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

I. DENSITY-OF-STATES EFFECTIVE MASS

The effective mass of charge carriers is defined as the reciprocal of the second derivative of the spherically averaged dispersion relation[1] and, thus, dependent on the shape of the conduction/valence band. Because the latter are not uniform in a semiconductor deviating masses for each principal direction are achieved. These direction-dependent values are then further combined to end up with more simplistic descriptions[2].

In this section we investigate the effective mass of electrons and holes in each principal direction and how these get merged into the density-of-states (DOS) and conductivity mass. We extend earlier overview publications[3–9] and focus primarily on the DOS masses because they are used in TCAD simulations in various occasions, e.g., the calculation of the charge carrier concentration or impact and incomplete ionization. We want to highlight that in TCAD tools many additional effective masses are used, e.g., tunneling masses, quantum well masses, effective mass at the contact or in a channel or thermionic relative masses, which must not be confused.

A. Theory

In the sequel we start with a short theoretical analysis of effective masses. For further information the interested reader is referred to the dedicated literature[2–7,10–12]. To increase the readability the effective masses are denoted relative to the free electron mass m_0, i.e., $m^* = m/m_0$[13].

1. Effective Masses along Principal Directions

For electrons the mass is specified in the directions starting in the conduction band minimum at the M point[4,14–17] (cp. **??**) towards the Γ, K and L point, denoted in the sequel as $m^*_{\mathrm{M\Gamma}}$, m^*_{MK} and m^*_{ML}. The first two are perpendicular to the c-axis and the last one parallel[15,18–20]. In the M point two conduction bands are very close together, such that both can influence the effective mass[7,17]. Zhao *et al.* [21] even used three conduction bands. If not otherwise stated we will focus in this paper solely on the lowest one.

The valence band maximum is in the Γ point[9,15,18]. Consequently, the three relative masses are termed $m^*_{\Gamma\mathrm{M}}$, $m^*_{\Gamma\mathrm{K}}$ (perpendicular) and $m^*_{\Gamma\mathrm{A}}$ (parallel) indicating the directions towards the M, K and A point[17,22]. At the Γ point three separate bands meet[11,14,18,22,23], whereat the two topmost are called heavy-hole (hl) and light-hole (ll) and the third one crystal split off (so)[11,23]. Although

all have to be considered for an accurate estimation often only a subset is used.

2. *Density-of-States (DOS) Mass*

The effective density of states for conduction (N_C) and valence (N_V) band[24–28]

$$N_C = 2\,M_C \left(\frac{2\pi m^*_{de} k_B T}{h^2}\right)^{3/2}$$
$$N_V = 2 \left(\frac{2\pi m^*_{dh} k_B T}{h^2}\right)^{3/2},$$

with M_C the number of conduction band minima in the first Brillouin zone[28], is, for example, used to evaluate the electron and hole concentration. The utilized effective density-of-states masses m^*_{de} and m^*_{dh} are defined as[6,12,18,29]

$$m^*_{de} = ({m^*_{de\perp}}^2 m^*_{de\parallel})^{1/3} = (m^*_{M\Gamma} m^*_{MK} m^*_{ML})^{1/3}$$
$$m^*_{dh} = ({m^*_{dh\perp}}^2 m^*_{dh\parallel})^{1/3} = (m^*_{\Gamma M} m^*_{\Gamma K} m^*_{\Gamma A})^{1/3}$$

with[11]

$$m^*_{de\perp} = \sqrt{m^*_{M\Gamma} m^*_{MK}}, \qquad m^*_{de\parallel} = m^*_{ML}$$
$$m^*_{dh\perp} = \sqrt{m^*_{\Gamma M} m^*_{\Gamma K}}, \qquad m^*_{dh\parallel} = m^*_{\Gamma A}\,.$$

In this case m^*_{de} is called the *single valley* DOS electron effective mass[6,15,29,30], as the factor M_C is not considered. It is also very common,e.g., in some TCAD tools, to add M_C to the effective mass[2,18,31–33], i.e.,

$$m^*_{de} = (M_C^2\, {m^*_{de\perp}}^2 m^*_{de\parallel})^{1/3}\,.$$

In this review we will only present the single valley values and highlight all publications where we found expressions including M_C.

For an effective mass of the holes it is also necessary to combine the masses of heavy (m^*_{hh}) and light (m^*_{lh}) holes, which can be achieved by[1,34,35]

$$m^*_{dh} = \left({m^*_{hh}}^{3/2} + {m^*_{lh}}^{3/2}\right)^{2/3}. \tag{1}$$

This expression is already a simplification, because for accurate results the energy difference between the bands has to be considered[18]. This leads to

$$m^*_h(T) = \left[m_{h1}^{3/2} + m_{h2}^{3/2} \exp\left(-\frac{\Delta E_2}{k_B T}\right) + m_{h3}^{3/2} \exp\left(-\frac{\Delta E_3}{k_B T}\right)\right]^{2/3} \tag{2}$$

where ΔE_2 and ΔE_3 denote the energy separation between the bands.

a. Temperature Dependency The changing amount of charge carriers with temperature can be compactly modeled by using a *thermal DOS effective mass*[12,36]. There is no explicit form available but it was calculated by Wellenhofer and Rössler[12] (electrons and holes separately) and Tanaka *et al.*[37] (average effective mass). Later Schadt[7], Hatakeyama, Fukuda, and Okumura[30] fitted the results from Wellenhofer and Rössler[12] with an equation of the form

$$m^*(T) = \left(\frac{z_0 + z_1 T + z_2 T^2 + z_3 T^3 + z_4 T^4}{1 + n_1 T + n_2 T^2 + n_3 T^3 + n_4 T^4} \right)^{\eta} \tag{3}$$

for both electrons and holes. Such a change in the effective DOS mass is not yet covered in TCAD simulations suites.

3. *Conductivity Effective Mass*

For investigations of the mobility in 4H-SiC[7,37–46] the mobility mass is a crucial simplification, e.g., in[4]

$$\mu = \frac{e\tau}{m_c^*},$$

with μ the mobility, e the elementary charge and τ the lifetime (see **??**). The conductivity mass must not be confused with the DOS mass since its definition[2,47]

$$m_{ce}^* = \frac{3 m_{ce\perp}^* m_{ce\parallel}^*}{m_{ce\perp}^* + 2 m_{ce\parallel}^*}$$
$$m_{ch}^* = \frac{3 m_{ch\perp}^* m_{ch\parallel}^*}{m_{ch\perp}^* + 2 m_{ch\parallel}^*}$$

with[38,39]

$$\frac{2}{m_{ce\perp}^*} = \frac{1}{m_{MK}^*} + \frac{1}{m_{M\Gamma}^*}, \qquad m_{ce\parallel}^* = m_{ML}^*$$
$$\frac{2}{m_{ch\perp}^*} = \frac{1}{m_{\Gamma M}^*} + \frac{1}{m_{\Gamma K}^*}, \qquad m_{ch\parallel}^* = m_{\Gamma A}^*$$

which results in[40]

$$\frac{3}{m_{ce}^*} = \frac{1}{m_{M\Gamma}^*} + \frac{1}{m_{MK}^*} + \frac{1}{m_{ML}^*}$$
$$\frac{3}{m_{ch}^*} = \frac{1}{m_{\Gamma M}^*} + \frac{1}{m_{\Gamma K}^*} + \frac{1}{m_{\Gamma A}^*}.$$

is fundamentally different. In the sequel we will solely concentrate on the DOS mass.

4. *Polaron Mass*

In the Si-C bond of silicon carbide, carbon atoms are more electronegative than silicon ones. This results in a partly ionic crystal[11]. Within this surrounding a charge carrier, together with its self-induced polarization, forms a quasiparticle, which is called a polaron[48]. This can also be described by longitudinal optical vibrations that generate an electric field along the direction of the vibration which interacts with the charge carriers[11,13]. Effectivly, the carrier is "dressed" by a charge leading to a deviating effective mass[49]. The adapted mass m_p, called *polaron mass*, is slightly higher than the bare mass m and can be calculated as[10,11,49]

$$m_\mathrm{p} = m\frac{1-8\times10^{-4}\alpha^2}{1-\alpha/6+3.4\times10^{-3}\alpha^2} \approx m\left(1-\frac{\alpha}{6}\right)^{-1}$$

with the Fröhlich constant α defined as

$$\alpha = \frac{1}{2}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_\mathrm{s}}\right)\frac{e^2}{\hbar\omega_\mathrm{LO}}\left(\frac{2m\omega_\mathrm{LO}}{\hbar}\right)^{1/2}\frac{1}{4\pi\varepsilon_\mathrm{s}}\,.$$

In the latter e denotes the elementary charge, $\varepsilon_\mathrm{s}/\varepsilon_\infty$ the static/high-frequency dielectric constant and ω_LO the longitudinal optical phonon frequency (see **??**). We want to highlight that in some definitions in literature[48,50,51] the last term $1/4\pi\varepsilon_\mathrm{s}$ is missing due to a differing unit system.

Note that in (optically detected) cyclotron resonance measurements always the polaron mass is extracted. For a better comparability it is thus necessary to adapt non-polaron masses, e.g., those achieved by calculations[17].

B. Results

In the following we show the results of our investigations. Note that we discarded conductivity masses, e.g., by Mikami, Kaneko, and Kimoto[52], and solely concentrate on the DOS mass here. We also did not include the results by Son *et al.*[53] since Son *et al.*[11] later stated that the smaller values are due to "errors caused by a broad and asymmetric ODCR line shape with the peak position slightly shifted to lower magnetic fields".

1. *Effective Mass along Principal Directions*

To determine the effective masses mainly band structure calculations are used. The most common ones are based on the density functional theory (DFT) local density approximation

(LDA)[12,16,17,19,54–57]. Differing methods, e.g., projector augmented wave (PAW)[22,58], (full-potential) linearized augmented plane wave ((FP)LAPW)[10,11,14,49,59], (orthogonalized) linear combination of atomic orbital ((O)LCAO)[60,61], full-potential linear muffin-tin orbital method (FPLMTO)[62] and hybrid pseudo-potential and tight-binding (HPT)[63], were utilized in this context. Other calculations include empirical pseudo potentials (EPM)[64,65] and RSP Hamiltonians (RSPH)[23].

Results achieved by these calculations are sometimes combined using Monte Carlo (MC)[54,56] simulations or genetic algorithm fitting (GAF)[68,69]. In some cases the literature values were used as starting point for further analyses. Based on the data from Son *et al.* [53] such a refinement was executed by Nilsson, Sannemo, and Petersson [56], whose results then served as starting point for a fitting by Mickevičius and Zhao [70]. Similarly, Mikami, Kaneko, and Kimoto [52] calculated the hole mass as the second derivative of the E-k dispersion by Persson and Lindefelt [14].

The calculations are complemented by measurements, for example by optically detected cyclotron resonance (ODCR)[13,46,53,66,71], photoluminescence[29], infrared absorption (IR)[28], Raman scattering[72] and Hall effect measurements[44,73–75]. However, for the relative masses in the principal directions (see Table I) calculations clearly dominate. Only two measurements[44,66] could be found for the electron masses whereat not a single experimental evaluation for hole masses was achieved.

In literature the hole bands are either denoted as heavy-hole (hh), light-hole (lh) and crystal split-off (so) or simply as 1, 2, 3. According to the found values we are confident to say that 1 $\equiv$ hh, 2 $\equiv$ lh and 3 $\equiv$ so.

2. *DOS Mass*

For a comprehensive overview on DOS masses we combine calculations based on the effective masses in the principal directions and values presented in literature (see Table II and Table III). Again, calculations clearly dominate, however, an increased amount of measurements[13,44,53,66,73–75], including some for the hole mass, could be acquired.

The values show significant deviation. In addition Schadt [7] stated that they are only valid close to the band minimum/maximum as they are calculated there or at very low temperature. Furthermore, Son *et al.* [11] claimed that if the polaron effect is added to the results from Persson and Lindefelt [14,59] the values $m^*_{\mathrm{dh}\perp} = 0.66$ and $m^*_{\mathrm{dh}\parallel} = 1.76$ are achieved, which fit the results from

TABLE I. Effective masses in principal directions. Multiple values for the same band are are calculated by differing algorithms.

	electron				hole					
ref.	$m^*_{M\Gamma}$ $[m_0]$	m^*_{MK} $[m_0]$	m^*_{ML} $[m_0]$	band	$m^*_{\Gamma M}$ $[m_0]$	$m^*_{\Gamma K}$ $[m_0]$	$m^*_{\Gamma A}$ $[m_0]$	band	method[a]	polaron
[Kack94][55]	0.62	0.13	0.39	-	4.23	2.41	1.73	hh	DFT-LDA	-
	-	-	-	-	0.45	0.77	1.73	lh	DFT-LDA	-
	-	-	-	-	0.74	0.51	0.21	so	DFT-LDA	-
[Karc95][16]	0.66	0.31	0.3	-	-	-	-	-	DFT-LDA	-
[Lamb95][62]	0.58	0.28	0.31	-	-	-	-	-	DFT-LDA	-
[Wenz95][57]	0.6	0.28	0.19	-	-	-	-	-	DFT-LDA	-
[Nils96][56]	0.43	0.43	0.28	1	-	-	-	-	DFT-LDA	-
	0.52	0.21	0.45	2	-	-	-	-	DFT-LDA	-
[Pers96][14]	0.57	0.28	0.31	-	-	-	-	-	DFT-LDA	-
[Volm96][66]	0.58 ± 0.01	0.31 ± 0.01	0.33 ± 0.01	-	-	-	-	-	ODCR	y
[Chen97][63]	1.2	0.19	0.33	-	-	-	-	-	DFT-LDA	-
[Pers97][49]	0.57	0.28	0.31	1	-	-	-	-	DFT-LDA	-
	0.59	0.31	0.34	1	-	-	-	-	DFT-LDA	-
	0.61	0.29	0.33	1	-	-	-	-	DFT-LDA	y
	0.78	0.16	0.71	2	-	-	-	-	DFT-LDA	-
	0.8	0.18	0.75	2	-	-	-	-	DFT-LDA	-
	0.85	0.17	0.77	2	-	-	-	-	DFT-LDA	y
[Pers98a][67]	-	-	-	-	0.7	3.04	1.64	1	fit	-
	-	-	-	-	0.6	0.34	1.64	2	fit	-
[Bell00][64]	0.57	0.23	0.27	-	-	-	-	-	EPM	-
[Zhao00a][61]	0.62 ± 0.03	0.27 ± 0.02	0.31 ± 0.02	-	-	-	-	-	DFT-LDA	-
[Penn01][65]	0.60 ± 0.05	0.20 ± 0.02	0.36 ± 0.02	-	-	-	-	-	EPM	-
[Iwat03][19]	0.59	0.29	-	-	-	-	-	-	DFT-LDA	-
[Iwat03a][44]	0.58	0.3	-	-	-	-	-	-	Hall	-
[Dong04][17]	0.53	0.27	0.3	-	0.86	0.95	1.58	1	DFT-LDA	-
	-	-	-	-	0.55	0.52	1.32	2	DFT-LDA	-
	-	-	-	-	1.13	1.30	0.21	3	DFT-LDA	-
[Chin06][60]	0.47	-	0.38	-	-	-	-	-	DFT-LDA	-
[Ng10][68]	0.66	0.31	0.34	-	-	-	-	-	GAF	-
[Kuro19][22]	0.54	0.28	0.31	-	0.54	0.54	1.48	-	DFT-LDA	-
[Lu21][58]	0.54	0.3	-	-	2.77	1.82	1.52	-	DFT-LDA	-

[a] for explanation see text

TABLE II. First half of DOS masses. Multiple values for the same band are are calculated by differing algorithms.

	electron				hole					
ref.	m^*_{de} $[m_0]$	$m^*_{de\perp}$ $[m_0]$	$m^*_{de\parallel}$ $[m_0]$	band	m^*_{dh} $[m_0]$	$m^*_{dh\perp}$ $[m_0]$	$m^*_{dh\parallel}$ $[m_0]$	band	method[h]	polaron
[Loma73][74]	0.20[a]	0.21	0.19	-	-	-	-	-	Hall	-
[Loma74][75]	0.20[a]	0.21	0.19	-	-	-	-	-	Hall	-
[Gotz93][28]	0.19	0.176	0.224	-	-	-	-	-	IR	-
[Kack94][55]	0.31[a]	0.28[b]	0.39[c]	-	2.60[a]	3.19[b]	1.73[c]	hh	DFT-LDA	-
	-	-	-	-	0.84[a]	0.59[b]	1.73[c]	lh	DFT-LDA	-
	-	-	-	-	0.43[a]	0.61[b]	0.21[c]	so	DFT-LDA	-
[Hari95][72]	0.35[a]	0.30 ± 0.07	0.48 ± 0.12	-	-	-	-	-	Raman	-
[Karc95][16]	0.39[a]	0.45[b]	0.30[c]	-	-	-	-	-	DFT-LDA	-
[Kord95][46]	-	0.42	-	-	-	-	-	-	ODCR	y
[Lamb95][62]	0.35[a]	0.4	0.27	-	-	-	-	-	DFT-LDA	-
[Son95][53]	0.37[a]	0.42	0.29 ± 0.03	-	-	-	-	-	ODCR	y
[Wenz95][57]	0.32[a]	0.41[b]	0.19[c]	-	-	-	-	-	DFT-LDA	-
[Nils96][56]	0.37[a]	0.43[b]	0.28[c]	1	-	-	-	-	DFT-LDA	-
	0.37[a]	0.33[b]	0.45[c]	2	-	-	-	-	DFT-LDA	-
[Pers96][14]	0.37[a]	0.40[b]	0.31[c]	-	-	-	-	-	DFT-LDA	-
[Volm96][66]	0.39[a]	0.42[b]	0.33[c]	-	-	-	-	-	ODCR	y
[Bako97][18]	-	-	-	-	0.84	-	-	1	-	-
	-	-	-	-	0.79	-	-	2	-	-
	-	-	-	-	0.78	-	-	3	-	-
[Chen97][63]	0.42[a]	0.48[b]	0.33[c]	-	-	-	-	-	DFT-LDA	-
[Hemm97][32]	-	-	-	-	1	-	-	-	-	-
[Lamb97][23]	-	-	-	-	0.85[a]	0.62	1.6	hh	RSPH	-
	-	-	-	-	0.84[a]	0.62	1.55	lh	RSPH	-
	-	-	-	-	0.81[a]	1.58	0.21	so	RSPH	-
[Pers97][49]	0.37[a]	0.40[b]	0.31[c]	1	0.82[a]	0.59	1.56	1	DFT-LDA	-
	0.40[a]	0.43[b]	0.34[c]	1	0.82[a]	0.59	1.6	1	DFT-LDA	-
	0.39[a]	0.42[b]	0.33[c]	1	0.82[a]	0.59	1.56	2	DFT-LDA	y
	0.44[a]	0.35[b]	0.71[c]	2	0.82[a]	0.59	1.6	2	DFT-LDA	-
	0.48[a]	0.38[b]	0.75[c]	2	0.78[a]	1.49	0.21	3	DFT-LDA	-
	0.48[a]	0.38[b]	0.77[c]	2	0.79[a]	1.49	0.22	3	DFT-LDA	y

[a] $m^*_{de} = (m^*_{de\perp}{}^2 m^*_{de\parallel})^{1/3}$
[b] $m^*_{de\perp} = \sqrt{m^*_{MI} m^*_{MK}}$
[c] $m^*_{de\parallel} = m^*_{ML}$
[d] $m^*_{dh} = (m^*_{dh\perp}{}^2 m^*_{dh\parallel})^{1/3}$
[e] $m^*_{dh\perp} = \sqrt{m^*_{\Gamma M} m^*_{\Gamma K}}$
[f] $m^*_{dh\parallel} = m^*_{\Gamma A}$
[h] explanation see text

TABLE III. Second half of DOS masses. Multiple values for the same band are are calculated by differing algorithms.

	electron				hole					
ref.	m^*_{de} $[m_0]$	$m^*_{de\perp}$ $[m_0]$	$m^*_{de\parallel}$ $[m_0]$	band	m^*_{dh} $[m_0]$	$m^*_{dh\perp}$ $[m_0]$	$m^*_{dh\parallel}$ $[m_0]$	band	method[h]	polaron
[Well97][12]	0.394	-	-	-	-	-	-	-	DFT-LDA	-
[Lind98][1]	-	-	-	-	1.7	-	-	hh	DFT-LDA	-
	-	-	-	-	0.48	-	-	lh	DFT-LDA	-
[Pers98a][67]	-	-	-	-	0.94	1.46[b]	1.64[c]	1	fit	-
	-	-	-	-	0.84	0.45[b]	1.64[c]	2	fit	-
	-	-	-	-	0.88	-	-	3	fit	-
[Egil99][29]	0.37	-	-	-	-	-	-	-	PL	-
[Pers99b][59]	-	-	-	-	0.85[a]	0.62	1.61	1	DFT-LDA	-
	-	-	-	-	0.84[a]	0.61	1.62	1	DFT-LDA	-
	-	-	-	-	0.78[a]	0.56	1.52	2	DFT-LDA	-
	-	-	-	-	0.78[a]	0.58	1.42	2	DFT-LDA	-
	-	-	-	-	0.78[a]	1.5	0.21	3	DFT-LDA	-
	-	-	-	-	0.76[a]	1.46	0.21	3	DFT-LDA	-
[Bell00][64]	0.33[a]	0.36[b]	0.27[c]	-	-	-	-	-	EPM	-
[Son00][13]	0.39[a]	0.45 ± 0.02	0.30 ± 0.02	-	0.91[a]	0.66 ± 0.02	1.75 ± 0.02	-	ODCR	y
[Zhao00][21]	0.37[a]	0.42	0.28	1	-	-	-	-	-	-
	0.44[a]	0.35	0.71	2	-	-	-	-	-	-
	0.40[a]	0.66	0.15	3	-	-	-	-	-	-
[Zhao00a][61]	0.37[a]	0.41 ± 0.02	0.31[c]	-	-	-	-	-	DFT-LDA	-
[Penn01][65]	0.34[a]	0.35 ± 0.02	0.31 ± 0.05	-	-	-	-	-	EPM	-
[Iwat03][19]	-	0.41[b]	-	-	-	-	-	-	DFT-LDA	-
[Iwat03a][44]	-	0.42[b]	-	-	-	-	-	-	Hall	-
[Dong04][17]	0.35[a]	0.38[b]	0.30[c]	-	1.09[a]	0.90[b]	1.58[c]	1	DFT-LDA	-
	-	-	-	-	0.72[a]	0.53[b]	1.32[c]	2	DFT-LDA	-
	-	-	-	-	0.67[a]	1.21[b]	0.21[c]	3	DFT-LDA	-
[Chin06][60]	-	-	0.38[c]	-	-	-	-	-	DFT-LDA	-
[Aktu09][54]	0.40	-	-	-	-	-	-	-	DFT-LDA	-
[Koiz09][73]	-	-	-	-	0.5	-	-	-	Hall	-
[Ng10][68]	0.41[a]	0.45[b]	0.34[c]	-	-	-	-	-	GAF	-
[Kuro19][22]	0.36[a]	0.39[b]	0.31[c]	-	0.76[a]	0.54[b]	1.48[c]	-	DFT-LDA	-
[Lu21][58]	-	0.40[b]	-	-	1.97[a]	2.25[b]	1.52[c]	-	DFT-LDA	-

[a] $m^*_{de} = (m^*_{de\perp}{}^2\, m^*_{de\parallel})^{1/3}$
[b] $m^*_{de\perp} = \sqrt{m^*_{M\Gamma} m^*_{MK}}$
[c] $m^*_{de\parallel} = m^*_{ML}$
[d] $m^*_{dh} = (m^*_{dh\perp}{}^2\, m^*_{dh\parallel})^{1/3}$
[e] $m^*_{dh\perp} = \sqrt{m^*_{\Gamma M} m^*_{\Gamma K}}$
[f] $m^*_{dh\parallel} = m^*_{\Gamma A}$
[h] explanation see text

TABLE IV. Fitting parameters in Eq. (3) to calculations by Wellenhofer and Rössler [12].

ref.	mass	z_0	z_1	z_2	z_3	z_4	n_1	n_2	n_3	n_4	η
[Scha97][7]	m^*_{de}	0.3944	-6.822×10^{-4}	1.335×10^{-6}	3.597×10^{-10}	0	-1.776×10^{-3}	3.65×10^{-6}	0	0	1
[Scha97][7]	m^*_{dh}	1.104	1.578×10^{-2}	3.087×10^{-3}	-7.635×10^{-8}	0	1.387×10^{-2}	1.126×10^{-3}	0	0	1
[Hata13][30]	m^*_{de}	0.394	0	3.09×10^{-8}	2.23×10^{-10}	-1.65×10^{-13}	0	0	0	0	1
[Hata13][30]	m^*_{dh}	1	6.92×10^{-2}	0	0	1.88×10^{-6}	0	6.58×10^{-4}	0	4.32×10^{-7}	2/3

ODCR measurements well. In the opinion of these authors it is also important to consider spin-orbit couplings for holes. Zhao *et al.* [21] is the only publication that also provided parameters for a third conduction band, which is, however, 2 eV above the lowest one in the M-point.

According was achieved over the last decades regarding the value of M_{C}. Although in early publications rather high values of $M_{\mathrm{C}} = 12$[76,77] or $M_{\mathrm{C}} = 6$[8,78,79] were encountered, almost all more recent publications agree upon $M_{\mathrm{C}} = 3$[1,6,7,18,24,26,27,30,32,36,43,67,80–85].

We found some deviations among the utilized formalisms. Pennington and Goldsman [86] used $\sqrt{m^*_{\mathrm{M\Gamma}} m^*_{\mathrm{MK}}}$ as the DOS effective mass of electrons, i.e., $m^*_{\mathrm{de}} = m^*_{\mathrm{de}\perp}$. Tilak, Matocha, and Dunne [87] reused the value of m^*_{de} but calculated the perpendicular one themselves, which lead to almost identical values. Persson and Lindefelt [67] used for the calculation of the effective mass, i.e., $m^*_{\mathrm{de}} = (m^*_{de\perp 1}{}^2\, m^*_{\mathrm{de}\parallel})^{1/3}$ only one of the perpendicular masses, which was in the sequel reused[35]. In contrary, Gao *et al.* [88] used $m^*_{\mathrm{de}} = m^*_{\mathrm{de}\parallel}$. Ivanov, Magnusson, and Janzén [89] used $m^*_{\mathrm{de}\perp} = \sqrt{m^*_{\mathrm{ML}} m^*_{\mathrm{MK}}} = 0.32$ resp $m^*_{\mathrm{de}\parallel} = m^*_{\mathrm{ML}} + 0.58$ by citing Faulkner [90]. We were unable to retrace these equations. Transformed to the set of equations used in this paper we, thus, get $m^*_{\mathrm{de}\perp} = 0.42$ and $m^*_{\mathrm{de}\parallel} = 0.33$. A more comprehensive listing of all inconsistencies is presented in **??**.

3. *Temperature*

The temperature dependency of the DOS masses was calculated by Tanaka *et al.* [37] and Wellenhofer and Rössler [12] (see Fig. 1). Since these calculations can not be described implicitly there exist two fittings for the latter[7,30] using Eq. (3). The respective parameters are shown in Table IV.

The temperature scaling of the hole mass considering the separation between the three valence bands in the Γ point[18] (see Eq. (2), also shown in the figure) is described by the coefficients $m_{\mathrm{h1}} = 0.84$, $m_{\mathrm{h2}} = 0.79$, $m_{\mathrm{h3}} = 0.78$, $\Delta E_2 = 9\,\mathrm{meV}$ and $\Delta E_3 = 73\,\mathrm{meV}$. Bakowski, Gustafsson,

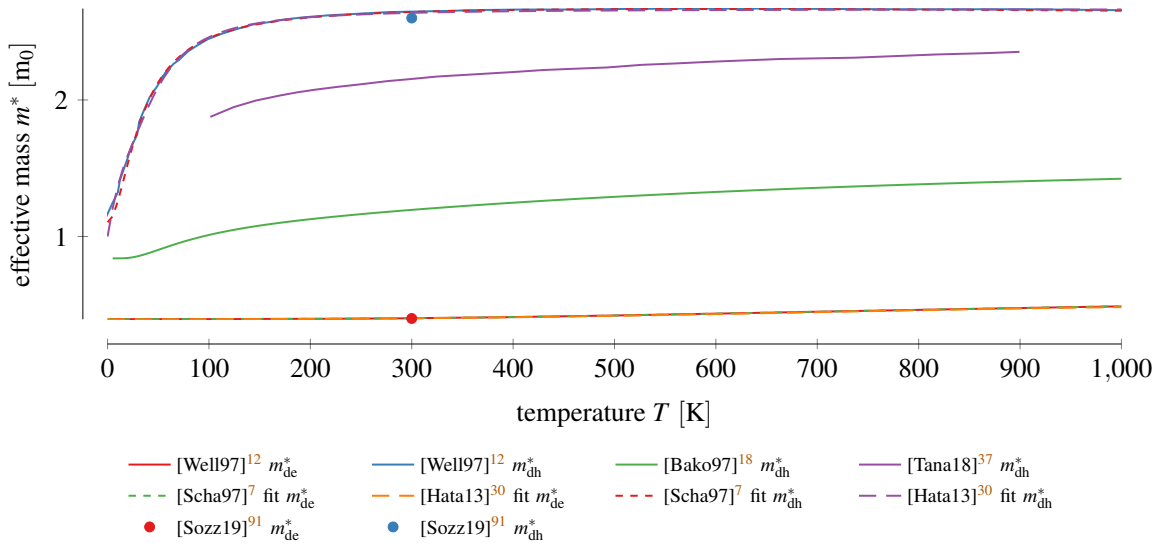

FIG. 1. Temperature dependency of the DOS mass.

and Lindefelt [18] stated that these are only valid for low temperatures, which might explain the big deviations compared to the calculations by Wellenhofer and Rössler [12]. Also shown in the figure are the parameters extracted by Sozzi *et al.* [91] from Wellenhofer and Rössler [12] at 300 K, i.e., $m^*_{de} = 0.4$ and $m^*_{dh} = 2.6$.

4. *Effective DOS Mass for TCAD Tools*

For TCAD simulations solely the effective electron and hole masses are interesting. We, therefore, collected all values found for m^*_{de} and m^*_{dh} (see Fig. 2). We also added values that we calculated from fundamental masses according to the formalism presented earlier. We just used the first conduction band for m^*_{de} and Eq. (1) to calculate m^*_{dh} considering the first two valence bands only.

For electrons the masses are dominantly using values of 0.37 ± 0.05. For holes the spread is more significant. Although the majority used 1 ± 3 there are also values > 2.6 available. This can be retraced to the significant temperature dependency. Ambivalent in this context is $m^*_{dh} = 1.2$. While Bakowski, Gustafsson, and Lindefelt [18] calculated this value for the mass at 300 K others[31,92] seemingly calculated $m^*_{dh} = \sqrt{m^*_{dh\perp} {m^*_{dh\parallel}}^2}$, i.e., twice the parallel instead of the perpendicular component, resulting in $m^*_{dh} = 1.26$[93] based on the masses by Son *et al.* [13]. Crude rounding then leads to the desired value.

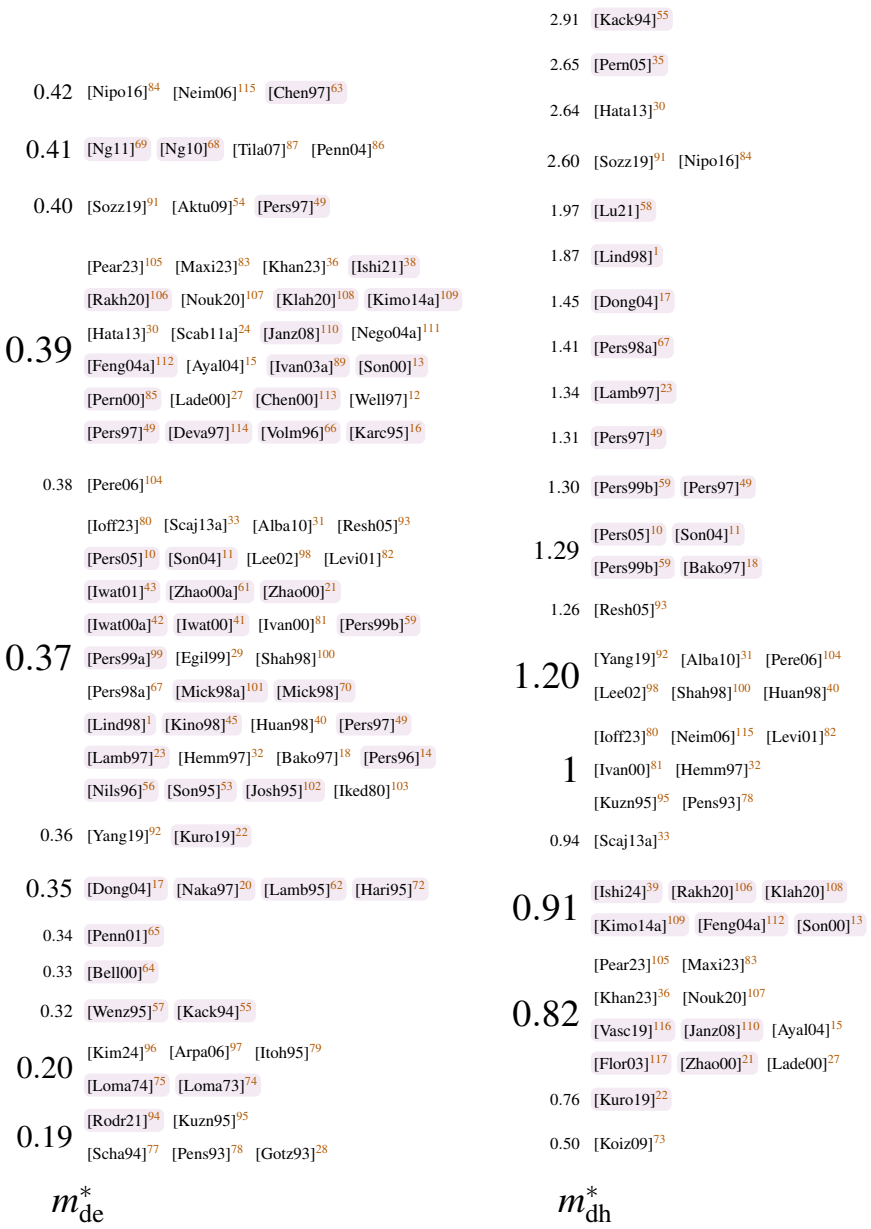

FIG. 2. Effective DOS masses for TCAD tools. A purple background denotes values that we calculated from more fundamental masses using the equations presented in this paper.

C. Discussion

The majority of the investigations on the density-of-states masses in 4H-SiC have been conducted in a time frame of one decade between 1994 and 2004. Although the earliest studies in the 70s were measurements, nowadays dominantly calculations are utilized. For the hole mass, actually, up to this day only two measurements could be identified.

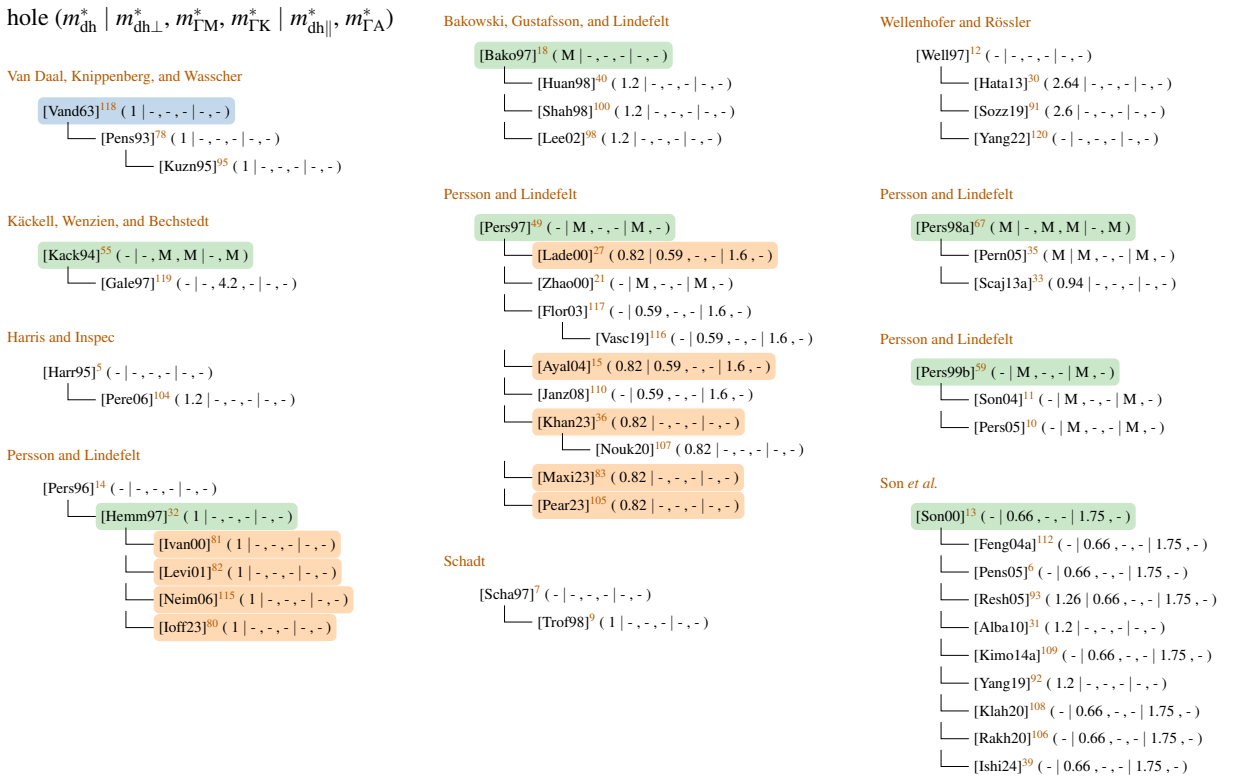

FIG. 3. DOS reference chain for holes. 'M' denotes that multiple values are found in the publication. Entries with green background show fundamental investigations, orange references we inferred based on the used data.

Our investigations showed that the value for m^*_{dh} has to be carefully picked, as a significant change with temperature was observed. Many of the available values, especially those based on calculations, are only valid close to 0 K. For more realistic results a much higher mass has to be used. Nevertheless, almost all temperature dependency fittings are based on the same calculation by Wellenhofer and Rössler [12]. Despite these large variations, temperature is rarely considered[9,26]. Rakheja *et al.* [106] explicitly claims the presented values to correspond to 300 K, although the reference investigation[13] was carried out at 4.4 K.

From the references (see Fig. 4 and Fig. 3) we are able to identify the publications by Persson *et al.*[14,49,59,67] but also by Volm *et al.* [66], [12] and[13] as very influential.

At last we shortly want to notice that there have been hints that the DOS mass is also doping dependent[2]. This was shown for 6H-SiC[99] but not yet for 4H.

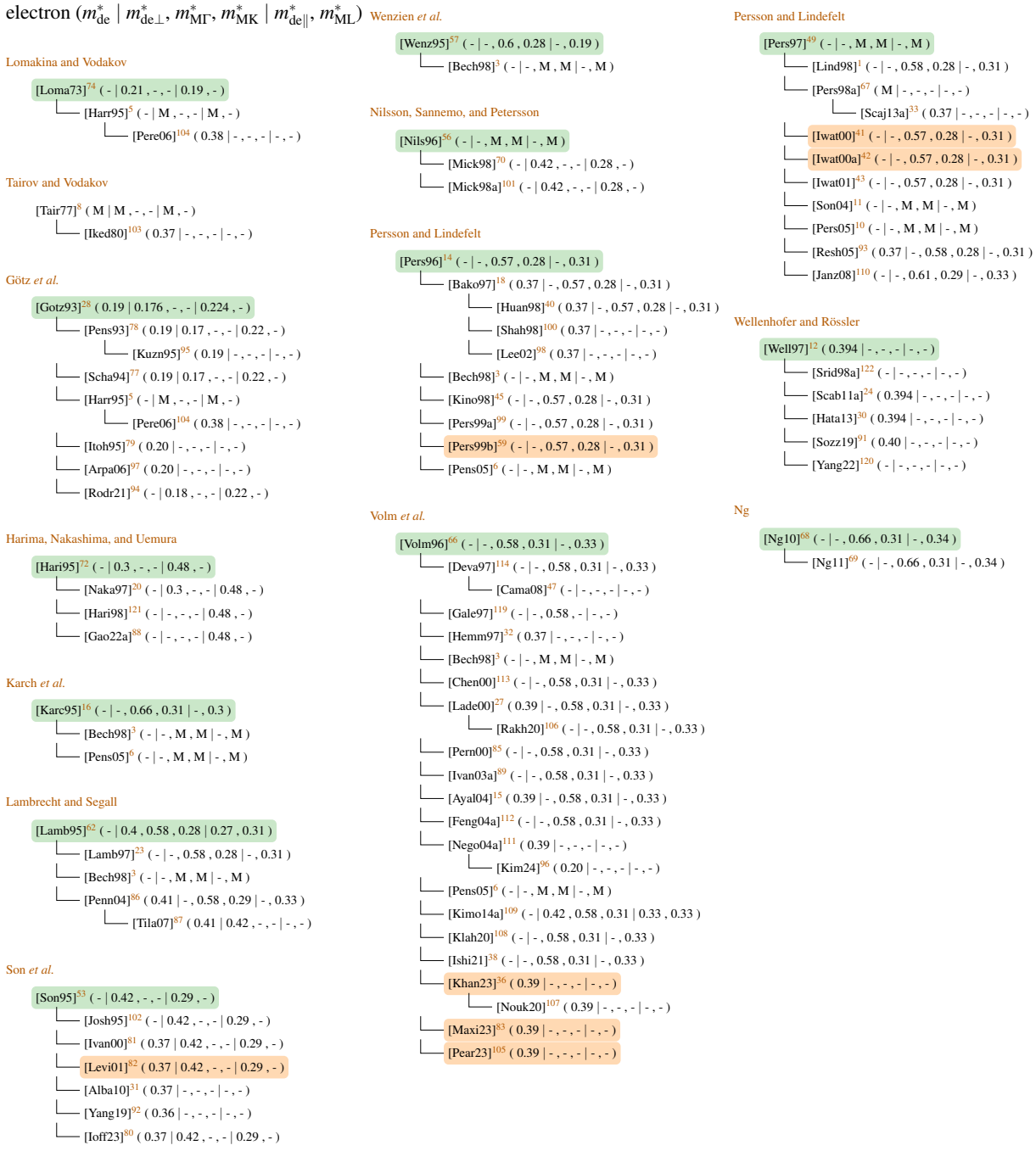

FIG. 4. DOS reference chain for electrons. 'M' denotes that multiple values are found in the publication. Entries with green background show fundamental investigations, orange references we inferred based on the used data and blue investigation based not on 4H.

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