An incomplete ionization model for indium in silicon

Victor Siu, Shuai Nie, Yan Zhu, Ziv Hameiri

The University of New South Wales, Sydney, Australia

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 ($E_{dop,0}$) and the degeneracy factor (g) that can be found in the literature [2].
- Four fitting parameters (N_{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]:

$$\frac{N_{acc}^-}{N_{acc}} = 1 - \frac{bp}{p + gp_1}$$

$$where \quad b = \frac{1}{1 + (N_{dop}/N_b)^d}, \qquad p_1 = N_V e^{-E_{dop}/kT}, \qquad and \ E_{dop} = \frac{E_{dop,0}}{1 + (N_{dop}/N_{ref})^c}$$

The ionization fraction for p-type silicon is the ratio of ionized acceptor concentration to the total acceptor concentration $\frac{N_{acc}^-}{N_{acc}}$, p is the free hole density, N_{dop} is the total dopant density which is equivalent to N_{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 ($p = N_{acc}^-$). In this study, we have used the ratio of hole density and the total dopant density (p/N_{dop}) from data published only recently by Murphy *et al.* [6], and the ratio of conductivity mobility and Hall mobility (μ_{cond}/μ_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_{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_{ref} on $E_{dop,0}$. In this study, the same procedure is used to estimate N_{ref} for indium.

Table 1: Indium-doped silicon wafer samples used for ionization parameterization

| Author	Sample ID	Indium Doping Concentration (cm^{-3})
Murphy *et al.*	IN-1	3.3×10^{16}
Murphy *et al.*	IN-2	2.7×10^{16}
Murphy *et al.*	IN-3	2.8×10^{16}
Murphy *et al.*	IN-4	2.5×10^{16}
Murphy *et al.*	IN-5	1.9×10^{16}
Murphy *et al.*	IN-6	1.6×10^{16}
Murphy *et al.*	IN-7	4.0×10^{15}
Linares	SIN17-1	6.44×10^{16}
Linares	SIN16-2	4.64×10^{16}

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 2.4×10^{19} 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, 3.2×10^{19}, 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$\pm$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 2.4×10^{19} cm^{-3} and even worse for values below. Therefore the estimate of N_{ref} to be 2.4×10^{19} cm^{-3} using the procedure proposed by Steinkemper *et al* seems plausible.
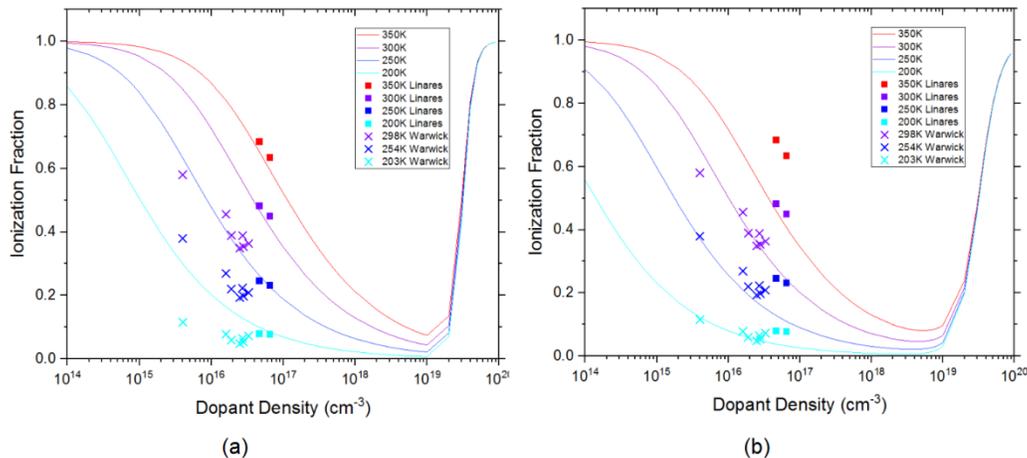
Figure 1: The ionization fraction of Indium as a function of dopant density with temperature as a parameter as fitted with (a) values from literature and (b) with $E_{dop,0}$ = 190 meV

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 (1×10^{18}–1×10^{20} cm^{-3}) will be beneficial for a more accurate model.
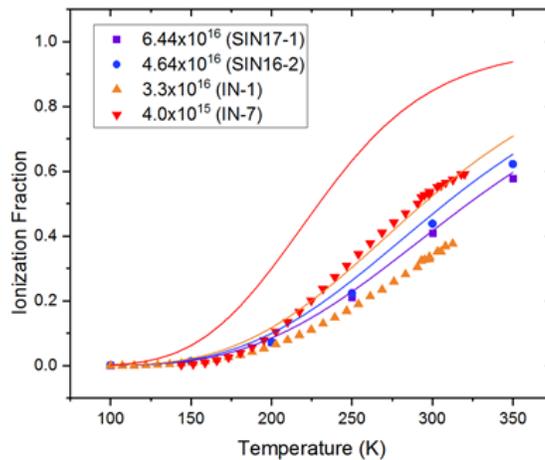
Figure 2: The ionization fraction of Indium as a function of temperature with dopant density as a parameter. The solid lines represent the modelled ionization fraction based off our estimated parameters from literature.

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.

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