Recent advances in Emission Channeling measurements and relevance to Hyperfine Interactions

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on behalf of IS453 EC-SLI experiment
Emission Channeling with Short-Lived Isotopes

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ABOUT EMISSION CHANNELING
principles and recent progress

LATTICE LOCATION CASE STUDIES

\(^{121}\text{Sn} \ (27\text{h}) : \text{Ge (off-line)}

\(^{56}\text{Mn} \ (2.6\text{h}) : \text{Ge (on-line)}

\(^{27}\text{Mg}(9.46\text{m}) : \text{GaN, AlN (on-line preliminary)}

“BRIEF BRIEFING”
of Timepix 512x512 ch detectors
(high position resolution + energy)
Interest of **accurate** impurity lattice location studies

- Functional properties of impurities are influenced by lattice location
- Local crystal field near impurity influences electronic configuration, magnetic spin
- High quality input information for atomic scale models and simulations

**EMMISSION CHANNELING ALLOWS:**
- determining lattice sites of impurities in **single-crystalline** materials
- **substitutional** site vs. many different interstitial sites
- **quantitative** determination

- highly sensitive: down to ppm range
- lattice location accuracy: down to 0.1 - 0.2 Å
- unique worldwide

(a consequence of the variety and purity of ISOLDE radioactive beams combined with position sensitive electron detectors)
Channeling (RBS/C) versus Emission Channeling

- **positively** charged particles: channeling in between rows of atoms
Electron Emission Channeling

- negatively charged particles
- electrons are emitted by radioactive isotope (C.E. or $\beta^-$)
- channeling or blocking effect – depends on lattice location of impurity
- anisotropic electron emission
2D energy- and position-sensitive detector

analysis = fitting experimental pattern to library of calculated patterns
What do you need to do Emission Channeling

Si PAD electron detectors

5μm kapton
2μm SiO2
0.3mm p (B) implant

Position-sensitive detector

Good energy resolution ~3 keV
Large pad – 1.4x1.4 mm2
Dead / unbonded channels
Leakage current limiting depletion
15keV << E(e^-) << 300 keV
Readout → 200Hz ... 5 kHz(new)!!
New ITN on-line emission channeling setup: side view

- ISOLDE beam is collimated by 2 apertures (1\textsuperscript{st} variable size, 2\textsuperscript{nd} $\varnothing$ 1 mm) on the sample
- sample mounted in remote controlled 3-axis goniometer
New ITN on-line emission channeling setup: top view

- detector at 17° backward geometry for simultaneous implantation and measurement
- valve in front of detector allows to maintain detector vacuum during sample exchange
- lead shielding around 1st collimator lowers background
NEW on-line EC-SLI setup for short lived isotopes

GHM beam line

NEW pad-Si FAST 2D electron detector

Goniometer

NEW cooling system down to 50K

Inside view during sample annealing
Elements for which emission channeling experiments have been published

<table>
<thead>
<tr>
<th>Elements</th>
<th>2007</th>
<th>2009</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>Be</td>
<td>β−</td>
</tr>
<tr>
<td>Na</td>
<td>Mg</td>
<td>2009</td>
</tr>
<tr>
<td>K</td>
<td>Ca</td>
<td>Sc</td>
</tr>
<tr>
<td>Rb</td>
<td>Sr</td>
<td>Y</td>
</tr>
<tr>
<td>Cs</td>
<td>Ba</td>
<td>La</td>
</tr>
<tr>
<td>Fr</td>
<td>Ra</td>
<td>Ac</td>
</tr>
<tr>
<td>Th</td>
<td>Pa</td>
<td>U</td>
</tr>
</tbody>
</table>

- β−: Beta minus
- β+: Beta plus
- CE: Channeling
- α: Alpha
- -emitters

Periodic table with highlighted elements and years where experiments were published.
Lattice location study of implanted $^{121}\text{Sn} \ (27 \text{h}) : \text{Ge}$

**MOTIVATION**
- group IV impurity = expected on S site in Ge
- no direct experimental info
- Sn-related defects $\rightarrow$ important for growth of GeSn!

**EXPERIMENTAL**
- radioactive isotope: $^{121}\text{Sn} \ (27 \text{ h})$
- implantation @ ISOLDE (CERN, Geneva)
- 60 keV, room temperature
- fluence: $2 - 4 \times 10^{12} \text{ cm}^{-2}$
- measurements @ room temperature
  - as implanted
  - after several annealing steps up to $500^\circ \text{C}$
    (10 min in vacuum)
- triangulation along 4 different directions:
  - $[111]$, $[100]$, $[110]$ and $[211]$

Decoster et al.
PRB 81, 155204 (2010)
Ge lattice

{110} plane
visual inspection of spectra: **substitutional** Sn

detailed fitting procedure:
  majority on S site but also fraction on BC site!

**BC** fraction is observed …
  …in three different samples (slightly different implantation fluence) …up to 400°C annealing!

No direct experimental observation of Sn on BC site reported in literature

Indications for BC behavior from **ab initio** calculations…
Ab initio calculations for Sn defects complexes in Ge

**STABILITIES**

Single vacancy + Sn (S) NOT STABLE

\[ \Delta H_{f, \text{subst.}} + \Delta H_{f, \text{vacancy}} > \Delta H_{f, \text{BC}} \]

Spontaneous capture of vacancies by substitutional Sn

<table>
<thead>
<tr>
<th>Sn on ...</th>
<th>( \Delta H_f ) (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sn on S site</td>
<td>0.19</td>
</tr>
<tr>
<td>Sn on T site</td>
<td>3.96</td>
</tr>
<tr>
<td>Sn on BC site (split-vacancy)</td>
<td>1.86</td>
</tr>
<tr>
<td>Sn on BC site (no vacancies)</td>
<td>3.83</td>
</tr>
<tr>
<td>Sn on S site + Ge self-interstitial</td>
<td>3.51</td>
</tr>
<tr>
<td>Ge vacancy</td>
<td>2.23</td>
</tr>
</tbody>
</table>

Previous – controversial - publications Höhler et al., PRB 71, 035212 (2005) and Coutinho et al., PRB 73, 235213 (2006)
**SIMULATIONS**

<table>
<thead>
<tr>
<th></th>
<th>(\Delta H_f) (eV)</th>
<th>(\delta_{(\text{calc})}) (mm/s)</th>
<th>(\Delta E_{Q(\text{calc})}) (mm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\text{Sn}_S)</td>
<td>0.19</td>
<td>1.75</td>
<td>0.0</td>
</tr>
<tr>
<td>(\text{Sn}_T)</td>
<td>3.96</td>
<td>3.19</td>
<td>0.0</td>
</tr>
<tr>
<td>(\text{Sn}_{BC}) (split vacancy)</td>
<td>1.86</td>
<td>2.24</td>
<td>0.10</td>
</tr>
<tr>
<td>(\text{Sn}_{BC}) (no vacancies)</td>
<td>3.83</td>
<td>3.25</td>
<td>0.82</td>
</tr>
<tr>
<td>(\text{Sn}_S+\text{Ge}_T) (self-int.)</td>
<td>3.51</td>
<td>1.84</td>
<td>0.64</td>
</tr>
<tr>
<td>unknown</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Mossbauer**

<table>
<thead>
<tr>
<th></th>
<th>Mössbauer spectroscopy line(^{a,b})</th>
<th>(\delta_{(\text{exp})}) (mm/s)</th>
<th>(\Delta E_{Q(\text{exp})}) (mm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(\text{Sn(BC)})-V</td>
<td>1.41</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>(\text{Sn}(S))</td>
<td>1.90</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>(\text{Sn}(S)-\text{V})</td>
<td>2.36</td>
<td>0.3(^{a}) – 0.4(^{b})</td>
</tr>
<tr>
<td>4</td>
<td>(\text{Sn}(T))</td>
<td>3.27</td>
<td>0.0</td>
</tr>
</tbody>
</table>

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Good agreement for \(\text{Sn}\) on S and T site.

Mossbauer values for “\(\text{Sn}(S)\)-V defect” is in very good agreement with \(\text{Sn}-\text{V}\) defect in split-vacancy configuration (i.e. with \(\text{Sn}_{BC}\))!!

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G. Weyer et al., Hyp. Int. 10, 775 (1981)
From EC: Majority of Sn on S site + significant fraction on BC site

From ab initio calculations:
- vacancies will be trapped by substitutional Sn
- Sn(S)-V defect relaxes towards split-vacancy configuration, i.e., Sn on BC site

Our experiments:
- Implantation creates many vacancies
- vacancy creation during MBE-growth of GeSn?

Ventura et al., PRB 79, 155202 (2009):
Split-vacancy defect in diluted GeSn could be nucleation point of metallic Sn
Mn-doped Ge → spintronic devices, Mn$_x$Ge$_{1-x}$ → ferromagnetic 25 and 116 K, TC increases linearly 0.6% $<[\text{Mn}]<$ 3.5%.

Cho et al. showed ferromagnetic ordering in Ge$_{0.94}$Mn$_{0.06}$ close to room temperature (285 K). The origin of ferromagnetism is not fully understood and has been related to Mn-rich precipitates.

Lattice location study of implanted $^{56}\text{Mn}$ (2.6h) : Ge

Implantation at 300°C (accepted by Applied Physics Letters 2010)
2009
First emission channeling experiments with $^{27}\text{Mg}(9.46\text{m})$

(no precise data analysis yet)
HIGHLY PIXILATED and energy resolving electron detectors TIMEPIX
(MEDIPIX COLLABORATION @ CERN)

TIMEPIX 512 x 512 ch; 30 x 30 mm²; 300 μm thick

89Sr : SrTiO3
After air annealing 1050 °C <100>
Highly pixilated and ENERGY RESOLVING electron detectors
TIMEPIX
(MEDIPIX COLLABORATION @ CERN)

Energy determination
Time Over Threshold (TOT) method

Energy (keV)
Counts (arbitrary units)

73As → 73Ge

Auger + L13 keV
X rays from decay of 73As

K53 keV
L53 keV

γ + e^−

f(x) = ax + b - \frac{c}{x - t}

Energy (keV)

0 5 10 15 20 25 30 35 40 45 50 55 60

Counts (arbitrary units)

0 10 20 30 40 50 60

Energy (keV)

0 20 40 60