Ab initio study bistable $C_sC_i$ defect pair in silicon

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Defects in Semiconductors

Defects can be either; **Primary** or **Secondary**

![Diagram showing the vacancy, self-interstitial, substitutional defects](image)

3.2.1 **Vacancy Defect**

If an atom is removed from its regular lattice site the empty lattice site is called a vacancy defect (V), and is shown in Fig. 3-1. The vacancy in some semiconductors (e.g. in Ge and Si) can have up to five charge states, V$^\text{++}$, V$^+$, V$^0$, V$^-$ and V$^\text{-}$. In order
Defects in Semiconductors

- The ever increasing applications of semiconductors has lead to their intensive and extensive study.
Defects in Semiconductors

- Defects can modify the properties of semiconductors and thus influence the performance of devices fabricated thereon.
- Defects can be introduced in the semiconductor lattice:
  1. Intentionally by **radiating** with energetic particles or
  2. Unintentionally during **processing** stages

**The knowledge of how defects influence the device performance is key**
Defect metastability

- **Metastable defects**: Defects with levels that reversibly appear and disappear or shift due to the history of the sample.

- Experimentally, defect metastability can be detected by e.g. Deep Level Transient Spectroscopy (DLTS)

Importance of metastability

• Leads to **erratic behaviour** (Thermal donors in Si)
  - Silicon solar cells

• Involved in **Staebler-Wronski** in amorphous silicon
  - Light-induced metastable changes in the properties of hydrogenated amorphous silicon

• Interesting physics (**MODELLING???)**

• Possible future memory elements?
$C_sC_i$ defect pair in silicon

- $C_sC_i$: Carbon-substitutional-Carbon-interstitial

- $C_s$ is a common impurity in Si

- $C_i$ is formed by the displacement of $C_s$ by mobile interstitial Si atoms produced by displacement damage during irradiation. (Highly mobile)

- $C_i$ migrates and are trapped by $C_s$ atoms to form the $C_sC_i$ pair.

- No \textit{ab initio} work has reported bistability in this system yet.

Figure 1. $C_sC_i$ diagrams and sketches showing the metastable transformation of the $C_sC_i$ pair in Silicon. (Song, 1988)
**C_sC_i** defect pair in silicon

Apparently the effect of the small but real chemical difference between carbon and silicon is accidentally compensated by the effect of their size differences to make these two configurations so close in energy. It should be a real challenge to a theorist to duplicate these results and provide a good physical picture for the driving forces and the effect of charge state.


Computational details

Density functional theory (DFT)

Parameters
- 64 atoms Si supercell
- $2 \times 2 \times 2$ k-mesh
- 500 eV cut-off energy
- LDA pseudopotential

Codes
VASP & Quantum ESPRESSO

$$E^f_{(C_sC_i^q)} = E_{\text{tot}}(Si) + \mu Si - 2\mu C + q\left[ E_F + \varepsilon_V \right]$$

$$\varepsilon_V = -(IP) = E_T \left[ n_{Si} \right]^0 - E_T \left[ n_{Si} \right]^{+1}$$
Results & Discussions

Figure 1: C-C diagrams and sketches showing the metastable transformation of the C-C pair in Silicon. (Song, 1988)

Results & Discussions

Table 1. Formation energies (in eV) of CsCi defect pair in Si for different charge states.

<table>
<thead>
<tr>
<th>Functional</th>
<th>Configuration</th>
<th>-2</th>
<th>-1</th>
<th>0</th>
<th>+1</th>
<th>+2</th>
</tr>
</thead>
<tbody>
<tr>
<td>LDA</td>
<td>A</td>
<td>5.01</td>
<td>4.20</td>
<td>3.53</td>
<td>3.36</td>
<td>3.33</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>4.84</td>
<td>4.30</td>
<td>3.90</td>
<td>4.02</td>
<td>4.26</td>
</tr>
</tbody>
</table>

Units (eV)

LDA Configuration-coordinate energy curves for $q = -2$ and $q = -1$ charge states.

DFT

Expt [3,4] Configuration-coordinate energy curves for $q = -1$ and $q = 0$ charge states.

Expt


Conclusions

• Configuration A is the most stable in many charge states. Similar to what was observed experimentally (Song et. al)

• Song et. al. observed metastability to occur at 0 & -1 and +1 & 0 charge states.

• In our study however, even though we observed Metastability, its occurs at a charge state lower. (Choice of XC functional)
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AHSANTE SANA!!!!!