TCAD Parameters for 4H-SiC: A Review

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(Dated: 1 October 2024)

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 dopand 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

I. IMPACT IONIZATION

In high electric fields, charge carriers are able to pick up enough kinetic energy to create an additional electron-hole pair, which is called impact ionization. This effect is sometimes deliberately used, e.g., in avalanche diodes, to increase the responsiveness[1] but often is an undesired effect that leads to breakdown and the destruction of the device. Consequently, impact ionization simulations are crucial to predict the safe operation regions of a device. In TCAD tools impact ionization is modeled as a (electric field dependent) multiplicative factor that denotes the increase of charge carriers per unit distance.

A. Theory

The impact ionization is described by the charge carrier generation rate[2,3]

$$G_{II} = \frac{1}{q}\left(\alpha J_\mathrm{n} + \beta J_\mathrm{p}\right) = \frac{1}{q}\left(\alpha n v_n + \beta p v_p\right)$$

with n resp. p the amount of electron resp. holes, v_n resp. v_p their velocity and J_n resp. J_p the electron resp. hole current. The impact ionization coefficients for electrons (α) and holes (β) represent the number of secondary carriers a single charge carrier generates per cm in an electric field F, i.e.,[1]

$$\alpha = \frac{1}{n}\frac{\mathrm{d}n}{\mathrm{d}x}\mathrm{cm}^{-1} \quad , \quad \beta = \frac{1}{p}\frac{\mathrm{d}p}{\mathrm{d}x}\mathrm{cm}^{-1} \, .$$

Many models to describe α and β were proposed. We will provide a short introduction to the topic, whereat more detailed descriptions are available in literature[1,4–7]. One of the earliest models is the still very popular empirical Chynoweth's law[8,9]

$$\alpha, \beta(F) = a \, \exp\left[-\frac{b}{F}\right] \, , \tag{1}$$

often also called Van Overstraeten-de Man model[10]. This empirical fitting was a necessity at the time of its publication because a physical explanation was only available for strong electric fields as[11]

$$\alpha, \beta(F) = \frac{eF}{E_\mathrm{i}} \exp\left[-\frac{3E_\mathrm{p}E_\mathrm{i}}{(eF\lambda)^2}\right] \, .$$

This changed with Shockley [12] who modeled the impact ionization coefficient by

$$\alpha, \beta(F) = \frac{eF}{E_\mathrm{i}} \exp\left[-\frac{E_\mathrm{i}}{eF\lambda}\right] \, , \tag{2}$$

In this case, e denotes the electron charge, λ the mean free path and E_i the ionization energy, i.e., the energy to create an electron-hole pair. The prefactor is the inverse of the length required to gain the ionization energy, i.e., how often per unit length this energy is reached, while the exponential term denotes the chance of doing that without collisions. This model is often called Shockley's "lucky electron"[13]. In Lackner[14] the close relationship between Eq. (1) and Eq. (2), which can be easily retraced by setting $a = eF/E_i$ and $b = E_i/e\lambda$, is highlighted, leading to a physically based calculation of parameters a and b. The author suggests an additional scaling factor, depending on the electric field and the parameter b for both α and β, to cover the parameter variations with changing electric field strength.

The low- and high-field cases were finally combined in Baraff's theory[15], which expresses $\alpha, \beta \propto \exp[-b/F]$ for low fields and $\alpha, \beta \propto \exp[-c/F^2]$ for high ones. It was later extended by Thornber[16] to the expression[4]

$$\alpha, \beta(F) = \frac{eF}{\langle E_\mathrm{i} \rangle} \exp\left[-\frac{\langle E_\mathrm{i} \rangle}{[(eF\lambda)^2/3E_\mathrm{p}] + eF\lambda + E_{k_\mathrm{B}T}} \right] , \tag{3}$$

with $\langle E_\mathrm{i} \rangle$ the effective ionization threshold[4], E_p the optical phonon energy and $E_{k_\mathrm{B}T}$ a temperature contribution that is often neglected in the literature. Konstantinov *et al.*[13] even only used the high-field part for the electrons and dropped the factor $3E_\mathrm{p}$ for the holes in the equation presented in the paper. We assume a typographical error as the division sign is still visible. For the ionization energy E_i originally a value of $3/2E_\mathrm{g}$ (E_g the band gap; see **??**) was assumed, which represents the ideal case[17]. Recent measurements, however, revealed for 4H-SiC values between 7.28 and 8.6 eV[18].

Since Baraff's theory was not able to satisfy all demands[19], Okuto and Crowell[20] extended Chynoweth's law by adding the electric field as a multiplicative factor, an exponential parameter m and a temperature dependency via c and d. The overall fitting model has the form

$$\alpha, \beta(F) = a\{1 + c(T - 300)\}\, F^n \exp\left[-\left(\frac{b\{1 + d(T - 300)\}}{F} \right)^m \right] \tag{4}$$

where T denotes the temperature in Kelvin. In all investigated publications $n = 0$ so we will not consider this parameter any further, leading to a simplified model that is often referred to as Selberherr model[5].

More advanced models were also proposed, which are, however, not yet used in TCAD simulations. These include a more sophisticated temperature dependency in Eq. (4)[21] and models based on multi-stage[22] and inelastic collision events[23]. Other popular methods to investigate the effects

of impact ionization are Monte Carlo simulations[24–34], non-localized models[35,36] and the impact of defects[37] in the presence of a magnetic field[38,39]. Some researchers[40–42] even combine α and β to an effective coefficient and model it by a power law, i.e., $\alpha, \beta \propto E^n$, to achieve an analytic expression suitable for calculations.

The impact ionization is anisotropic, meaning that the breakdown field in $\langle 1\,1\,\bar{2}\,0 \rangle$ is about three quarters of the one in $\langle 0\,0\,0\,1 \rangle$ direction[43]. For that reason the impact ionization coefficients have been determined parallel and perpendicular to the c-axis. These can be combined, using a formalism introduced by Hatakeyama[44], to achieve suitable amplification factors for any desired lattice direction. Jin *et al.*[45] reused the parameter values but introduced a new approach to calculate the "driving force" by considering also the field direction for constant carrier temperature. Nida and Grossner[46] adapted the field strength to an effective $F^* = (m/m_{\parallel})^{1/2} F$, with m resp $m_{\parallel}$ the effective masses (see **??**.

To depict the changing behavior with temperature either the built-in parameters, as is the case for the Okuto-Crowell model (see Eq. (4)), or a multiplicative factor[47]

$$\gamma = \frac{\tanh\left(\frac{\hbar\omega_{\mathrm{OP}}}{2k_{\mathrm{B}}T_0}\right)}{\tanh\left(\frac{\hbar\omega_{\mathrm{OP}}}{2k_{\mathrm{B}}T_{\mathrm{L}}}\right)} \tag{5}$$

to scale the parameters a and b of Eq. (1) is used[44,48–50] with T_0 a reference temperature (often 300 K), T_{L} the lattice temperature and ω_{OP} the optical phonon energy. We are very confident that the latter corresponds to the longitudinal optical phonon energy ω_{LO} (see **??**) as their respective values match well. Hatakeyama[44], however, pointed out that for a good fit $\omega_{\mathrm{OP}} = 190\,\mathrm{meV}$ had to be used, which contradicts experimental results of $\omega_{\mathrm{LO}} = 120\,\mathrm{meV}$. Niwa, Suda, and Kimoto[51] use a polynomial of degree two to scale the parameters while Bartsch, Schörner, and Dohnke[40] utilize the ratio $T/300\,\mathrm{K}$ for this purpose. In contrast, Hamad *et al.*[52] explicitly present parameter values for different temperatures. Nida and Grossner[46] scaled the mean free path by $\sqrt{\gamma}$ and the ionization energy by the ratio of the bandgap at temperature T_{L} and at 300 K.

B. Results

To measure the impact ionization coefficients an equal amount of charge carriers is generated in a space charge region, either by (pulsed) electron (electron beam induced current (EBIC))[53] or optical beams (optical beam induced current (OBIC))[13,51,52,54–60]. Defects have a significant impact on the coefficients such that EBIC is used to extract parameters at defect-free regions[61].

The charge carrier generation is executed at varying field strengths. Recording the respective terminal currents enables a comparison against the no-field current and, thus, the determination of the effective amplification. The readout of the current can be executed in DC mode[13,54] (whereat Raghunathan and Baliga[53] state that elimination of leakage current in this case is hard), AC mode[53,57,58] or both combined[55,56]. Additional challenges are the selection of a suitable test structure, e.g., p-n/n-p diodes or pnp/npn transistors) and the proper separation of electron and hole multiplication phenomena, which we will not further cover in this review. Instead we refer the interested reader to the dedicated literature[13,51,57,59,62,63].

Monte Carlo simulations are also used for the investigation of the impact ionization. While some are able to extract the impact coefficients as the reciprocal of the average distance[34,64] others solely present simulated values without fitting to any of the earlier presented model[24–33,65]. Fitting is, however, crucial to use the results in TCAD simulations tools. For this purpose Stefanakis *et al.*[66] provides fittings to Monte Carlo simulation[25,67],Nouketcha *et al.*[17] used a genetic algorithm to fit to multiple sources[46,54–56,68,69], Nida and Grossner[46] fitted their model to values from[13,44,53,55,68] and Stefanakis *et al.*[66] achieved a "global fit" in regard to many 4H investigations[13,55,56,58,60,69], but also a 6H one[70], and Monte Carlo simulations[25,67]. Kyuregyan[62] calculated the average of available parameter values without conducting any fitting. According to the authors this is supposed to remove statistical inaccuracies and uncertainties introduced by the characterization methods. Even multiple fittings on the same data were executed. Baliga[61], Banerjee[71], Choi *et al.*[72], Sheridan *et al.*[73], Zhao *et al.*[74], Morisette[75] all used the data from Konstantinov *et al.*[13], however, the ones for Sheridan *et al.*[73] exactly match values achieved for 6H by Ruff, Mitlehner, and Helbig[70].

TABLE I. Parameters for fundamental fittings of the Okuto-Crowell model found in literature. If only a single value spanning across two columns is presented the crystal direction was not specified.

	electron							hole							
ref.	$a_\parallel$	$a_\perp$	$b_\parallel$	$b_\perp$	c	d	m	$a_\parallel$	$a_\perp$	$b_\parallel$	$b_\perp$	c	d	m	F region
	[10^6 cm^{-1}]		[MV cm^{-1}]		[10^{-3}]	[10^{-3}]	[1]	[10^6 cm^{-1}]		[MV cm^{-1}]		[10^{-3}]	[10^{-3}]	[1]	[MV cm^{-1}]
[Ragh99][53]	-	-	-	-	0	0	1	3.09		17.9 ± 0.4		-3.46	0	1	2.5–3.2
[Bert00][76j]	0.4	48	15		0	0	1.15	1.8	45	15		0	0	1	-
[Sher00][73dl]	-	-	-	-	0	0	1	5.18	-	14	-	0	0	1	-
[Mori01][75d]	-	-	-	-	0	0	1	-	-	-	-	0	0	1	-
[Ng03][56]	1.98		9.46		-2.02[a]	0	1.42	4.38		11.4		-0.913[a]	0	1.06	1.8–4
[Zhao03][74d]	7.26		23.4		0	0	1	6.85		14.1		0	0	1	-
[Hata04][77]	176	21	33	17	0	0	1	341	29.6	25	16	0	0	1	2–5
[Choi05][72d]	16.5		25.8		0	0	1	5.5		13.5		0	0	1	1.5–5
[Loh08][55]	2.78		10.5		0	0	1.37	3.51		10.3		0	0	1.09	1–5
[Loh09][78]	-	-	-	-	0	0	1	3.321		10.385		-2.78	0.48[k]	1.09	1.33–2
[Nguy11][57]	0.46		17.8		0	0	1	15.6		17.2		0	0	1	1.5–2.7
[Gree12][63h]	0.019		2.888		0	0	4.828	0.06		1.387		0	0	0.96	1.6–4
[Nguy12][58]	3.36		22.6		0	0	1	8.5		15.97		0	0	1	1.5–4.8
[Sun12][34]	1.803		13.52		0	0	1.2	1.861		9.986		0	0	1.11	1.5–5
[Niwa14][51]	8190		39.4		0	0	1	4.513		12.82		0[f]	0	1	1.4–2.7
[Hama15][52]	0.99		12.9		0	0	1	1.61		11.5		0	0	1	2.5–7
[Niwa15][68]	0.143	-	4.93	-	0[c]	0[c]	2.37	3.14	-	11.8	-	6.3[c]	1.23[c]	1.02	1–2.8
[Shar15][79]	186	-	28	-	0	0	1	301	-	20.5	-	0	0	1	-
[Kyur16][62i]	38.6 ± 15.0		25.6 ± 0.1		0	0	1	5.31 ± 0.30		13.10 ± 0.01		0	0	1	1–5
[Zhan18][80]	1.31		13		-1.47	0	1	2.98		13		-1.56	0	1	-
[Bali19][61d]	313		34.5		0	0	1	8.07		15		0	0	1	1.1–5
[Zhao19][60]	0.339	-	5.15	-	0	0	2.37	3.56	-	11.7	-	6.19	1.15	1.02	1–3.2
[Stef20][59]	-	6.4	-	12.5	0	0	1	-	6	-	13.3	0	0	1	1.3–2
[Bane21][71d]	100		40.268		0	0	1	41.915		46.428		0	0	1	0.1–1
[Chea21][64g]	0.932		7.19		0	0	1.95	1.75		6.56		0	0	1.45	1.6–10
[Stef21][66e]	2.8	-	20.7	-	-1[b]	-0.29[b]	1	2.5	-	12.1	-	1.74[b]	0.59[b]	1	-

[a] provided by Cha *et al.* [81]

[b] provided by Steinmann *et al.* [82]

[c] different values suggested by Steinmann *et al.* [82]

[d] values fitted to Konstantinov *et al.* [13]

[e] values fitted to [13,25,55,56,58,60,67,69,70]

[f] temperature dependency stated in the paper that could not be transferred to model formalism

[g] a and b presumably stated in m^{-1} and MV m^{-1} in paper, converted to cm^{-1} and MV cm^{-1}

[h] for $F > 2.5\,\mathrm{MV\,cm^{-1}}$ the parameters α from Ng *et al.* [56] are used

[i] values achieved by averaging of [13,51,54–56,63,78,83]

[j] fitted to Nilsson *et al.* [84]

[k] we changed $b = 8.9 \times 10^6 - 4.95 \times 10^3\,T$ to $b = 8.9 \times 10^6 + 4.95 \times 10^3\,T$ to better match the results in the paper

[l] same values achieved as 6H investigation by Ruff, Mitlehner, and Helbig [70]

TABLE II. Parameters for fundamental fittings of the Thurnber model found in literature. For $E_{k_BT} = k_BT$ this parameter scales with temperature.

ref.	dir	electron				hole				F region
		$\langle E_i \rangle$ [eV]	λ [Å]	E_p [meV]	E_{k_BT} [meV]	$\langle E_i \rangle$ [eV]	λ [Å]	E_p [meV]	E_{k_BT} [meV]	[MV cm^{-1}]
[Kons97][13f]	∥	10	29.9	120	0	7	32.5	120	0	1.5–10
[Nida19][46a]	∥	10.61	27	120	k_BT	10.87	39.49	85	k_BT	1–10
[Nouk20][17c]	-	7.5	10	92.5	14	6.62	4.8	9	102	0.9–10
[Stei23][82e]	-	10.6	27	87	k_BT	10.9	80	87	k_BT	1–10

[a] values picked from specified ranges, fitting to[13,44,53,55,68]

[c] $3/2\,E_g$ instead of $\langle E_i \rangle$ used in the exponential, fitting to[46,54–56,68,69]

[e] initial values taken from Nida and Grossner[46]

[f] linear term in denominator not used for α

A wide range parameters for the Okuto-Crowell (see Table I) and Thornber (see Table II) model could be identified in literature. We were unable to match the temperature variation of β with $b = 8.9 \times 10^6 - 4.95 \times 10^3 T$[78] with the data presented in the same publication. We achieved much better results with $d = 8.9 \times 10^6 + 4.95 \times 10^3 T$ with T the temperature in Kelvin. In Stefanakis *et al.*[59] the fitting for α also deviates slightly from the plots in the paper. Due to the minor deviation we kept the values as they were. In Cheang, Wong, and Teo[64] the values of parameters a and b are two orders of magnitude too high. We suspect that they are specified in m^{-1} resp. MV m^{-1} although in the paper it is explicitly stated as cm^{-1} resp. MV cm^{-1}. Despite these changes we were not able to exactly recreate the plots shown in the paper. We had to exclude the publication by Ng *et al.*[83] as no data are shown in the paper and Cheong *et al.*[85], Kimoto *et al.*[86] who only specify that SiC is investigated but not the polytype.

A graphical representation of the models describing the impact ionization coefficient for electrons (see Fig. 1) show a spread of approximately one order of magnitude, whereat the deviations increase for low fields. For the crystal direction perpendicular to the c-axis much higher values are determined. This matches qualitatively early estimations, however, the quantities of $\alpha_\perp/\alpha_\parallel = 3.5$ used by Bakowski, Gustafsson, and Lindefelt[2], Lades[48] seems to be too low. For low resp. high fields the fittings of Zhang and You[80] resp. Sharma, Hazdra, and Popelka[79] are too high meaning that the models have to be handled with care in these regions.

For holes (see Fig. 2) the spread in values is much smaller, especially close to a field strength

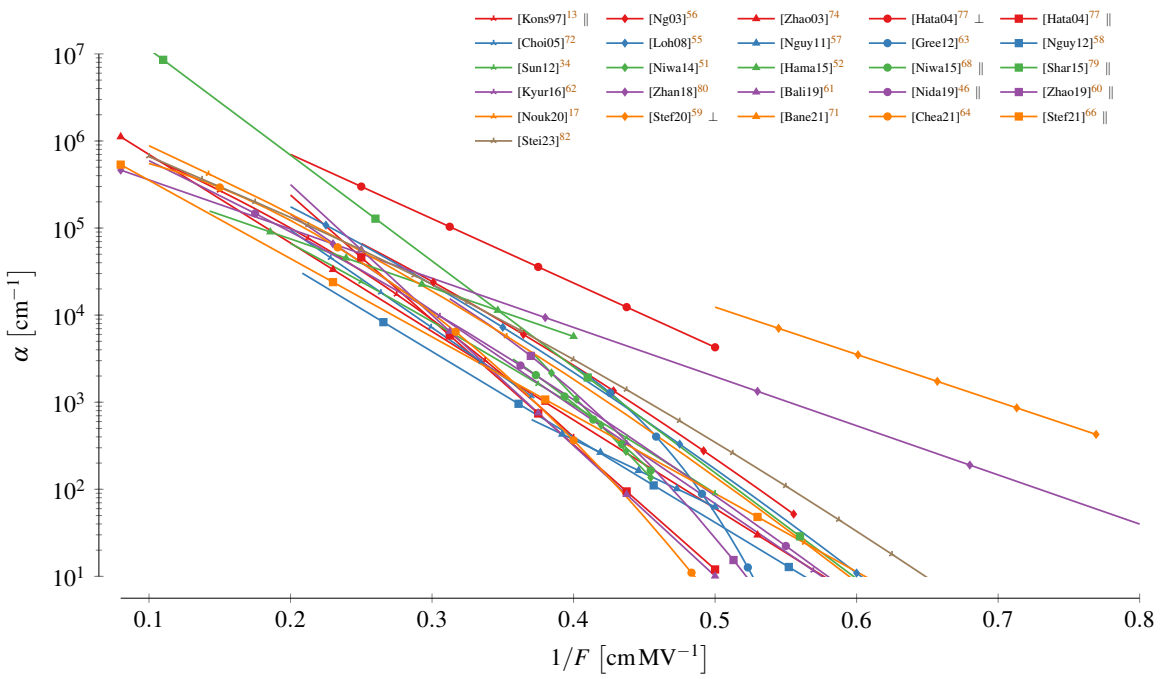

FIG. 1. Impact ionization coefficient α for electrons. Each model is limited to the interval used for characterization. The colors are altered to increase the readability.

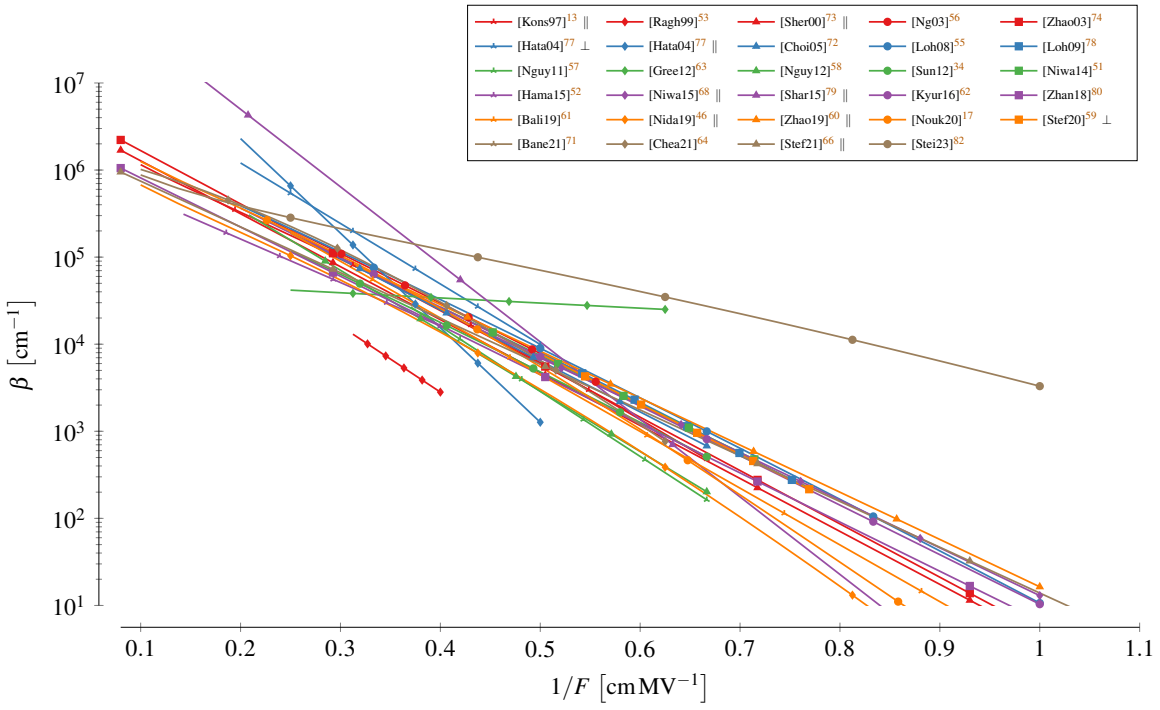

FIG. 2. Impact ionization coefficient β for electrons. Each model is limited to the interval used for characterization. The colors are altered to increase the readability.

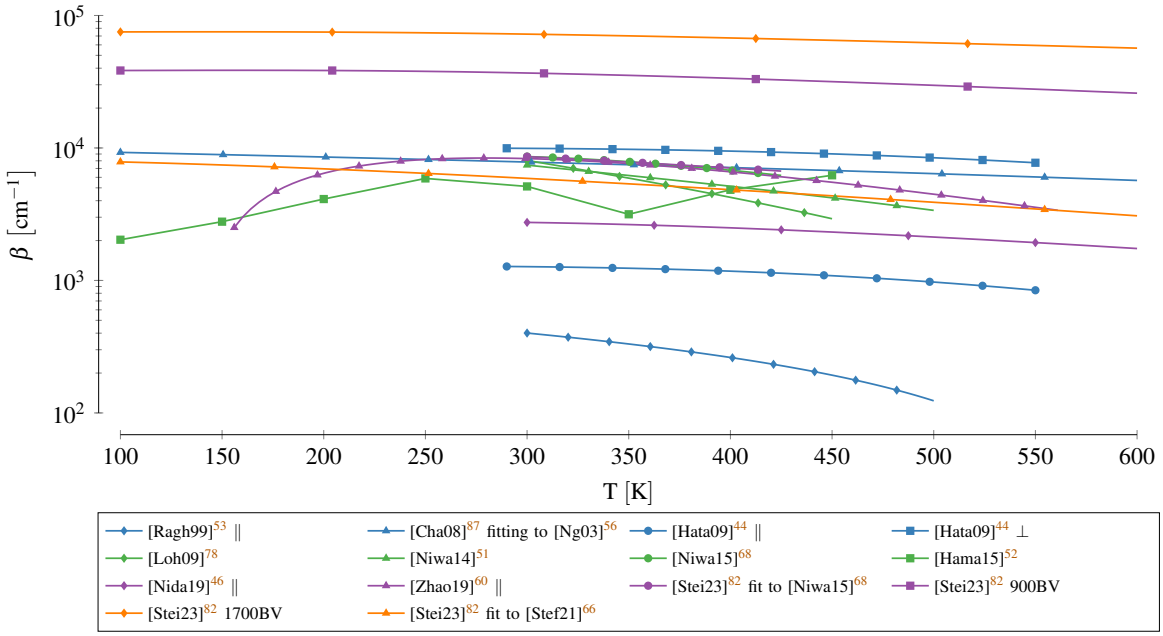

FIG. 3. Temperature dependence of the hole impact ionization coefficient. The single models are evaluated for an electric field of 2 MV cm^{-1} and are ordered according to their publication date. The colors simply are used to improve the readability.

around 2 MV cm^{-1}. Nevertheless, there are also fittings we want to highlight. The results of Steinmann *et al.*[82] are too high possibly correlating to the fitting of a rather high breakdown voltage. The values from Raghunathan and Baliga[53] are too low, which was attributed to the direction dependency of α[6,76], i.e., that the coefficient in the direction perpendicular to the c-axis is much stronger. Feng and Zhao[6] thus conclude that the results in[53] deviate from practical results since the focused beam used in the analyses caused them to miss a large share of the intrinsic defects. Although Fig. 2 supports this statement, the statement that the perpendicular impact ionization of holes is a lot stronger, could not be confirmed. The results suggest rather $\beta_\perp = \beta_\parallel$, which was also used for 6H[2]. Finally, the fittings by Green *et al.*[63] show a significantly slower increase with field than all other models.

Important for TCAD simulations is also the temperature dependency of the impact ionization coefficients. For holes (see Fig. 3) all models predict a decreasing value, which matches the reports of increasing breakdown voltage with increasing temperature. Hatakeyama[44] uses the temperature scaling shown in Eq. (5) (multiplication with γ), which is also used in Lades[48], Schröder[88]. Clearly visible is the decline of β with increasing temperature. Steinmann *et al.*[82] proposed two

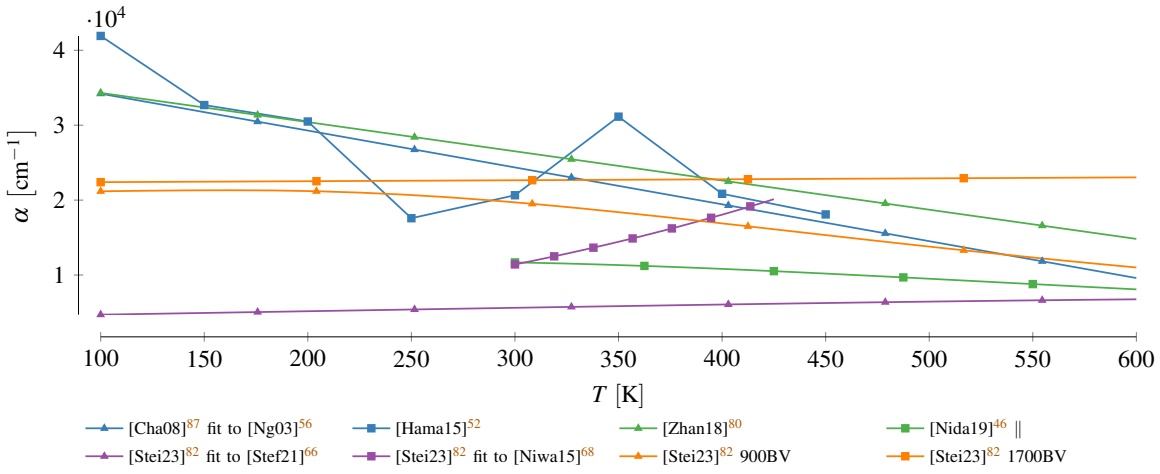

FIG. 4. Temperature dependence of the electron impact ionization coefficient. The single models are evaluated for an electric field of 3.33 MV cm^{-1} and are ordered according to their publication date. The colors simply are used to improve the readability.

fittings for two different breakdown voltages of the investigated device, i.e., 900 V and 1700 V.

For electrons (see Fig. 4) the results are quite inconclusive. Some models even propose an increase of α with temperature. This is, however, compensated by the decrease in β with increasing temperature due to the relatively small variations of α compared to β (linear vs. logarithmic y-axis).

C. Discussion

The majority of the currently utilized impact ionization coefficients are based on 4H measurements (see Fig. 5). Care has to be taken especially for publications prior to the year 2000, as those often are based on 6H[2,70,89,90]. These outdated results have later found their way in various publications[7,48,91–93]. In early publications[2] 6H was still used because 4H values were not available or simply[74,94] because the early available fittings from Konstantinov *et al.*[54], Raghunathan and Baliga[69] deviated significantly. Based on the results from Bakowski, Gustafsson, and Lindefelt[2] Lades[48] turned these further upside down by calculating values at 273 K and introducing a typographical for the hole coefficient a which was stated as 2.24×10^6 instead of 3.24×10^6. We found more such issues, which we summarize in **??**.

The most influential publications are arguably by Raghunathan and Baliga[53,69] and Hatakeyama *et al.*[77]. However, twelve investigations in the last decade reveal that this is still an active field

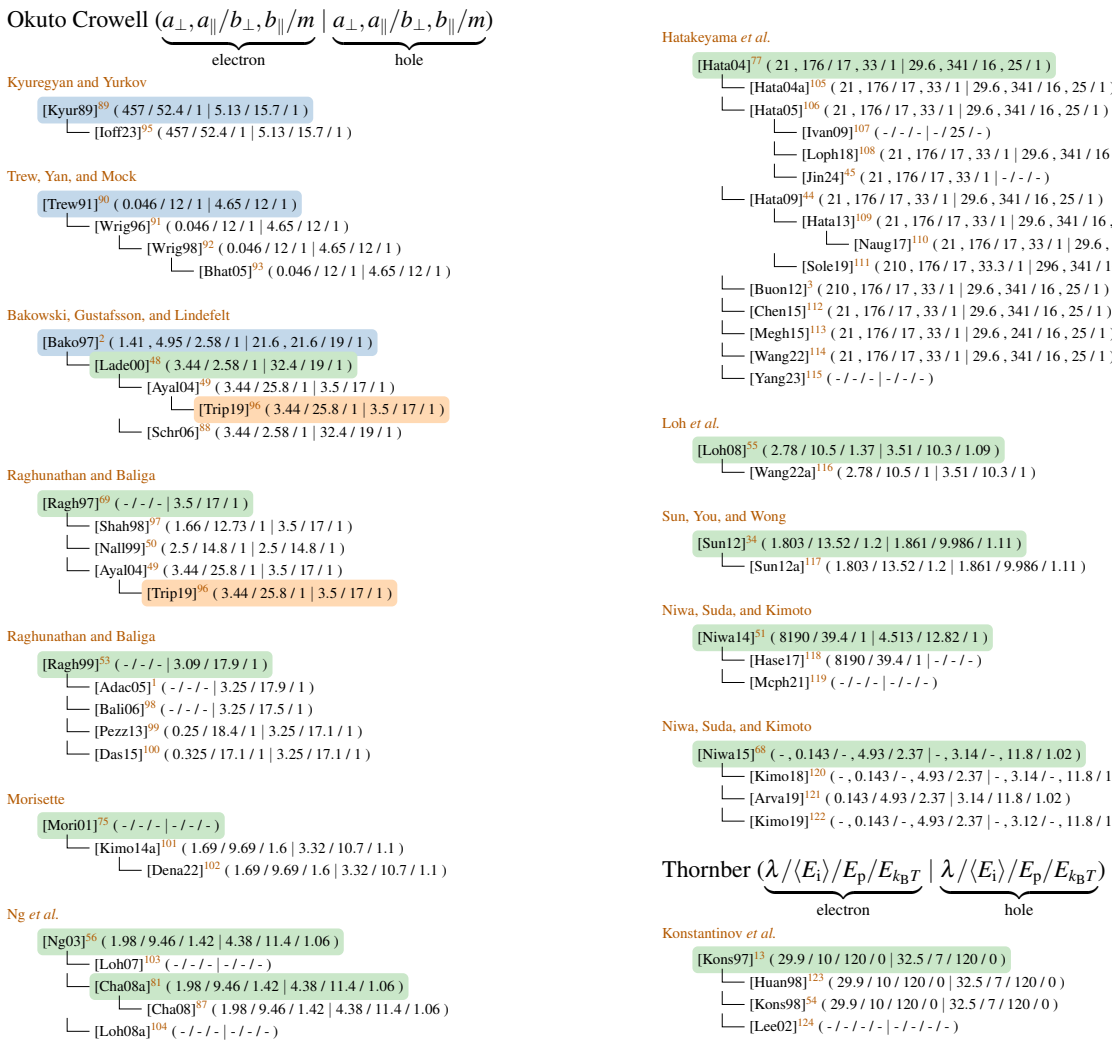

FIG. 5. Reference chain for impact ionization parameters. Publications with blue background are not focused on 4H-SiC, those in green are novel analyses on 4H-SiC and orange color indicates that the reference was guessed based on the values but not explicitly stated in the publication. The values for a and b were scaled by 1×10^6 for improved readability.

of research. Nevertheless, only very few values for the impact ionization perpendicular to the c-axis is available. Since the few available data suggest a higher coefficient and thus earlier breakdown these direction, further in detail investigations are required in the future. Also very few temperature analyses are available. Some of the temperature dependencies were later proposed by other authors, e.g., by Cha and Sandvik[87] or by Steinmann *et al.*[82], who fitted the linear and quadratic temperature coefficients of the breakdown voltage. Nida and Grossner[46] present the high temperature evolution of some models.

In contrast to Silicon, 4H-SiC shows higher hole than electron current amplification, i.e., $\beta > \alpha$[1,125], which is attributed to discontinuities in the electron spectrum[126]. Consequently, the Shockley approximation of the "lucky electron" can only be applied to holes, as the electrons energy can not continuously increase[13]. Kimoto *et al.* [120] name these "minigaps" as the reason for the low temperature dependence of α. Nevertheless, the breakdown voltage still increases with temperature[87,127] because the impact coefficient of the holes decreases with temperature[1], which prevents thermal runaway.

Although models can be use for any arbitrary field strengths, they are most accurate within their often very narrow characterization range. In general, the highest accuracy is required around the critical electric field, i.e., where breakdown occurs. In the literature commonly 2–3 $\mathrm{MV\,cm^{-1}}$[128–136] are used, whereat some explicitly state a dependence on the doping concentration[13,42,43,53,60,61,68,120,122,137–141]. Be advised that these values are, most commonly, determined for uniformly doped non-punch through diodes using power law approximations of the impact coefficients[53]. Consequently such values have to be interpreted with a grain of salt and have to be corrected according to the actual structure and doping level[68,142]. Over short distances a higher field is required to achieve breakdown than for thick devices, where charges can multiply over long distances.

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