

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 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. RELATIVE PERMITTIVITY

The permittivity ϵ describes the dielectric properties that influence electromagnetic wave propagation within a material and their reflections on interfaces¹. These effects are, for example, essential to describe the impact of an external electric field, which determines the capacitance values in a device. In general, the user has to provide the relative permittivity $\epsilon_r = \epsilon/\epsilon_0$, i.e., the ratio compared to the vacuum permittivity $\epsilon_0 = 8.854 \times 10^{-12} \text{ F m}^{-1}$, to the TCAD tools.

A. Theory

In the frequency domain, the complex relative permittivity can be written as

$$\epsilon_r^*(\omega) = \epsilon'(\omega) + i\epsilon''(\omega).$$

The real part ϵ' represents the energy stored in the material when exposed to an electric field and the imaginary part ϵ'' the losses (e.g., absorption and attenuation)¹. ϵ' and ϵ'' are tightly interconnected via the Kramers-Kronig (KK) relation²

$$\epsilon'(\omega) = 1 + \frac{2}{\pi} \int_0^\infty \frac{\omega' \epsilon''(\omega')}{\omega'^2 - \omega^2} d\omega' \quad (1a)$$

$$\epsilon''(\omega) = -\frac{2\omega}{\pi} \int_0^\infty \frac{\epsilon'(\omega')}{\omega'^2 - \omega^2} d\omega' \quad (1b)$$

In TCAD simulations of semiconductor devices ϵ'' is of diminishing importance, but ϵ' is required to calculate capacitances or the electric field distribution. Consequently, we will focus on ϵ' in the sequel.

In the literature the static (ϵ_s) and high-frequency resp. optical (ϵ_∞) relative permittivity are distinguished. The former is $\epsilon'(\omega \rightarrow 0)$ but a definition of the latter is more complicated. It denotes ϵ' at the end of the reststrahlen range towards higher frequencies, where the real part of the refractive index is null³. In publications that focus on optical high-frequency analysis ϵ_∞ is sometimes denoted as $\epsilon'(0)$ ⁴, which must not be confused with ϵ_s . These inconsistencies were explained in the following fashion⁵: “We shall use ϵ_∞ to denote the extrapolation . . . to zero frequency. This somewhat contradictory notation arose because ϵ_∞ the "optical" dielectric constant, was often set . . . at a frequency much higher than the lattice frequency, but low compared with electronic transition frequencies. In many substances no suitable frequency exists, and it is preferable to extrapolate optical data to zero frequency . . .”

To clarify: ϵ_∞ is measured at frequencies well above the long-wavelength longitudinal optical (LO) phonon frequency ω_{LO} ². ω_{LO} translates ϵ_s into ϵ_∞ and vice versa in conjunction with the transversal optical (TO) phonon frequency ω_{TO} and the Lyddane-Sachs-Teller (LST) relationship⁶

$$\frac{\epsilon_s}{\epsilon_\infty} = \left(\frac{\omega_{LO}}{\omega_{TO}} \right)^2. \quad (2)$$

For ω_{LO} we encountered the energy values 120 meV (approximately 29 THz)⁷⁻¹¹, 104 to 121 meV¹² and 104.2 meV¹³ in our search. Instead of the energy often the respective wave numbers are presented, i.e., (in cm^{-1}) $\omega_{TO} = 793$ and $\omega_{LO} = 974$ ¹⁴, $\omega_{LO}^\parallel = 964.2$, $\omega_{LO}^\perp = 966.4$, $\omega_{TO}^\parallel = 783$ and $\omega_{TO}^\perp = 798$ ¹⁵, $\omega_{TO} = 783$ and $\omega_{LO} = 964$ ¹⁶ and $\omega_{LO} \in [967, 971]$ ¹⁷.

B. Results

Various approaches have been used to determine the relative permittivity: One possibility are calculations using the density functional theory (DFT) based local density approximation (LDA)^{4,7,18-23} or the effective mass theory²⁴. With these the band structure and, thus, ϵ'' is calculated and then transformed into ϵ' using the Kramers-Kronig relations (Eq. (1)). Measurements use either some form of resonator (RES)²⁵⁻²⁷, spectroscopy (SPEC)²⁸⁻³⁰, spectroscopic ellipsometry (SE)^{31,32} or the refractive index (RI)^{5,15,33}. In some cases the transversal and longitudinal optical phonon frequencies is determined and used in the LST relationship (Eq. (2))^{31,32}. Furthermore, the tight relationship between relative permittivity and complex refractive index, i.e., $n^*(E) = \sqrt{\epsilon(E)}$ ², with $E = \hbar\omega$, is utilized if ϵ'' is negligible. For fitting purposes the representation

$$n^2 = 1 + \frac{\epsilon_g}{1 - (hf/E_g)^2} \approx \epsilon_\infty + \epsilon_g \left(\frac{hf}{E_g} \right),$$

with hf the photon energy, E_g an "average band gap" and ϵ_g proportional to the oscillator strength⁵, is used to extract ϵ_∞ ^{5,15,29,33}. Finally, fitting to $\ln(J/E)$ ³⁴, with J the current density, is also deployed.

The relative permittivity was furthermore investigated at mm-wave frequencies (MM) (10 GHz to 10 THz)^{26,35-38} (nicely summarized by Li *et al.*²⁷, Yanagimoto *et al.*³⁹). Unfortunately, there are often fluctuations in the data or just single data points available, which makes an interpolation to zero frequency ($= \epsilon_s$) not possible. For these reasons we had to discard most of the respective data. We also excluded publications whose values got refined in succeeding experiments^{40,41}, that

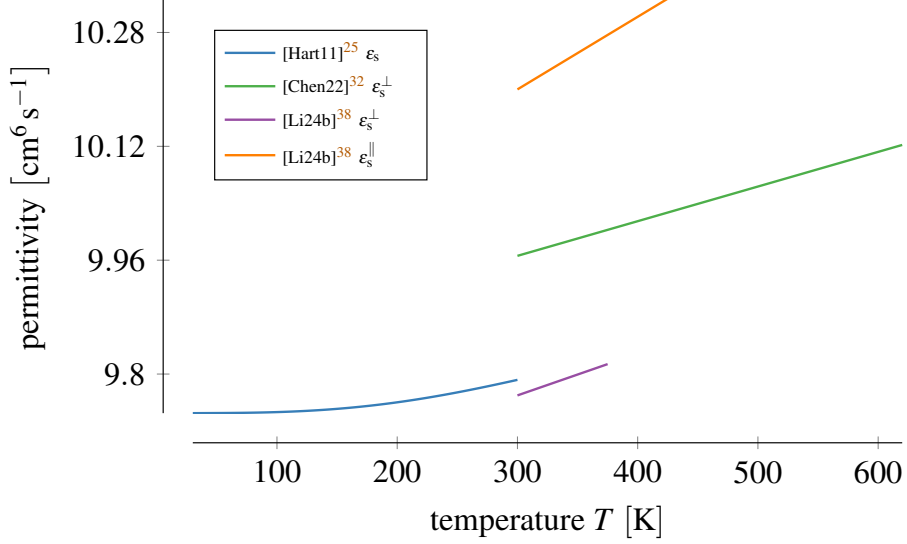


FIG. 1. Temperature dependency of the permittivity.

did not specify the investigated polytype^{42–45} or where an extraction of the data values was not possible⁴⁶.

With the listed characterization approaches values in the range of [9.6, 10.65] for the static relative permittivity and [6.25, 7.61] for the high-frequency one have been achieved (Table I). In the table we also show two references that exclusively provide 6H values because these are often referenced for 4H investigations. Wherever necessary we calculated the relative permittivity according to $\epsilon_s = (\epsilon_s^{\parallel} \epsilon_s^{\perp 2})^{\frac{1}{3}}$ resp. $\epsilon_{\infty} = (\epsilon_{\infty}^{\parallel} \epsilon_{\infty}^{\perp 2})^{\frac{1}{3}}$ ^{47–51}, which far more often used than $\epsilon_s = (\epsilon_s^{\parallel} \epsilon_s^{\perp})^{\frac{1}{2}}$ proposed by Ivanov *et al.*²⁴.

In TCAD tools the permittivity is a constant although research showed that there is a frequency²⁵ and temperature^{25,32} dependency. For a frequency around 40 GHz Hartnett *et al.*²⁵ provided the approximation

$$\epsilon_s(T) = 9.7445 + 3.1862 \times 10^{-5} T - 6.3026 \times 10^{-7} T^2 + 5.9848 \times 10^{-9} T^3 - 8.2821 \times 10^{-12} T^4 ,$$

with the temperature T in K. Cheng, Yang, and Zheng³² approximated $\epsilon_s^{\perp} = 9.82 + 4.87 \times 10^{-4} T$ and Li *et al.*³⁸ $\epsilon_s^{\perp} = 9.77 * (1 + 6 \times 10^{-5} (T - 300 \text{ K}))$ and $\epsilon_s^{\parallel} = 10.2 * (1 + 1 \times 10^{-4} (T - 300 \text{ K}))$. All approximations show an increase of the permittivity with temperature (Fig. 1).

TABLE I. Published relative permittivity values.

ref.	ϵ_s	ϵ_s^{\parallel}	ϵ_s^{\perp}	ϵ_{∞}	$\epsilon_{\infty}^{\parallel}$	$\epsilon_{\infty}^{\perp}$	method ^a	SiC	doping
[Patr70] ⁵	9.78 ^c	10.03	9.66	6.58 ^c	6.7	6.52	RI	6H	-
[Ikeda80] ³³	9.94 ^c	10.32	9.76	-	-	-	RI	4H	-
[Nino94] ³¹	9.83 ^c	9.98	9.76	6.62 ^c	6.67	6.59	SE	6H	-
[Hari95] ¹⁵	-	-	-	6.63 ^c	6.78	6.56	RI	4H	-
[Karc96] ¹⁸	10.53 ^c	10.9	10.352	7.02 ^c	7.169	6.946	DFT-LDA	4H	-
[Well96] ¹⁹	-	-	-	7.02 ^c	7.17	6.95	DFT-LDA	4H	-
[Adol97] ²⁰	-	-	-	7.56 ^c	7.61	7.54	DFT-LDA	4H	-
[Ahu02] ⁷	-	-	-	7.11 ^c	7.47	6.94	DFT-LDA	4H	n-type
[Peng04] ²¹	-	-	-	6.31 ^c	6.44	6.25	DFT	4H	-
[Pers05] ⁵²	9.73 ^c	9.94	9.63	6.47 ^c	6.62	6.4	DFT-LDA	4H	intrinsic
[Chin06] ⁴	-	-	-	6.81	-	-	DFT-LDA	4H	intrinsic
[Dutt06] ³⁵	9.97 ± 0.02 ^b	-	-	-	-	-	MM	4H	high purity
[Ivan06] ²⁴	9.93 ± 0.01	-	-	-	-	-	EMT	4H	intrinsic
[Hart11] ²⁵	9.77 ^d	-	-	-	-	-	RES	4H	high purity
[Jone11] ²⁶	9.6	-	-	-	-	-	RES	4H	high purity
[Naft16] ²⁸	10.11 ^c	10.53 ^f	9.91 ^f	-	-	-	SPEC	4H	undoped
[Cout17] ²³	10.13 ^c	10.65	9.88	-	-	-	DFT-LDA	4H	-
[Tare19] ²⁹	-	-	-	6.587 ± 0.003	-	-	SPEC	4H	-
[Chen22] ³²	9.97 ^g	-	-	-	-	-	SE	4H	-
[Gao22a] ³⁰	-	-	-	6.51	-	-	SPEC	4H	-
[Yang22a] ³⁴	10.21	-	-	-	-	-	ln(J/E)	4H	p-type
[Li23] ²⁷	-	10.27 ± 0.03	-	-	-	-	RES	4H	high purity
[Li24b] ³⁸	9.91 ^c	10.20 ± 0.05	9.77 ± 0.01	-	-	-	RES	4H	high purity

^a description of the single methods in the text

^b frequency range 131–145 GHz, for lower resp. higher frequencies $\epsilon_s = 9.74$ was achieved

^c $\epsilon_s = (\epsilon_s^{\perp 2} \epsilon_s^{\parallel})^{1/3}$

^d temperature and frequency dependent

^e calculated from refractive index n as $\epsilon_s = n^2$

^f wavelength-dependent refractive index presented

^g temperature dependent

C. Discussion

We identified two very influential publications, largely dominating the permittivity values found in literature. Ikeda, Matsunami, and Tanaka³³ published, based on measurements from Shaffer⁵³, in 1980 the first 4H-SiC permittivity data. Although these values are broadly used in liter-

ature^{22,54–58}, we never found a citation of that particular paper. Not even cross-references among the citing publications exist.

In 1970, so ten years prior to the first 4H values, Patrick and Choyke⁵ determined, based on measurements published in 1944⁵⁹, the permittivity of the 6H polytype. Many publications on 4H-SiC used these results (see Fig. 2) despite the deviating polytype. Some authors claimed that dedicated 4H values were not available^{12,48,60–63}, a mistake as we showed before. Nevertheless, it is still claimed up to this day³². This shows, how hard it is to get a comprehensive overview over 4H-SiC TCAD parameters. In contrast to early analysis, that clearly highlight that 6H values were used⁶⁴, the majority of publications simply adopts the parameters without further remark, which leaves the false impression that proper 4H values were used.

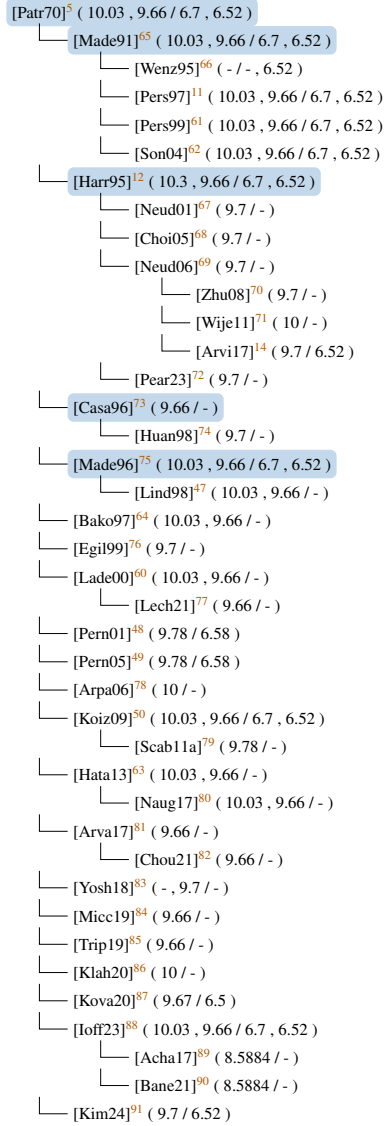
Rounding of the original values, e.g., $9.66 \rightarrow 9.7 \rightarrow 10$ ^{67,78} (see Fig. 2), and mere typographical errors, e.g., turning 9.66 into 9.67⁸⁷ (a comprehensive analysis of all encountered inconsistencies is shown in ??), expanded the range of available values (see Figs. 3 and 4). In these figures we connected those values where at least one direct connection could be found. Due to missing references we can, however, not guarantee that all authors made their selection based on the same data. In many cases, e.g., for the prominent values $\epsilon_s = 9.7$ or $\epsilon_s = 10$, it is not unreasonable to assume that simply the permittivity in one principal direction was picked.

An interesting case is $\epsilon_s = 8.5584$ ^{89,90}, which is supposed to be based on $\epsilon_s^\perp = 9.66$ and $\epsilon_s^\parallel = 10.03$ ⁸⁸. We were not able to achieve this value analytically since the result is lower than both constituents. Only when we added the high-frequency relative permittivity to the calculations we achieved a somewhat close value of 8. Such a combination is, however, not justifiable.

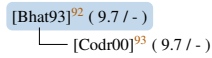
Overall, the missing awareness regarding 4H related permittivity values is striking. One explanation why the same old values are reused over and over again are the often very long citation (see Fig. 2). Combined with often missing references this makes it difficult to pinpoint the origin of a value and thus assess its suitability. Another interpretation of the achieved results is that the permittivity has little impact in TCAD simulations, such that somewhat accurate 6H values are already sufficient. Nevertheless, even if this was the case, we highly encourage the scientific community to adopt the most recent measurement 4H-SiC in future publications to make these values more prominently known and, thus, lead to a wider distribution.

Permittivity (ϵ_s^\parallel , ϵ_s^\perp / $\epsilon_\infty^\parallel$, ϵ_∞^\perp)

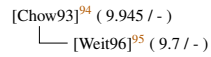
Patrick and Choyke



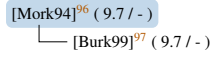
Bhatnagar and Baliga



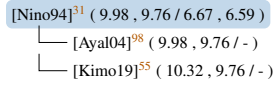
Chow and Tyagi



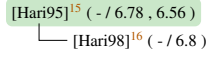
Morkoç *et al.*



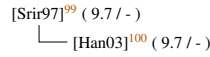
Ninomiya and Adachi



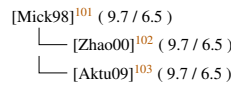
Harima, Nakashima, and Uemura



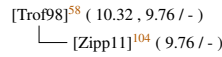
Sriram *et al.*



Mickevicius and Zhao



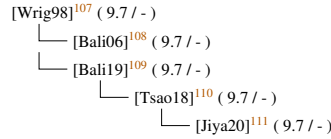
Troffer



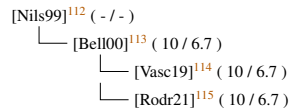
Weitzel



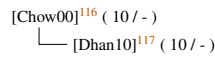
Wright *et al.*



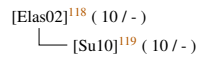
Nilsson *et al.*



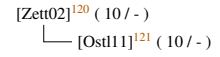
Chow



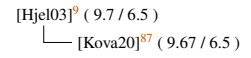
Elasser and Chow



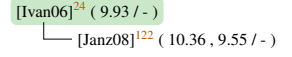
Zetterling



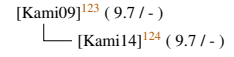
Hjelm *et al.*



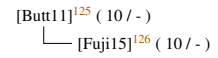
Ivanov *et al.*



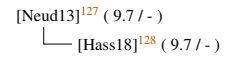
Kaminski



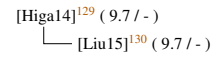
Buttay *et al.*



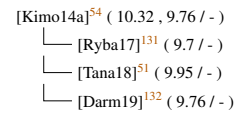
Neudeck



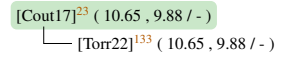
Higashiwaki *et al.*



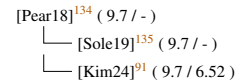
Kimoto and Cooper



Coutinho *et al.*



Pearton *et al.*



Li *et al.*

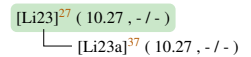


FIG. 2. Reference chains found for the relative permittivity. Publications with blue background are not focused on 4H-SiC, while those in green are novel analyses on 4H-SiC.

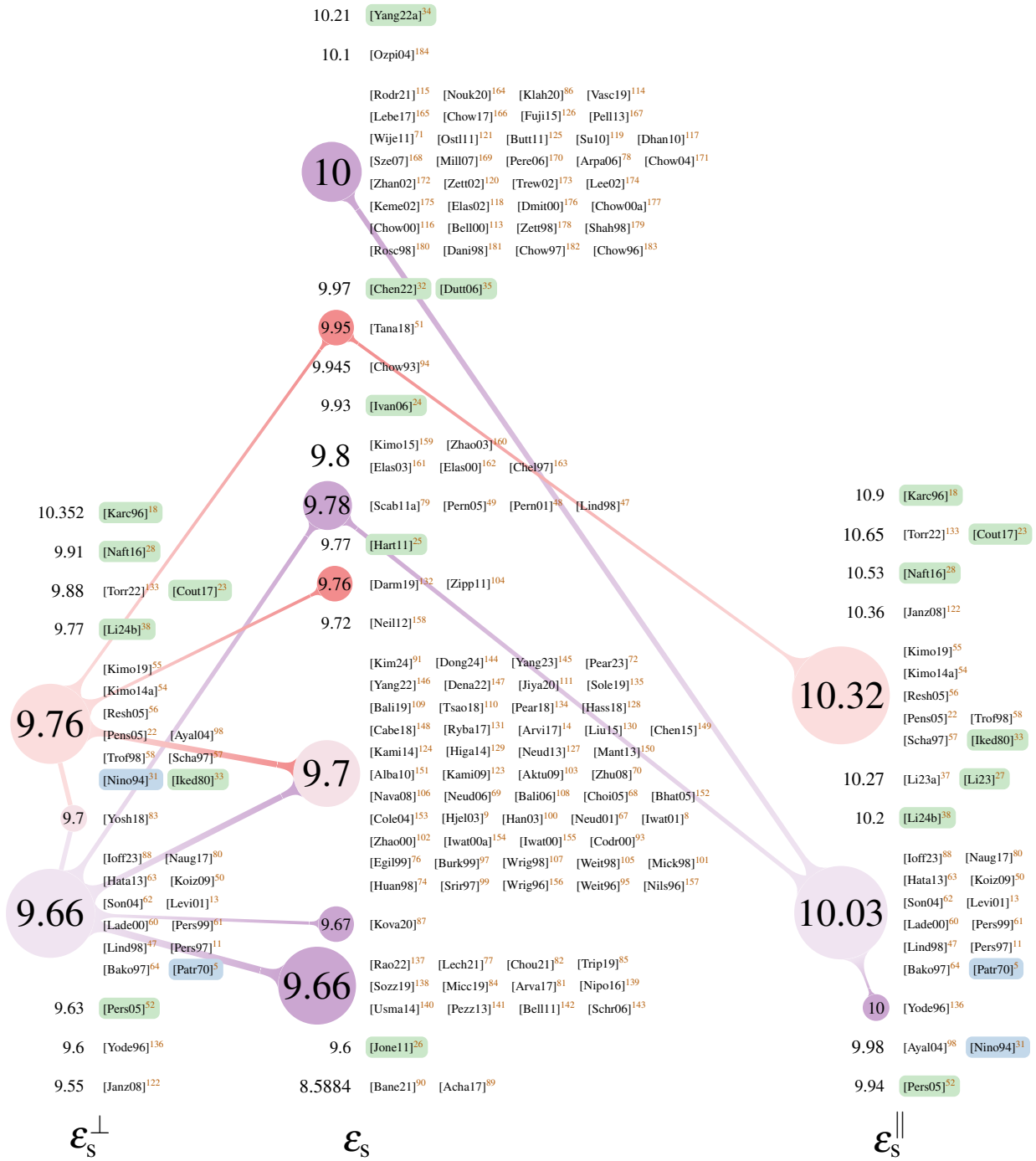


FIG. 3. Published values for the static permittivity. Connected values indicated that at least one connection has been found. References with blue background indicate investigations of non-4H silicon carbide while green background denotes basic 4H-SiC investigations.

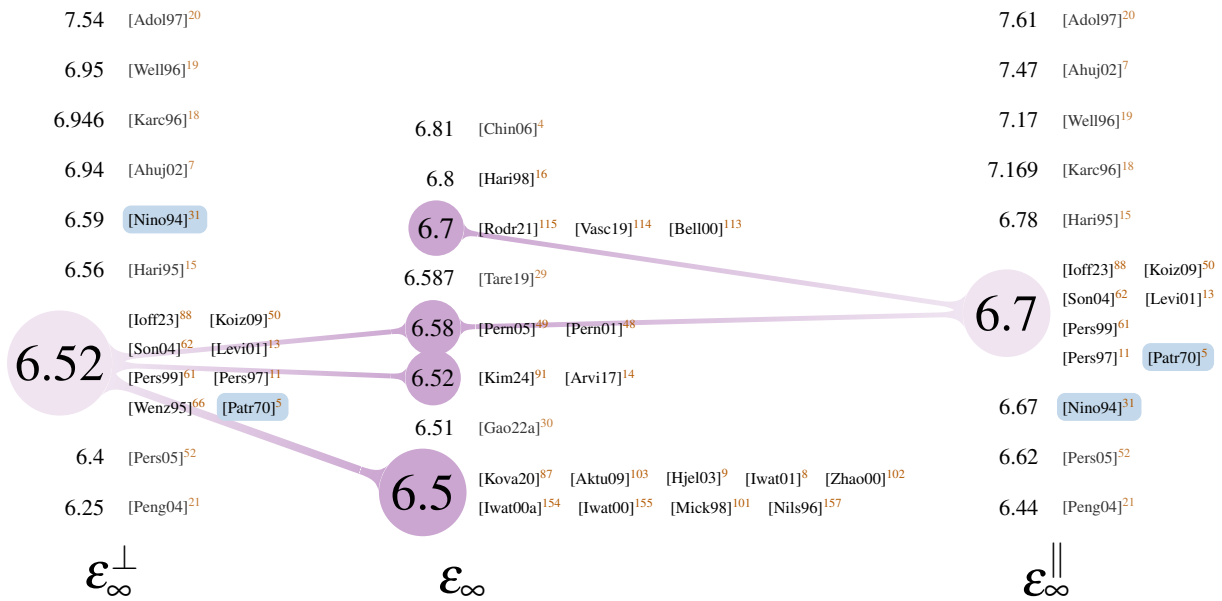


FIG. 4. Published values for the high-frequency permittivity. Connected values indicated that that at least one connection has been found. References with green background indicate investigations of non-4H silicon carbide while blue background denotes basic 4H-SiC investigations.

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