: $T_V \ & T_{\text{II-IV}}$
ZnGeP$_2$: II-IV pseudo-T-site

*Unequal charge on Zn (+1.2$q_e$) & Ge (+1.8$q_e$) → distorted 1s $\Psi$
→ anisotropy with [110] axial symmetry

$$\vec{E} = \mp \frac{1}{4\pi\varepsilon_0} \frac{32\sqrt{3}}{9} (q_{Zn} - q_{Ge}) [110]$$

Seen in LF but not TF
$\Rightarrow$ not promptly formed, but visited throughout lifetime

The Sample

Single Crystal

Nominally undoped

7.1x8.5x1.1 mm$^3$

Orientation: [001]
Summary: Mu0 Centers in ZnGeP$_2$

1) Implantation

2) Formation of Mu$^0$ in $T_V$
   with isotropic: $A_1 = 1961.8 \pm 2.3$ MHz
   (Visible in TF)

3) Mu$^0$ hops w/ ID change ea. hop (not discussed)

4) Mu$^0$ in $T_{II-IV}$ with anisotropic:
   $A_2 = 3185$ MHz D = 374 MHz (+/- 10%)
   (Visible in LF Repolarization data)

This completes our discussion of the Muonium centers in ZnGeP$_2$
Thank You
Hyperfine Spectroscopy of ZnGeP$_2$  
(from TF-$\mu$SR)

\[
A(T \rightarrow 0) = 1961.8 \text{ MHz (} +/\- 2.3) 
\]

ZnGeP$_2$: Structure

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