An incomplete ionization model for indium in silicon

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Introduction

Ionization level of dopants in silicon as a function of temperature is a critical electronic parameter. Several studies have developed models for ionization levels of phosphorus, arsenic, boron [1, 2] and even aluminium in silicon [3]. Based on these models, it is usually assumed that the dopants in silicon are completely ionized at room temperature due to their shallow energy levels [4]. However, there is insufficient literature and experimental data regarding the ionization of indium in silicon. This is despite the interest in Indium-doped wafers which can solve various degradation processes, such as light-induced degradation [5], of p-type wafers. The much higher ionization energy of indium, compared to other p-type dopants, suggests incomplete ionization even in the temperature range near room-temperature. This study aims to develop a model for the ionization level of indium as a function of temperature.

Method

According to Altermatt et al., there are six key parameters which are required in order to parameterize the ionization level:

- The ground state doping energy \( E_{\text{dop},0} \) and the degeneracy factor \( g \) that can be found in the literature [2].
- Four fitting parameters \( (N_{\text{ref}}, c, N_b, d) \) that are obtained by fitting the ionization fraction as a function of dopant density.

The fitting parameters are related to the ionization fraction as described by the following equations [2]:

\[
\frac{N_{\text{acc}}^-}{N_{\text{acc}}} = 1 - \frac{bp}{p + gp_1},
\]

where

\[
b = \frac{1}{1 + \left( N_{\text{dop}}/N_h \right)^d}, \quad p_1 = N_v e^{-E_{\text{dop}}/kT}, \quad \text{and} \quad E_{\text{dop}} = \frac{E_{\text{dop},0}}{1 + \left( N_{\text{dop}}/N_{\text{ref}} \right)^c}
\]

The ionization fraction for p-type silicon is the ratio of ionized acceptor concentration to the total acceptor concentration \( \frac{N_{\text{acc}}^-}{N_{\text{acc}}} \), \( p \) is the free hole density, \( N_{\text{dop}} \) is the total dopant density which is equivalent to \( N_{\text{acc}} \) for p-type silicon, \( N_v \) is the density of states in the valence band as a function of temperature, and \( T \) is the absolute temperature.

For p-type wafers, the hole density is approximately equal to the ionized dopant density \( (p = N_{\text{acc}}^-) \). In this study, we have used the ratio of hole density and the total dopant density \( (p/N_{\text{dop}}) \) from data published only recently by Murphy et al. [6], and the ratio of conductivity mobility and Hall mobility \( (\mu_{\text{cond}}/\mu_H) \) from the data of Linares [7]. In Ref. [6] the hole densities of indium-doped wafers were directly calculated using the Van der Pauw method [8], while Linares [7] used four-probe and Hall effect to measure the conductivity and the Hall coefficient, respectively. These were then used to calculate the conductivity mobility and Hall mobility. Information regarding the samples used in these two studies is summarised in Table 1.

The fitting parameter \( N_{\text{ref}} \) is obtained using the linear regression method proposed by Steinkemper et al., when parameterized an incomplete ionization model for aluminium [3]. They suggested a linear dependency of \( N_{\text{ref}} \) on \( E_{\text{dop},0} \). In this study, the same procedure is used to estimate \( N_{\text{ref}} \) for indium.
Table 1: Indium-doped silicon wafer samples used for ionization parameterization

<table>
<thead>
<tr>
<th>Author</th>
<th>Sample ID</th>
<th>Indium Doping Concentration (cm⁻³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Murphy et al.</td>
<td>IN-1</td>
<td>3.3 x 10¹⁶</td>
</tr>
<tr>
<td>Murphy et al.</td>
<td>IN-2</td>
<td>2.7 x 10¹⁶</td>
</tr>
<tr>
<td>Murphy et al.</td>
<td>IN-3</td>
<td>2.8 x 10¹⁶</td>
</tr>
<tr>
<td>Murphy et al.</td>
<td>IN-4</td>
<td>2.5 x 10¹⁶</td>
</tr>
<tr>
<td>Murphy et al.</td>
<td>IN-5</td>
<td>1.9 x 10¹⁶</td>
</tr>
<tr>
<td>Murphy et al.</td>
<td>IN-6</td>
<td>1.6 x 10¹⁶</td>
</tr>
<tr>
<td>Murphy et al.</td>
<td>IN-7</td>
<td>4.0 x 10¹⁵</td>
</tr>
<tr>
<td>Linares</td>
<td>SIN17-1</td>
<td>6.44 x 10¹⁶</td>
</tr>
<tr>
<td>Linares</td>
<td>SIN16-2</td>
<td>4.64 x 10¹⁶</td>
</tr>
</tbody>
</table>

### Result and discussion

We have used values from literature for $E_{dop,0}$ (155.58 meV) and $g$ (0.25) [2]. Using the linear regression analysis and Table 1 from Ref. [2], we have estimated $N_{ref}$ to be 2.4 x 10¹⁹ cm⁻³ for indium.

Using the fitting procedure used for boron and aluminium [2,3], we have estimated the ionization fitting parameters $c$, $N_b$ and $d$ for indium to be 5.6, 3.2 x 10¹⁹, and 5.3, respectively. The modelled ionization curves based on these parameters are presented in Fig. 1(a). It is interesting that the modelled ionization curves are able to closely fit the data from Linares [7], but not the data from Murphy et al. [6]. We are only able to fit the data of Ref [6] when using $E_{dop,0} >$ 190 meV [see Fig. 1(b)], which is substantially larger than the reported value (155.58±0.02 meV) [9]. It should be noted that the degeneracy factor $g$ is fixed at 0.25, as it is the well-known value for p-type silicon [2]. Furthermore, the quality of the fit was found to be insensitive to $N_{ref}$ values above 2.4 x 10¹⁹ cm⁻³ and even worse for values below. Therefore the estimate of $N_{ref}$ to be 2.4 x 10¹⁹ cm⁻³ using the procedure proposed by Steinkemper et al seems plausible.

![Figure 1: The ionization fraction of Indium as a function of dopant density with temperature as a parameter as fitted with (a) values from literature and (b) with $E_{dop,0} =$ 190 meV](image)

Our results suggest that either Altermatt et al. ionization model is insufficient for indium or that the measurement of Murphy et al. [6] need to be validated as they do not fit to a plausible ionisation model. Additionally, experimental data for heavily-doped indium wafers ($1 x 10^{18}$–$1 x 10^{20}$ cm⁻³) will be beneficial for a more accurate model.
Figure 2: The ionization fraction of Indium as a function of temperature with dopant density as a parameter. The solid lines represent the modelled ionization fraction based off our estimated parameters from literature.

Figure 2 presents the ionization fraction as a function of temperature. Again, the significant deviation between the values from Murphy et al. and the modelled ionization fraction can be observed. Based on this data, it seems the samples from Murphy et al. are displaying much higher levels of incomplete ionization than what is theoretically expected.

Conclusions

Ionisation level of dopants in silicon semiconductors has a critical impact on key material parameters, such as resistivity and carrier mobility. This is especially important for semiconductor dopants with large ionization energies, such as indium, which are incompletely ionized at room temperature as a result. Our study demonstrates that more experimental data is required to parameterize an incomplete ionization model for indium, especially from heavily-doped wafers. Furthermore, our inability to parameterize the recent data suggests that the theoretical model is insufficient for indium or that these measurements should be validated.

References