

## TCAD Parameters for 4H-SiC: A Review

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In this paper we review the models and their parameters to describe the relative permittivity, bandgap, impact ionization, mobility, charge carrier recombination/effective masses and incomplete dopant ionization of 4H silicon carbide in computer simulations. We aim to lower the entrance barrier for newcomers and provide a critical evaluation of the status quo to identify shortcomings and guide future research. The review reveals a rich set of often diverging values in literature based on a variety of calculation and measurement methods. Although research for all the selected parameters is still active, we show that sometimes old values or those determined for other kinds of silicon carbide are commonly used.

Keywords: 4H-SiC, TCAD simulations, simulation parameters, silicon carbide

## CONTENTS

<b>I. Incomplete Ionization</b>	3
A. Theory	3
B. Results	6
C. Discussion	11
<b>References</b>	17

## I. INCOMPLETE IONIZATION

It is indispensable to add a doping to a semiconductor, i.e., to introduce impurity atoms, in order to create sophisticated electronic devices. These so-called dopants add energy levels near to the conduction (n-type doping) resp. valence band (p-type doping) such that free charge carrier can be injected at moderate temperatures. In this fashion the electrical characteristics of the material can be altered. Partial overviews on available doping elements and their respective activation energies in 4H-SiC are available<sup>1-21</sup>. Uncommon elements were also investigated. Ab initio calculations by Miyata, Higashiguchi, and Hayafuji<sup>22</sup> identified Arsenic<sup>23</sup>, Gallium<sup>24</sup> or Antimony as, energy level wise, fitting. Group IV elements were investigated by Krieger *et al.*<sup>25</sup>, Feng and Zhao<sup>5</sup>, Huang *et al.*<sup>26</sup> focused on Tantalum and Chromium and Dalibor and Schulz<sup>3</sup>, Dalibor *et al.*<sup>27</sup> on Vanadium. Additional factors such as the activation rates<sup>28</sup> or the impact of hydrogen<sup>29</sup> might, however, prevent the deployment of these dopants.

Due to the wide bandgap of 4H-SiC the respective dopant activation energies are large such that the often used assumption of full ionization is not applicable. Quite the opposite: incomplete ionization has to be carefully considered to correctly predict the amount of free charge carriers and, thus, achieve a realistic conductivity<sup>30,31</sup>.

In this section we will, thus, review measurements, models and TCAD parameters used to describe the amount of ionized dopants depending on temperature and doping concentration. We focus on the four most common doping species in 4H-SiC<sup>32-34</sup>: Aluminum (analysis by Darmody and Goldsman<sup>35</sup>) and Boron for p-type resp. Nitrogen and Phosphorous for n-type doping. We limit ourselves to simple model, e.g., a single energy level per lattice site (cubic or hexagonal). Depending on various parameters, e.g., binding type and location<sup>36-39</sup> or whether the impurity is located in a non-neutral regions or not<sup>31</sup>, rather elaborate descriptions would be necessary to account otherwise<sup>40</sup>.

### A. Theory

A good overview on the physical descriptions of incomplete ionization is provided by<sup>32</sup>. In brief, the amount of ionized dopants can be modeled by the Fermi-Dirac distribution<sup>12,41-44</sup>, also

known as steady-state Gibbs distribution<sup>31</sup>, as

$$\begin{aligned} N_D^+ &= \frac{N_D}{1 + g_D \exp\left(\frac{E_{F,n} - E_D}{k_B T}\right)} \\ N_A^- &= \frac{N_A}{1 + g_A \exp\left(\frac{E_A - E_{F,p}}{k_B T}\right)} \end{aligned} \quad (1)$$

where  $N_A$  resp.  $N_D$  are the active acceptor resp. donor concentrations,  $E_A$  resp.  $E_D$  the acceptor resp. donor energy levels,  $E_{F,n}$  resp.  $E_{F,p}$  the electron resp. hole Fermi level and  $g_D$  resp.  $g_A$  the degeneracy factors. The latter denote the degeneracy of the energy levels<sup>45</sup>, whereat in the literature commonly the values  $g_A = 4$  (spin up and spin down plus two valence bands) and  $g_D = 2$  (spin up and down)<sup>30,46</sup> are used. There are, however, exception: Troffer<sup>47</sup> used  $g_D = 6$ , Scaburri<sup>32</sup>, Laube *et al.*<sup>48</sup> a spin degeneracy of  $g_D = 4$  for Phosphorous, Balachandran, Chow, and Agarwal<sup>49</sup>, Nawaz<sup>50</sup>  $g_A = g_D = 3$ , Persson and Lindefelt<sup>51</sup>  $g_A = 2$ , Lv *et al.*<sup>52</sup>  $g_A = g_D = 2$  and Pernot *et al.*<sup>53</sup>  $g_k = 6$  resp.  $g_h = 2$  for the cubic resp. hexagonal site of Nitrogen. There were also efforts to introduce a temperature dependency as  $G_A(T)$  and  $G_D(T)$ <sup>17,32,47,54-57</sup>, whereat the description by Lophitis *et al.*<sup>58</sup> (equ. (11)) deviates significantly.

If solely Boltzmann statistics are considered Eq. (1) can be simplified to<sup>20,32,59-61</sup>

$$\begin{aligned} N_D^+ &= \frac{N_D}{1 + g_D \frac{n}{N_C} \exp\left(\frac{\Delta E_D}{k_B T}\right)}, & n &= N_C \exp\left(\frac{E_{F,n} - E_C}{k_B T}\right) \\ N_A^- &= \frac{N_A}{1 + g_A \frac{p}{N_V} \exp\left(\frac{\Delta E_A}{k_B T}\right)}, & p &= N_V \exp\left(\frac{E_V - E_{F,p}}{k_B T}\right) \end{aligned} \quad (2)$$

with  $N_C$  resp.  $N_V$  the effective density of states in the conduction resp. valence band (see ??) and  $\Delta E_D = E_C - E_D$  resp.  $\Delta E_A = E_A - E_V$  the ionization energies of donors and acceptors relative to the conduction ( $E_C$ ) and valence band ( $E_V$ ). This representation is often preferred in TCAD simulation tools, which commonly operate on charge carrier concentrations.

For completeness we want to highlight that using the neutrality equation<sup>32</sup>

$$N_D^+(E_F) + p(E_F) = N_A^-(E_F) + n(E_F) \quad (3)$$

it is possible to even get rid of the carrier concentration. If we assume a highly donor doped material ( $p(E_F)$  can be neglected) and no compensation ( $N_A^-(E_F) = 0$ ) Eq. (3) results, by inserting Eq. (2) for  $N_D^+$ , in a quadratic equation for  $n$  which can be solved to<sup>34,62-67</sup>

$$N_D^+ = N_D \frac{-1 + \sqrt{1 + 4 g_D \frac{N_D}{N_C} \exp\left(\frac{\Delta E_D}{k_B T}\right)}}{2 g_D \frac{N_D}{N_C} \exp\left(\frac{\Delta E_D}{k_B T}\right)}.$$

We have to highlight that the solution of the quadratic expression for  $n$  by Scaburri<sup>32</sup> is incorrect, which makes it impossible to retrace the presented, correct, equation for  $N_D^+$ . Accordingly an expression for  $N_A^-$  can be achieved.

The ionization energies also depend on the doping concentration. This can be explained by the changing potential energy of the charge carriers when they are closer to the ionized atoms, effectively shielding them<sup>68</sup>. To model the decrease in the ionization energy the Pearson-Bardeen<sup>68</sup> expression

$$\Delta E(N) = \Delta E_0 - \alpha N^{1/3} \quad (4)$$

is used.

The literature is inconsistent on what dopants should be included into the overall doping concentration  $N$  in Eq. (4). Some authors include both donors and acceptors  $N_A + N_D$ <sup>59,60</sup>, others only the respective donor concentration ( $N_A$  or  $N_D$ )<sup>54,69–73</sup>, while a third group just uses the ionized ones<sup>74</sup>. Kajikawa<sup>75</sup> even argues that the compensating dopants, i.e., donors for the acceptor levels and vice versa, have the bigger impact and should be used instead of the overall donor and acceptor concentrations. There have also been proposals to include the compensating dopants into the factor  $\alpha$ <sup>32,76</sup>. Finally, a completely different approach focuses on the degree of compensation depicted by a screening of free charge carriers<sup>32,77</sup>, which introduces an additional temperature dependency.

An alternative approach to the Pearson-Bardeen expression in Eq. (4) is given by Altermatt, Schenk, and Heiser<sup>78</sup>, Altermatt *et al.*<sup>79</sup>, who used the logistic equation

$$\Delta E(N) = \frac{\Delta E_0}{1 + (N/N_E)^c} \quad (5)$$

to model the decrease in ionization energy, with  $N_E$  a reference concentration where the ionization energy is half its original value  $\Delta E_0$ . Darmody and Goldsman<sup>35</sup> argue that with Eq. (4) it is possible to shift the dopant level into the conduction/valence band and thus ionize all dopants immediately, which is neither physically reasonable nor possible with Eq. (5). Despite these arguments, the described approach has not yet found its way into the major simulation tools.

Dopants have differing ionization energies depending on whether they are located in a hexago-

nal or a cubic lattice site<sup>80</sup> (see ??). Consequently Eq. (2) has to be adapted to<sup>23,60</sup>

$$N_D^+ = \frac{\frac{1}{2}N_D}{1 + g_D \frac{p}{N_C} \left( \frac{\Delta E_{Dh}}{k_B T} \right)} + \frac{\frac{1}{2}N_D}{1 + g_D \frac{p}{N_C} \left( \frac{\Delta E_{Dc}}{k_B T} \right)}$$

$$N_A^- = \frac{\frac{1}{2}N_A}{1 + g_A \frac{p}{N_V} \left( \frac{\Delta E_{Ah}}{k_B T} \right)} + \frac{\frac{1}{2}N_A}{1 + g_A \frac{p}{N_V} \left( \frac{\Delta E_{Ac}}{k_B T} \right)}$$

with  $E_{Dc}$  and  $E_{Dh}$  the cubic resp. hexagonal ionization energies for donors and  $E_{Ac}$  and  $E_{Ah}$  for acceptors. The factors 1/2 denote that both lattice sites are equally probable<sup>61</sup>. In TCAD simulations it is often the case that these separate values are merged to an effective energy level, ending up once again in a description as shown in Eq. (2)<sup>13,59,65,81,82</sup>. The effects of such simplifications have been investigated by Lades<sup>83</sup>, Ayalew *et al.*<sup>84</sup>.

For more accurate approximation of dynamic processes around the dopant, i.e., (de)trapping of charge carriers, the electron and hole cross sections are crucial (see ??). There are multiple description available in literature, which differ in their temperature scaling<sup>85</sup>. The multi-phonon capture model is independent of temperature<sup>86–88</sup> while the cascade capture model is proportional to  $T^{-289-91}$ . Kaindl *et al.*<sup>92</sup> argue that the latter delivers a better fit. A scaling with  $T^{-3}$  was used by Kuznetsov and Zubrilov<sup>93</sup>. Note that we discovered large discrepancies between the single tools regarding which models are supported.

## B. Results

The most commonly method to determine the ionization energy of dopants in literature is to fit the neutrality equation, i.e., for p-type doping

$$p + N_K = \frac{N_A}{1 + \frac{g_A p}{N_V} \exp \left( \frac{\Delta E_A}{k_B T} \right)}.$$

to Hall measurements, e.g., conductivity or charge carrier concentration, for varying temperature<sup>24,38,46,47,53,56,57,66,69,71,73,75,91,94–122</sup>. The compensation doping density  $N_K$  is only required for fitting purposes, such that we solely use  $N_A$  as the doping density to present our results. Due to the anisotropy of the Hall effect it is possible to achieve direction dependent ionization energies this way<sup>56</sup>. Other approaches based on Hall measurements include the fitting to the activation ratio<sup>123</sup> or free carrier concentration spectroscopy (FCCS)<sup>54,70,124</sup>. Further used electrical measurements are (thermal)<sup>125–128</sup> admittance spectroscopy (AS)<sup>24,47,56,73,91,92,102,129</sup>, electron spin resonance (ESR) measurement<sup>130</sup>, deep level transient spectroscopy (DLTS)<sup>56,93,131,132</sup> and minority

carrier transient spectroscopy (MCTS)<sup>131</sup>, which are often combined with Hall measurements for more accurate results. Troffer<sup>47</sup> notes that DLTS is more sensitive but admittance spectroscopy allows to depict time constants below 1  $\mu$ s.

These electrical methods are complemented by optical ones, e.g., (fourier transform infrared) photothermal ionization spectroscopy (PTIS)<sup>133</sup>, donor-acceptor pair (DAP) luminescence<sup>80,134–136</sup>, free to acceptor (FTA) spectroscopy<sup>80</sup>, infrared absorption (IA)<sup>98</sup>, photoluminescence (PL)<sup>102,137–140</sup>, time-resolved spectroscopy (TRS)<sup>137</sup> or delay measurements (DM)<sup>137</sup>. In these cases electrons are empowered and the resulting photon emission is recorded. The latter can be caused by transitions among traps or between traps and the conduction/valence band<sup>56</sup>. Note that different methods lead to slightly deviating results, even when applied to the same device<sup>98</sup>. Also possible are calculations, e.g., Faulkner model (FM) calculations<sup>141</sup>, density functional theory (DFT)<sup>22,142</sup>, effective mass approximation (EMA)<sup>143</sup>, first principles calculations (FPC)<sup>26,29,39</sup> or *ab initio* supercell calculations (AISC)<sup>144</sup>. Finally, some authors define a value range based on measurements in literature<sup>34,61,83</sup>, calculate an average values<sup>145</sup> or fit to existing data<sup>35,60,146</sup>.

In the sequel we are going to present the ionization energies  $\Delta E_D$  resp.  $\Delta E_A$  found in literature with their respective doping concentration. In order to draw the measurements we dropped uncertainties and replaced the sometimes stated exciton energy  $E_x$  with 20 meV (see ??). We had to discard results where the samples were solely described as "high purity" or "unintentional doping"<sup>96,138–140</sup> and Laube *et al.*<sup>48</sup>, which was superseded by a publication of the same authors. We mark results for the hexagonal lattice site by a trailing "h" and result for the cubic one by a trailing "c". The latter is often also denoted by the letter "k", which, most probably, corresponds to the german word "kubisch" for cubic. In fact, some of the literature is written in german<sup>47,56</sup>, making it hard to retrace the results for the international community.

For Aluminum (see Fig. 1) many measurements and model fittings have been proposed. The values are equally distributed across the last three decades, meaning that the improvements in material quality did not result in significant changes. The model proposed by Achatz *et al.*<sup>72</sup> uses the critical aluminum concentration for the doping-induced metal-insulator transition to set  $\Delta E_A = 0$  and then fit the parameters. This is in contrast to the logistic equation in Eq. (5) used by Darmody and Goldsman<sup>35</sup>, where a much slower decrease of  $\Delta E_A$  below 100 meV can be observed.

For low-doped and compensated devices a second energy level is required to properly describe the measurements<sup>71</sup>. The origin of this deep level is still discussed in literature. Matsuura *et al.*<sup>54</sup>,

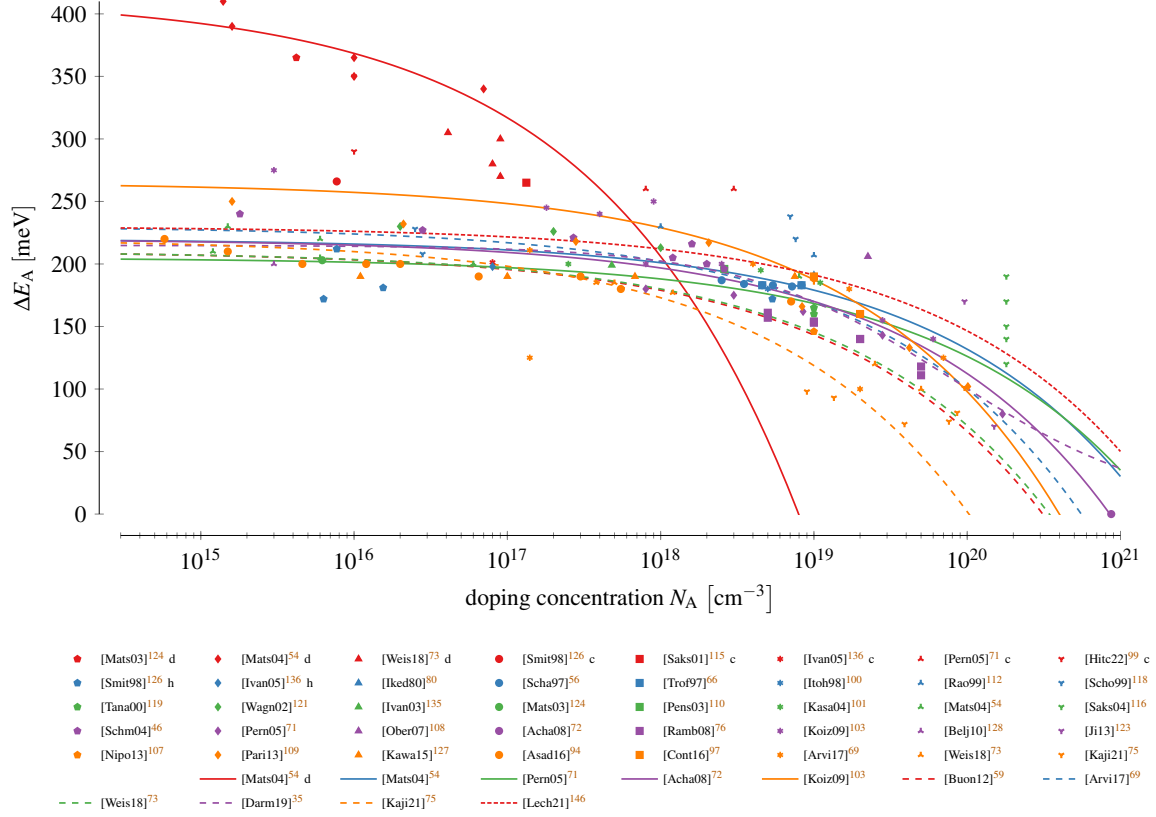


FIG. 1. Aluminum ionization energy. Marks refer to measurements and lines to fittings. The letter 'd' after the reference indicates a deep level whose origin is still discussed (see text). Colors are used solely to increase the readability.

<sup>124</sup> were not able to provide any explanation, Weiße *et al.* <sup>73</sup> suspect excited states of the aluminum ground state and Pernot, Contreras, and Camassel <sup>71</sup>, Smith, Evwaraye, and Mitchel <sup>126</sup> describe them as the cubic lattice site. In fact, Smith, Evwaraye, and Mitchel <sup>126</sup> states that for higher concentration only the hexagonal site is measured. Nevertheless, in our plots we show the data as presented by the original authors, with the exceptions of the ones by Saks *et al.* <sup>115</sup>, which Pernot, Contreras, and Camassel <sup>71</sup> pointed out to denote the cubic lattice site.

Aluminum is the single dopant where a fitting using the logistic approximation (see Eq. (5)) was used. Darmody and Goldsman <sup>35</sup> achieved  $\Delta E_0 = 214.86 \text{ meV}$ ,  $N_E = 8.12 \times 10^{19} \text{ cm}^{-3}$  and  $c = 0.632$ .

The available measurements for Boron (see Fig. 2) are very few and date back to the last millennium. We suspect the main cause in the deep D-center <sup>35,39,47</sup> that comes with a Boron doping. It introduces an energy level in a range of 495–630 meV <sup>47,80,91,93,131,134</sup>, which results



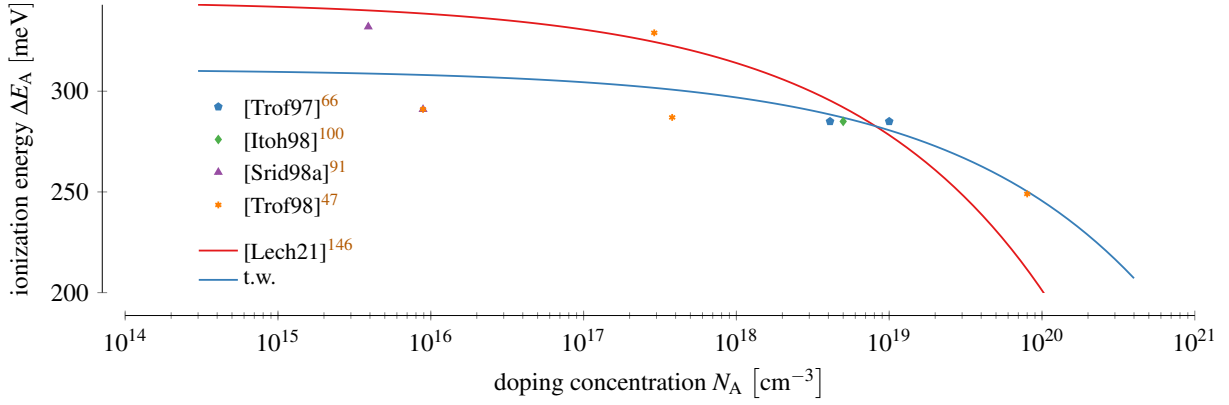


FIG. 2. Boron ionization energy. Marks refer to measurements and lines to fittings. Colors are used solely to increase the readability.

in a very effective recombination center. In some publications and also in some simulation tools the D-center level is used as the actual Boron one<sup>9,80,134,140,147–150</sup>. Since only a single fitting according to Eq. (4) is available for Boron we used all the available data to generate an additional one (t.w.).

For the n-type donor Nitrogen (shown in Fig. 3) almost all publications distinguish between cubic and hexagonal site. However, there is also a big spread in the data, especially towards higher doping concentrations. The results suggest that the ionization energy does not decrease (especially for the cubic lattice site) even as the solubility limit ( $1 \times 10^{19} \text{ cm}^{-3}$  for annealing at 1700 K up to  $3 \times 10^{20} \text{ cm}^{-3}$  for annealing at 2500 K<sup>16,136,150–152</sup>) is approached.

For Nitrogen only fittings according to Eq. (4) are available. Kagamihara *et al.*<sup>70</sup> provided a fitting for both hexagonal and cubic lattice site, which were combined by Hatakeyama, Fukuda, and Okumura<sup>60</sup> to an effective ionization energy model. The remaining fittings also represent effective levels but are surprisingly low. In the case of Buono<sup>59</sup> this can be explained by the selection of  $\Delta E_0$ , which was picked as the effective value of 65 meV determined by Bakowski, Gustafsson, and Lindefelt<sup>81</sup> based on the values from Götz *et al.*<sup>98</sup>. The latter, as can be seen in the figure, were, however, determined for a doping of  $1 \times 10^{17} \text{ cm}^{-3}$  resp.  $1 \times 10^{18} \text{ cm}^{-3}$ .

Compared to Nitrogen a lot less measurements are available for Phosphorous (see Fig. 4), all roughly two decades old. Again, hexagonal and cubic lattice site are always distinguished, but the results especially for the latter largely deviate. Due to the lack of fittings according to Eq. (4) we used the available data to generate very crude fittings. Even as the solubility limit ( $6 \times 10^{18} \text{ cm}^{-3}$  for annealing at 1700 K up to  $2 \times 10^{20} \text{ cm}^{-3}$  for annealing at 2500 K<sup>16,136,150–152</sup>) is reached high



ionization energies for the cubic lattice site are observable.

The parameters for the Pearson-Bardeen model (see Eq. (4)) fittings, which were shown in Figs. 1 to 4, are summarized in Table I. We also added our own fitting parameters (t.w.). To take the described inconsistency for  $N$  in Eq. (4) into account column N denotes either the total doping (tot), the n- resp. p-type doping (dop), the compensation (comp) or fitting (fit). For the figures we used uniformly the specific doping concentration  $N_A$  resp.  $N_D$  (x-axis).

Cross-sections with varying temperature were heavily investigated at the end of the last century (see Table II). The column  $\sigma$  denotes the cross section with the charge carrier in the energetically closer band (conduction or valence) because the interaction with the other band is significantly lower<sup>47,92</sup>.

Finally we also investigated single energy values used in overviews or in TCAD simulations (see Fig. 5). We do not show fundamental values here as these are always linked to a specific doping concentration. For Aluminum many publications use a value that corresponds to the deeper (cubic site?) energy level. Also for Boron some values refer to the deep D-center. Altogether, a wide range of values is used, especially for Nitrogen, where again hexagonal and cubic sites are almost always distinguished. We want to highlight that for the Boron ionization energy of 293 meV<sup>31,58,153</sup> no direct connection to any fundamental investigation could be inferred.

In some publications the dopant is not clearly specified. Instead only the acceptor and donor energy level are provided (see Fig. 6). While the acceptor values clearly correspond to Aluminum the n-type values could belong to both Nitrogen and Phosphorous.

## C. Discussion

In contrast to other properties that have been investigated within this review, there exist a lot of fundamental studies and measurements for incomplete ionization. Nevertheless, the results acquired over the last decades deviate sometimes significantly, making it impossible to distill them to common values. This is, by the way, not caused by less mature samples in the past. Even by limiting our analysis to the last two decades we did reveal a large spread in measurement results. The situation is worsened by the fact that values for hexagonal and cubic lattice sites are often used without appropriate notation. In this fashion significant errors can be introduced, especially for Boron where the deep levels is approximately twice the shallow one.

Overall, almost all publications utilize values determined from 4H-SiC measurements. Only



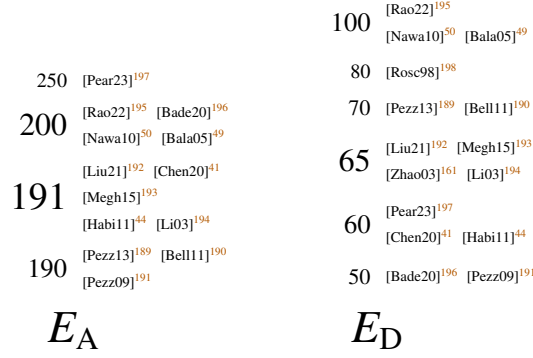


FIG. 6. Energy levels used in literature for acceptors and donors without closer specification of dopant element.

### n-type (Don | N | P)

Hagen, Van Kemenade, and Van Der Does De Bye

[Hage73]<sup>137</sup> (- | -, 80, 130 | -, -, -)  
 [Pank14]<sup>16</sup> (- | -, 33, 90 | -, -, -)

Lomakina and Vodakov

[Loma73]<sup>105</sup> (- | 29, -, - | -, -, -)  
 [Loma74]<sup>181</sup> (- | 33, -, - | -, -, -)  
 [Pank14]<sup>16</sup> (- | -, 33, 90 | -, -, -)

Suzuki, Matsunami, and Tanaka

[Suzu77]<sup>140</sup> (- | 55+7, -, - | -, -, -)  
 [Made91]<sup>150</sup> (- | -, 66, 124 | -, -, -)

Ikedo, Matsunami, and Tanaka

[Iked80]<sup>80</sup> (- | -, 66, 124 | -, -, -)  
 [Made91]<sup>150</sup> (- | -, 66, 124 | -, -, -)  
 [Izzo08]<sup>187</sup> (- | -, 66, 124 | -, -, -)  
 [Fan14]<sup>149</sup> (- | -, 66, 124 | -, -, -)  
 [Dona18]<sup>31</sup> (- | -, 70, 120 | -, 55, 102)  
 [Ioff23]<sup>147</sup> (- | -, 66, 124 | -, -, -)

Götz *et al.*

[Gotz93]<sup>78</sup> (- | -, 52.1, 91.8 | -, -, -)  
 [Pens93]<sup>40</sup> (- | -, 45, 100 | -, -, -)  
 [Gao01]<sup>159</sup> (- | 100, -, - | -, -, -)  
 [Heni13]<sup>177</sup> (- | 100, -, - | -, -, -)  
 [Bako97]<sup>81</sup> (- | 65, 52.1, 91.8 | -, -, -)  
 [Wang99]<sup>162</sup> (- | 65, 52.1, 91.8 | -, -, -)  
 [Zhao03]<sup>161</sup> (65 | -, -, - | -, -, -)  
 [Buon10]<sup>170</sup> (- | 65, -, - | -, -, -)  
 [Usma12]<sup>169</sup> (- | 65, -, - | -, -, -)  
 [Greu97]<sup>148</sup> (- | -, 52.1, 91.8 | -, -, -)  
 [Lebe99]<sup>10</sup> (- | -, 52, 92 | -, -, -)  
 [Arva17]<sup>153</sup> (- | 71, -, - | -, -, -)  
 [Pers99a]<sup>183</sup> (- | -, 52.1, 91.8 | -, -, -)  
 [Zett02]<sup>20</sup> (- | -, 50, 92 | -, 53, 93)  
 [Feng04a]<sup>5</sup> (- | -, 52, 92 | -, -, -)  
 [Pers05]<sup>18</sup> (- | -, 52, 92 | -, -, -)  
 [Zhu08]<sup>21</sup> (- | -, 50, 92 | -, 54, 93)

Harris and Inspec

[Harr95]<sup>6</sup> (-, -, -, - | -, -, - | -, -, -)  
 [Bali06]<sup>165</sup> (- | 100, -, - | -, -, -)

Kimoto *et al.*

[Kimo95]<sup>102</sup> (- | -, 45, 105 | -, -, -)  
 [Sozz19]<sup>175</sup> (- | 50, -, - | -, -, -)

Evwaraye, Smith, and Mitchel

[Ewva96]<sup>125</sup> (- | -, 53, 100 | -, -, -)  
 [Gerh11]<sup>184</sup> (- | -, 53, 100 | -, -, -)

Choyke and Pensl

[Choy97d]<sup>96</sup> (- | -, 59, 102 | -, -, -)  
 [Iwa01]<sup>185</sup> (- | -, 59, 102 | -, -, -)  
 [Levi01]<sup>11</sup> (- | -, 59, 102 | -, -, -)  
 [Dona18]<sup>31</sup> (- | -, 70, 120 | -, 55, 102)

Pensl

[Pens98]<sup>199</sup> (- | -, -, - | -, -, -)  
 [Neud01]<sup>14</sup> (- | 45, -, - | 80, -, -)  
 [Neud06]<sup>15</sup> (- | 45, -, - | 80, -, -)

Capano *et al.*

[Capa00]<sup>95</sup> (- | -, 42, 84 | -, 53, 93)  
 [Hand00]<sup>28</sup> (- | -, -, - | -, 53, 93)  
 [Zett02]<sup>20</sup> (- | -, 50, 92 | -, 53, 93)  
 [Zhu08]<sup>21</sup> (- | -, 50, 92 | -, 54, 93)  
 [Dhan10]<sup>4</sup> (- | -, -, - | -, 53, 93)  
 [Zhan10]<sup>160</sup> (- | 42, -, - | -, -, -)

Lades

[Lade00]<sup>83</sup> (- | -, 50±5, 90±10 | -, -, -)  
 [Schr06]<sup>168</sup> (- | -, 50±5, 90±10 | -, -, -)

Adachi

[Adac03]<sup>200</sup> (- | -, -, - | -, -, -)  
 [Bhat05]<sup>82</sup> (- | 81, 60, 91 | -, -, -)

Ivanov, Magnusson, and Janzén

[Ivan03a]<sup>141</sup> (- | -, 61.4±0.5, - | -, -, -)  
 [Janz08]<sup>163</sup> (- | -, 61.4, 125.5 | -, -, -)  
 [Yang19]<sup>186</sup> (- | 61, -, - | -, -, -)  
 [Tian20]<sup>167</sup> (- | 61.4, -, - | -, -, -)

Kagamihara *et al.*

[Kaga04]<sup>70</sup> (- | -, 70.9, 123.7 | -, -, -)  
 [Tiwa19]<sup>174</sup> (- | 70.9, -, - | -, -, -)  
 [Tiwa19a]<sup>173</sup> (- | 70.9, -, - | -, -, -)

Ivanov, Henry, and Janzén

[Ivan05]<sup>136</sup> (- | -, -, 125.5 | -, 60.7, 120+20)  
 [Janz08]<sup>163</sup> (- | -, 61.4, 125.5 | -, -, -)  
 [Scab11]<sup>77</sup> (- | -, -, - | -, 60.7, 120)  
 [Scab11a]<sup>32</sup> (- | -, -, - | -, 60.7, 120)  
 [Kimo14a]<sup>164</sup> (- | -, 61, 126 | -, 60, 120)  
 [Kimo19]<sup>152</sup> (- | -, 61, 126 | -, 60, 120)  
 [Kimo15]<sup>8</sup> (- | -, 61, 126 | -, 60, 120)  
 [Nipo18]<sup>33</sup> (- | -, -, - | -, 60, 120)

Sullivan and Stanley

[Sul108]<sup>179</sup> (- | 80, -, - | -, -, -)  
 [Rakh20]<sup>178</sup> (- | 65, -, - | -, -, -)

Tamaki *et al.*

[Tama08a]<sup>201</sup> (66 | -, -, - | -, -, -)  
 [Meno11]<sup>202</sup> (- | -, -, - | -, -, -)

Habib, Wright, and Horsfall

[Habi11]<sup>44</sup> (60 | -, -, - | -, -, -)  
 [Chen20]<sup>41</sup> (60 | -, -, - | -, -, -)

Buono

[Buon12]<sup>59</sup> (- | 65, 52.1, 91.8 | -, -, -)  
 [Joha19]<sup>176</sup> (- | 65, -, - | -, -, -)

Hatakeyama, Fukuda, and Okumura

[Hata13]<sup>60</sup> (- | 105, -, - | -, -, -)  
 [Uhne15]<sup>13</sup> (- | 105, -, - | -, -, -)  
 [Maxi23]<sup>203</sup> (- | 105, -, - | -, -, -)

FIG. 7. Reference chain for n-type doping. Entries with green background show fundamental investigations, orange references we inferred based on the used data and blue investigation based not on 4H.

TABLE I. Parameters for the Pearson-Bardeen model (see Eq. (4)). Column N denotes how the factor  $N$  is interpreted: either as active dopants (dop), all dopants (tot), just the compensating ones (comp) or simply used in a fitting (fit). The site denotes besides hexagonal and cubic also a combined effective energy level (eff) and the deep level for Aluminium (deep). If left blank no information were stated in the paper.

ref.	N	site	$\Delta E$ [meV]	$\alpha$ [meV cm]
<b>Nitrogen</b>				
[Kaga04] <sup>70</sup>	dop	hex	70.9	$3.38 \times 10^{-5}$
		cubic	123.7	$4.65 \times 10^{-5}$
[Buon12] <sup>59</sup>	tot	eff	65	$3.1 \times 10^{-5}$
[Hata13] <sup>60</sup>	tot	eff	105	$4.26 \times 10^{-5}$
[Lech21] <sup>146</sup>	tot		52.5	$3.38 \times 10^{-5}$
<b>Phosphorous</b>				
t.w.	fit	hex	57	$9.54 \times 10^{-6}$
		cubic	96	$2.71 \times 10^{-6}$
<b>Aluminum</b>				
[Mats04] <sup>54</sup>	dop		220	$1.9 \times 10^{-5}$
[Pern05] <sup>71</sup>	dop		205	$1.7 \times 10^{-5}$
[Acha08] <sup>72</sup>	dop		220	$2.32 \times 10^{-5}$
[Koiz09] <sup>103</sup>	dop		265	$3.6 \times 10^{-5}$
[Buon12] <sup>59</sup>	tot	eff	210	$3.1 \times 10^{-5}$
[Arvi17] <sup>69</sup>	dop		$230 \pm 10$	$(2.8 \pm 0.3) \times 10^{-5}$
[Weis18] <sup>73</sup>	dop		210	$3 \times 10^{-5}$
[Kaji21] <sup>75</sup>	comp		220	$4.7 \times 10^{-5}$
[Lech21] <sup>146</sup>	tot		230	$1.8 \times 10^{-5}$
<b>Boron</b>				
[Lech21] <sup>146</sup>	tot		345	$3.1 \times 10^{-5}$
t.w.	fit		311	$1.41 \times 10^{-5}$

seldomly 6H data were used<sup>178,180</sup>, whereat the values match those from 4H publications<sup>31,58,153</sup>.

TABLE II. Dopants and their respective cross sections with the charge carriers in the energetically closer band (conduction or valence). Different temperature dependencies are indicated in the column  $T^\alpha$ . We found no data for Nitrogen.

ref.	site	$T^\alpha$	$\Delta E$ [meV]	$\sigma$ [cm <sup>2</sup> ]
<b>Nitrogen</b>				
[Kain99] <sup>92</sup>	cubic	$T^0$	77	$7.92 \times 10^{-15}$
		$T^{-2}$	90	$3.57 \times 10^{-10}$
<b>Aluminum</b>				
[Kuzn95] <sup>93</sup>		$T^{-3}$	229	$8 \times 10^{-13}$
[Scha97] <sup>56</sup>		$T^0$	164–179	$2.2\text{--}7.6 \times 10^{-13}$
		$T^{-2}$	189–202	$1.7\text{--}5.6 \times 10^{-12}$
[Kain99] <sup>92</sup>		$T^0$	189	$2.58 \times 10^{-13}$
		$T^{-2}$	208	$2.57 \times 10^{-8}$
[Resh05] <sup>129</sup>		$T^0$	185	$1 \times 10^{-14}$
		$T^{-2}$	210	$1 \times 10^{-13}$
[Belj10] <sup>128</sup>		$T^0$	200	$1 \times 10^{-12}$
[Kawa15] <sup>127</sup>		$T^0$	190	$1.4 \times 10^{-13}$
[Kato22] <sup>132</sup>		$T^0$	120–170	$1\text{--}100 \times 10^{-17}$
<b>Boron</b>				
[Srid98a] <sup>91</sup>		$T^0$	259–262	-
		$T^{-2}$	284–295	-
[Trof98] <sup>47</sup>		$T^0$	292	$6 \times 10^{-15}$
		$T^{-2}$	314	$5 \times 10^{-14}$
[Kain99] <sup>92</sup>		$T^0$	312	$2.1 \times 10^{-14}$
		$T^{-2}$	375	$9.69 \times 10^{-9}$
[Zhan03] <sup>131</sup>		$T^0$	230–280	$2\text{--}30 \times 10^{-14}$

However, since the latter did not provide a reference for the picked values it is impossible to retrace where and how these values have been determined. Nevertheless we tried to create causality chains for n-type (see Fig. 7) p-type (see Fig. 8) values, whereat quite some values hat to be inferred due to missing information.

For n-type doping the values published by Ikeda, Matsunami, and Tanaka<sup>80</sup> are widely used

p-type (Acc | Al | B)

Hagen, Van Kemenade, and Van Der Does De Bye

[Hage73]<sup>137</sup> (- | 150 ± 5 + Ex, -, -, -, -, -)  
 [Pank14]<sup>16</sup> (- | 270, -, -, | 390, -, -, -)

Ikeda, Matsunami, and Tanaka

[Iked80]<sup>80</sup> (- | 191, -, -, | 647, -, -, -)  
 [Made91]<sup>150</sup> (- | 191, -, -, | 647, -, -, -)  
 [Bako97]<sup>81</sup> (- | 191, -, -, | -, -, -, -)  
 [Wang99]<sup>162</sup> (- | 191, -, -, | -, -, -, -)  
 [Zhao03]<sup>161</sup> (- | 191, -, -, | -, -, -, -)  
 [Greu97]<sup>148</sup> (- | 191, -, -, | 647, -, -, -)  
 [Pers98]<sup>51</sup> (- | 191, -, -, | -, -, -, -)  
 [Blue00]<sup>2</sup> (-, -, -, | -, -, -, | -, -, -, -)  
 [Mart02]<sup>145</sup> (- | 200, -, -, | -, -, -, -)  
 [Levi01]<sup>11</sup> (- | 190, -, -, | 650, -, -, -)  
 [Li03]<sup>194</sup> (191 | -, -, -, | -, -, -, -)  
 [Nego03]<sup>158</sup> (- | 190, -, -, | 285, -, -, -)  
 [Nego04]<sup>157</sup> (- | 190, -, -, | -, -, -, -)  
 [Zhan10]<sup>160</sup> (- | 191, -, -, | -, -, -, -)  
 [Habi11]<sup>144</sup> (191 | -, -, -, | -, -, -, -)  
 [Chen20]<sup>11</sup> (191 | -, -, -, | -, -, -, -)  
 [Wije11]<sup>156</sup> (- | 190, -, -, | 285, -, -, -)  
 [Fan14]<sup>149</sup> (- | 191, -, -, | 647, -, -, -)  
 [Megh15]<sup>193</sup> (191 | -, -, -, | -, -, -, -)  
 [Megh18]<sup>155</sup> (- | 190, -, -, | -, -, -, -)  
 [Yosh18]<sup>154</sup> (- | 190, -, -, | -, -, -, -)  
 [Liu21]<sup>192</sup> (191 | -, -, -, | -, -, -, -)  
 [Ioff23]<sup>147</sup> (- | 191, -, -, | 647, -, -, -)

Pensl and Choyke

[Pens93]<sup>140</sup> (- | 200, -, -, | -, -, -, -)  
 [Habe94]<sup>166</sup> (- | 200, -, -, | -, -, -, -)  
 [Zeit02]<sup>20</sup> (- | 200, -, -, | 285, -, -, -)  
 [Zhu08]<sup>21</sup> (- | 200, -, -, | 285, -, -, -)

Harris and Inspec

[Harr95]<sup>5</sup> (-, -, -, | -, -, -, | -, -, -, -)  
 [Bali06]<sup>165</sup> (- | 200, -, -, | -, -, -, -)

Kuznetsov and Zubrilov

[Kuzn95]<sup>93</sup> (- | -, -, -, | -, -, -, -)  
 [Blue00]<sup>2</sup> (-, -, -, | -, -, -, | -, -, -, -)  
 [Mart02]<sup>145</sup> (- | 200, -, -, | -, -, -, -)

Troffer *et al.*

[Trof97]<sup>66</sup> (- | 183, -, -, | 285, -, -, -)  
 [Blue00]<sup>2</sup> (-, -, -, | -, -, -, | -, -, -, -)  
 [Mart02]<sup>145</sup> (- | 200, -, -, | -, -, -, -)  
 [Zeit02]<sup>20</sup> (- | 200, -, -, | 285, -, -, -)  
 [Zhu08]<sup>21</sup> (- | 200, -, -, | 285, -, -, -)  
 [Pezz09]<sup>191</sup> (190 | -, -, -, | -, -, -, -)  
 [Wije11]<sup>156</sup> (- | 190, -, -, | 285, -, -, -)  
 [Pezz13]<sup>189</sup> (190 | -, -, -, | -, -, -, -)

Itoh, Troffer, and Pensl

[Itoh98]<sup>100</sup> (- | 180, -, -, | 285, -, -, -)  
 [Blue00]<sup>2</sup> (-, -, -, | -, -, -, | -, -, -, -)  
 [Mart02]<sup>145</sup> (- | 200, -, -, | -, -, -, -)  
 [Nego03]<sup>158</sup> (- | 190, -, -, | 285, -, -, -)

Pensl

[Pens98]<sup>199</sup> (- | -, -, -, | -, -, -, -)  
 [Neud01]<sup>14</sup> (- | 200, -, -, | 300, -, -, -)  
 [Neud06]<sup>15</sup> (- | 200, -, -, | 300, -, -, -)

Smith, Ewvarayee, and Mitchel

[Smit98]<sup>126</sup> (- | -, 212, 266 | -, -, -, -)  
 [Smit99]<sup>204</sup> (- | -, 212, 266 | -, -, -, -)

Sridhara *et al.*

[Srid98a]<sup>91</sup> (- | -, -, -, | 291+10, -, -, -)  
 [Gali99]<sup>205</sup> (- | -, -, -, | -, -, -, -)  
 [Gerh11]<sup>184</sup> (- | -, -, -, | -, -, -, -)

Lebedev

[Lebe99]<sup>10</sup> (-, -, -, | -, -, -, | -, -, -, -)  
 [Lu21]<sup>142</sup> (- | 220, -, -, | -, -, -, -)

Rao *et al.*

[Rao99]<sup>112</sup> (- | 230, -, -, | -, -, -, -)  
 [Blue00]<sup>2</sup> (-, -, -, | -, -, -, | -, -, -, -)  
 [Mart02]<sup>145</sup> (- | 200, -, -, | -, -, -, -)

Schöner *et al.*

[Scho99]<sup>118</sup> (- | 228, -, -, | -, -, -, -)  
 [Mart02]<sup>145</sup> (- | 200, -, -, | -, -, -, -)

Lades

[Lade00]<sup>83</sup> (- | 210 ± 20, -, -, | 320 ± 20, -, -, -)  
 [Schr06]<sup>168</sup> (- | 210 ± 20, -, -, | 320 ± 20, -, -, -)  
 [Buon10]<sup>170</sup> (- | 210, -, -, | -, -, -, -)  
 [Lutz11]<sup>12</sup> (- | 210, -, -, | 320, -, -, -)  
 [Usma12]<sup>169</sup> (- | 210, -, -, | -, -, -, -)  
 [Lutz18]<sup>13</sup> (- | 210, -, -, | 320, -, -, -)

Tanaka *et al.*

[Tana00]<sup>119</sup> (- | 160, -, -, | -, -, -, -)  
 [Bhat05]<sup>82</sup> (- | 191, -, -, | -, -, -, -)

Ayalew

[Ayal04]<sup>61</sup> (- | 220 ± 20, -, -, | 330 ± 30, -, -, -)  
 [Ayal05]<sup>84</sup> (- | 220 ± 20, -, -, | 330 ± 30, -, -, -)

Ivanov, Henry, and Janzén

[Ivan05]<sup>136</sup> (- | -, 197.9, 201.3 | -, -, -, -)  
 [Janz08]<sup>163</sup> (- | -, 197.9, 201.3 | -, -, -, -)  
 [Kimo14a]<sup>164</sup> (- | -, 198, 201 | 280, -, -, -)  
 [Kimo19]<sup>152</sup> (- | -, 198, 201 | -, -, -, -)  
 [Kimo15]<sup>8</sup> (- | -, 198, 201 | 280, -, -, -)  
 [Nipo18]<sup>23</sup> (- | -, 198, 210 | -, -, -, -)  
 [Tian20]<sup>167</sup> (- | 201.3, -, -, | -, -, -, -)

Pensl *et al.*

[Pens05]<sup>17</sup> (-, -, -, | -, -, -, | -, -, -, -)  
 [Sul108]<sup>179</sup> (- | -, -, -, | 300, -, -, -)  
 [Rakh20]<sup>178</sup> (- | -, -, -, | 300, -, -, -)

Pernot, Contreras, and Camassel

[Pern05]<sup>71</sup> (- | 180+3, -, 260+15 | -, -, -, -)  
 [Uhne15]<sup>43</sup> (- | 205, -, -, | -, -, -, -)  
 [Maxi23]<sup>203</sup> (- | 205, -, -, | -, -, -, -)

Tamaki *et al.*

[Tama08a]<sup>201</sup> (191 | -, -, -, | -, -, -, -)  
 [Meno11]<sup>202</sup> (- | -, -, -, | -, -, -, -)

Koizumi, Suda, and Kimoto

[Koiz09]<sup>103</sup> (- | 275, -, -, | -, -, -, -)  
 [Arva17]<sup>153</sup> (- | 265, -, -, | 293, -, -, -)  
 [Dona18]<sup>21</sup> (- | 265, -, -, | 293, -, -, -)  
 [Loph18]<sup>38</sup> (- | 265, -, -, | 293, -, -, -)  
 [Tiwa19]<sup>174</sup> (- | 265, -, -, | -, -, -, -)  
 [Tiwa19a]<sup>173</sup> (- | 265, -, -, | -, -, -, -)  
 [Joha19]<sup>176</sup> (- | 265, -, -, | -, -, -, -)  
 [Sozz19]<sup>175</sup> (- | 265, -, -, | -, -, -, -)

Arvinte

[Arvi17]<sup>69</sup> (- | 211, -, -, | -, -, -, -)  
 [Bade20]<sup>196</sup> (200 | -, -, -, | -, -, -, -)

Huang *et al.*

[Huan22a]<sup>26</sup> (- | 230, -, -, | -, -, -, -)  
 [Huan22b]<sup>172</sup> (- | 230, -, -, | -, -, -, -)

FIG. 8. Reference chain for p-type doping. Entries with green background show fundamental investigations, orange references we inferred based on the used data and blue investigation based not on 4H.

up until this day. Similarly, for p-type doping Götz *et al.*<sup>98</sup> provided for some time the values. However, recently the values by Ivanov, Henry, and Janzén<sup>136</sup>, Ivanov, Magnusson, and Janzén<sup>141</sup> are dominantly cited.

The most research has been clearly directed towards Aluminum. Overall, future research should be denoted to (i) gather additional data for Phosphorous and Boron and (ii) condense the already achieved values. For this purpose we added our own fittings based on the gathered data for cubic and hexagonal lattice site as well as for all values together (effective value).



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