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THz Measurements, Antennas, and Simulations: From the Past to the Future

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ABSTRACT In recent years, terahertz (THz) systems have become an increasingly popular area of research thanks to their unique properties such as extremely high data rates towards Tb/s, submillimeter localization accuracy, high resolution remote sensing of materials, and remarkable advances in photonics and electronics technologies. This article traces the progress of THz measurements, antennas and simulations, from historical milestones to the current state of research and provides an outlook on the remaining challenges.

INDEX TERMS Channel modeling, history, MTT 70th Anniversary Special Issue, on-chip antennas, ray-tracing, THz communications, THz measurements and simulations.

I. INTRODUCTION

No doubt, radio waves have been propagating since the beginning of the universe. However, twentieth century marks the era of radio communications initiated by the prediction of electromagnetic (EM) waves from J.C. Maxwell in 1865 based on his EM theory of light owing to the similarity between the two taking into account M. Faraday's existing experimental works (1831) on EM induction. Later, in the 1880 s, H. Hertz confirmed Maxwell's theoretical work with multiple laboratory experiments (original apparatus of Hertz can be seen at the Deutsches Museum in Munich) generating, radiating, and receiving EM waves of 66 cm wavelength in free space.

G. Marconi, inspired by Hertz brought the EM waves (long waves) from the confines of laboratory to the outer world with his epoch-making experiment of transmitting radio signals successfully across the Atlantic ocean in 1901 [1], laying the foundation for long-distance radio communications. Moving

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closer to the low THz band (i.e., between 0.1−1 THz), in 1895, J.C. Bose conducted pioneering millimeter-wave (mm-wave) experiments at 60 GHz [2] with radio waves ($\lambda \cong$ 5 mm) to ring bells and trigger explosions.

Almost 100 years later from the pioneering work by W. Herschel (1800) in both the visible and near-infrared portions of the EM spectrum, H. Rubens and his colleagues in Berlin advanced their infrared experiments towards the currently termed far-infrared (FIR) or THz region [3]. In 1897, Rubens with E.F. Nichols explicitly acknowledged the existence of a technology gap spanning between the optical and electronic sources of radiation. Later, in 1923, Nichols and J.D. Tear employed the interferometric method for obtaining wavelengths as low as 1.8 mm and finally succeeded in closing the THz gap, defined as the region between 0.1−10 THz, thus joining it to the already explored near-infrared. Along with the advances in the development of THz devices in the last decades, the application of THz waves for modern communication systems became possible. This brief history might perhaps miss some important incidents. Looking ahead at the next decade, the power, peril, and promise of THz technologies will witness even more progressive explorations overcoming the current challenges.

II. THZ CHANNEL MEASUREMENTS

Johannes M. Eckhardt, Tobias Doeker, Thomas Kürner, Naveed A. Abbasi, Jorge Gomez-Ponce and Andreas F. Molisch

First ideas on concepts of THz communications came up almost two decades ago [4], [5], [6]. This has triggered numerous activities on channel measurements and simulations - a necessary initial step when developing a wireless communication system in a new frequency range − at 100 GHz and beyond. Tutorial overviews on these activities are provided for example in [7], [8], [9]. Measurement equipment working at THz frequencies in the early stage was limited mainly to THz Time Domain Spectroscopy (THz-TDS). In this context, THz-TDS has been used to characterize the reflection and scattering properties of materials [10], [11]. These measurements have shown that at wave lengths below 1 mm, surface roughness of typical building materials like concrete and the thickness of paint on a concrete wall - causing a layered structure - significantly influence the scattering behaviour. This is quite different from the observations at lower frequencies, where walls are usually considered as flat surfaces. Based on these findings, ray-tracing has been applied to explore the potential of THz communication systems by simulations [12]. More details on THz simulations are provided in Section IV. Other early works have used first simple THz communication systems that have been built up by discrete components, allowing a rough estimation on potential inter-symbol interference (ISI) in kiosk downloading applications [13]. In outdoor environments, the impact of atmospheric gases in long-path outdoor environments [14] has also been measured by THz-TDS. A comparison of the measured attenuation and achievable bit error rate (BER) in THz and infra-red systems in dust-clouds and fog has been performed by Su et al. [15], [16] revealing advantages of THz communications in case of low visibility conditions.

With the availability of frequency extenders of vector network analyzer (VNA) at the 100–500 GHz range (and more recently up to 1100 GHz) [17], [18], frequency domain channel sounding has been applied to investigate a multitude of more complex scenarios. In [19] the impact of blocking and diffraction has been described including a comparison of these effects at 60 GHz and 300 GHz. Complete indoor scenarios cover office environments [20], data centers [21], intra-device communications [22], [23], and kiosk downloading [24]. The high path loss and limited dynamic range of the measurement equipment requires the use of high-gain antennas for most of the applications. Rotational units as described in [20] enable automatic spatial scanning at the transmitter (TX) and receiver (RX), thus allowing to derive spatial channel characteristics.

VNA based channel sounding has a major limitation: It can be applied to static scenarios only. Alternative approaches are correlation-based channel sounding (CBCS) working in time domain. In the past years, various CBCS systems have become available [25], [26], [27], [28] allowing either dynamic measurements or reducing the measurement time in static environments significantly. CBCS have been widely used for measurements in various environments such as outdoor environments [27], office environments [26], industrial environments [29], data centers [30], trains [31], automotive [32], and aircrafts [33]. Recently, CBCS have also been used for channel characterisation with regard to the determination of key performance indicator (KPI) for physical layer security such as secrecy capacity [34], [35].

Nowadays, 300 GHz measurement systems are available and allow measurements of more system related KPIs such as bit error rates (BERs). In [36] the impact of diffuse scattering on the BER has been measured. A complementary approach to derive system related KPIs are simulations as described e.g. in [37]. The simulations can be based on either deterministic channel models calibrated from measurements [20] or on stochastic channel models, e.g. [38]. For example, the modeling framework described in [38] has been applied in developing IEEE Std 802.15.3d-2017 [39].

In the following, we will extract key findings on propagation at THz communication systems. Starting with some common insights based on measurement campaigns and simulation from the literature, we will provide more details for scenarios in outdoor environments and data center applications.

A. COMMON INSIGHTS

Measurements reported both in indoor [36], [23], [33], [29], and outdoor [40], [41] environments have shown that THz communications works also in non-line-of-sight (NLoS) situations by exploiting single or even multiple reflection or scattering processes, yielding a reduction of the received power level of compared to line-of-sight (LoS) as low as a few dB. Generally speaking, the pathloss coefficients for NLoS are in a similar range as those at cm-wave frequencies; however, shadowing is more severe, raising the probability of outage.

In highly reflective environments [23], [24], [33], the delay spread can be considerable - the order of multiple inverse bandwidths - despite the use of directional antennas. Again, this holds true for both indoor and outdoor environments. The measured multipath richness may cause inter-user interference [42], [48]. The use of directional antennas can reduce the multipath richness (though significant multipath might occur even when using directional antennas at both link ends, particularly in outdoor environments). Furthermore, in the presence of non-negligible antenna side lobes, which are hard to avoid for electronically steerable antennas THz [25], [43], multipath richness is further enhanced; in the extreme case of omni-directional antennas, hundreds of multipath component (MPC) have been observed.

THz channels also suffer from significant directional dispersion, which impacts inter-user interference in multi-user environments, due to two effects: i) the strongest paths of an interferer may arrive at the victim RX at such an angle that they fall within the side lobes of the antenna pattern, or ii) the directional dispersion makes (possibly weaker) MPC arrive within the main lobe of the victim RX. Due to the near-far effect, even attenuated interfering MPC can significantly impact the signal-to-interference ratio at a RX; thus channel models need to have high dynamic range. Due to the importance of directional dispersion, channel measurements should generally be double-directional [44], i.e., describe the channel characteristics for each transmit- and receive direction combination.

B. OUTDOOR ENVIRONMENTS

For outdoor environments, the main scenarios envisioned for THz applications are (i) microcells, (ii) hotspots, and (iii) device-to-device (D2D) communications, which have in common that typically links cover distances $<$100 m, are in urban environments, and have high anticipated user density; the main difference lies in the height of the "base station": 10 m in the case of microcells, 3 m to 5 m in the case of hotspots, and 1.5 m in the case of D2D communications.

In addition to these three scenarios, wireless backhaul is also a promising application, but has a significantly different setup (static TX and RX, and mostly static environment, possibly longer distances), and do not require double-directional measurements and thus requires different types of channel measurements.

The first double-directional outdoor measurements were performed in [45]. Though using a VNA, measurements over long distances were made possible by hauling the signal from the receive antenna (and its co-located frequency extender) to the VNA via an RF-over-fiber connection. Measurements used a frequency step of 1 MHz, a bandwidth of 1 GHz, and horn antennas with a beamwidth of 13°. Directional resolution at both TX and RX was achieved by mechanical rotation of the antennas via precision rotors.

FIGURE 1. Map of the outdoor plaza for microcellular environment measurements in [41].

The same setup was subsequently used for extensive (50,000 - 100,000 impulse responses) measurement campaigns in the D2D [40] and the microcellular scenarios [41], see Fig. 1. For both scenarios, the campaigns were performed in an urban environment, with mixtures of street canyons and open squares (plazas/quads or parking lots). In the D2D measurements only the horizontal plane was scanned, while in the microcellular measurements, azimuthal scans were performed for multiple elevation cuts. The same setup was also used for indoor measurements, see [46].

From the measurements, both the directional and the non-directional (omni) pathloss were evaluated. In LoS situations, the pathloss as well as the pathloss coefficient is somewhat smaller than in free space, in line with expectations, and behavior at lower frequencies. In NLoS situations, pathloss is typically higher by about 10 dB to 30 dB compared to free space, though care must be taken in the interpretation of those results: as pointed out in those papers, there is an inherent selection bias caused by the measurement locations chosen such that reasonable receive power could be anticipated; in practice there might be more locations in which complete outage occurs.

Delay dispersion is significant in outdoor scenarios, both for D2D and microcellular environments; a sample can be seen in the lower plot of Fig. 2. In LoS situations, on the order of 3(30) ns is observed for the directional (omni-directional) rms delay spread, while for NLoS, the corresponding values are 2(10) ns and 30(100) ns for microcellular and D2D situations, respectively. When analyzing the number of freely adjustable equalizer taps/Rake fingers to collect 99 % of the energy, values range from 5 to 20 for the chosen directional antennas (13° beamwidth) and bandwidth (1 GHz) [47].

Another important effect observed in these measurements is a strong directional dispersion, which impacts inter-user interference as described in Section II-II-A, with the detailed impact depending on the beamforming algorithm [48]. Energy is coming from multiple clusters that have different directions, see right plot of Fig. 2, with the clusters having different arrival times. Detailed descriptions, sample results, and statistical results for pathloss, delay- and angular dispersion can be found in [40], [41], [47].

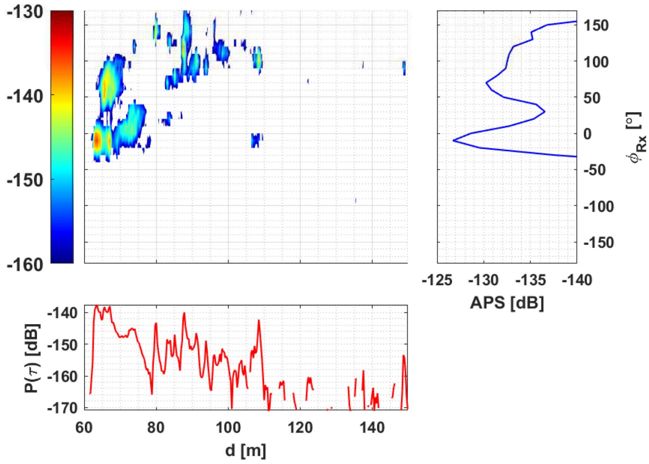


FIGURE 2. Angular delay power spectrum (APDS) of outdoor NLoS link, TX3-RX14 for $d_{TX-RX} = 62.6\,\text{m}$.

Several other measurement campaigns have been performed in recent years, including extensive measurements in an access point (AP) scenario (base station height 4 m) at 140 GHz [49], [50], and a street canyon at 300 GHz [51]. The qualitative insights from those campaigns are similar to the ones mentioned above.

For outdoor environments, blockage by both large and small objects needs to be considered. Large objects might include trucks, cars, and even people. Since most of these objects are essentially impermeable to THz radiation, diffraction around them is the main mechanism. Furthermore, due to the small wavelength, objects such as leaves, lantern masts, etc., which are not significant blockers at cm-wave frequencies, become relevant at THz. Their impact can be analyzed by ray-tracing, or a stochastic-geometry analysis [52], with the two methods showing good agreement.

C. INDOOR ENVIRONMENTS

THz applications can be further imagined in many indoor environments entailing revolutionary benefits. High-speed wireless AP in office premises or wireless D2D communications will influence the modern working world. Directional THz links will bring the mobile machine type communications in industrial environments to the next level and additional wireless THz links in data centers enhancing the flexibility and reconfigurability with comparable data rates to those of fibre connections. Similarly, THz entertainment systems in an aircraft cabin or a high speed train entertain a large number of people thus, upgrading the passenger experience and comfort. The requirements for the mentioned indoor use cases differ from long-distance outdoor applications. Within the paper, our methodology, tool chain, and work flow for the channel characterization of THz communications in indoor scenarios is presented and exemplarily discussed for the data center use case.

Compared to outdoor environments, the dimensions of the indoor measurement setups are smaller, thus reducing the synchronization and measurement distance between the TX and the RX making systems with ultra-high measurement rate possible. One possible realization of a CBCS system records the channel impulse response (CIR) with a measurement rate of 17,590 CIR/s in a 4×4 multiple-input multiple-output (MIMO) configuration. An ultra-wide band (UWB) module creates an M-sequence allowing a max. access delay of approximately 445 ns with a bandwidth of 8 GHz and serves as an excitation signal. Within the TX frequency extender, the baseband signal is upconverted to a center frequency of 304.2 GHz. All TX and RX are synchronized by a base unit. The same approach is followed for the downconversion in the RX frequency extender before the signal is sampled by analog-to-digital converter (ADC) [25].

The CBCS system measures a spatially limited CIR due to its dependency on highly directive antennas that compensate for the high free space path loss (FSPL) at THz frequencies. Using rotational units with an automatic mechanical steering, a power angular profile (PAP) can be created [53] that enables the processing of an omni-directional CIR [54]. Fig. 3 shows a classical measurement setup in a data center in this case. The equipment is complemented by tripods and a rail system [35].

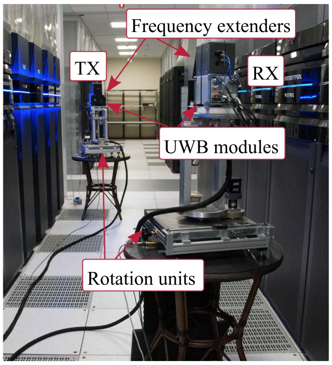
Aligning the measurement setup with the application-oriented use case, the measurement results are valuable in three different ways: First, various channel parameters are calculated and the propagation is characterized [33]. Second, the measurement data is used for calibration or validation of propagation simulations [31]. Third, the measurement data is directly applied for higher layer simulations of the specific use case.

In this context, measurement campaigns in various indoor environments have revealed the need for scenario-specific channel models at THz frequencies. Referring to the propagation characterization, the data center measurements verify the adequate modeling of FSPL and the importance of reflection and transmission effects that rely on the material properties [30]. Moreover, omni-directional and point-to-point measurements discover significant multipath propagation in all inter-rack measurement setups [8].

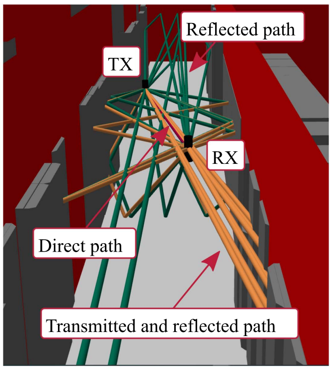
III. THZ ON-CHIP ANTENNAS

Benedikt Sievert, Jan Taro Svejda, Andreas Rennings and Daniel Erni

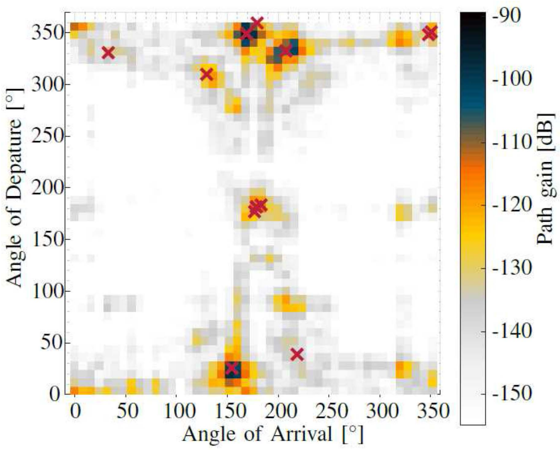
From a historical perspective, antennas and, even more remarkable, J.C. Bose's pioneering sub-THz emitters in 1895 based on a 60 GHz dielectric-lens antenna setup [55] are among the first devices ever developed in the dawn of RF engineering. Since then, antennas have played an essential role in advancing modern RF technology (and in particular the wireless revolution), adapting to increasing demands such as, e.g., smart and controllable functionalities, ultra-widedband and multi-band operation, high integration density, shape conformity, including the current access to the THz range [56], [57]. As early as the late 1960 s full-wave computational EM (CEM) simulations, numerical network analysis, and topological optimization [58] had already become the cornerstones



(a) Measurement setup.



(b) Ray-tracing simulation.



(c) PAP of the measurement setup and ray-traced MPCs.

FIGURE 3. Investigations in a data center.

of standard RF design techniques. (Sub-) THz chip antennas can be considered as operating at their physical limit, facing fundamental limitations in gain and radiation efficiency due to the high permittivity of the semiconductor substrates involved. It is therefore not surprising that holistic design concepts [59], such as e.g. those incorporating energy flux from the locally resolved radiation mechanisms in the antenna topology, are receiving increasing attention in current chip antenna research. Efficient (sub-) THz chip antenna optimization in particular invokes thus the full interplay between CEM simulations,

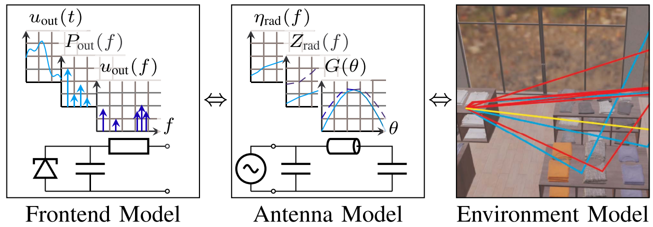


FIGURE 4. The interplay between the modeling of frontend, antenna, and environment is key for state of the art THz systems.

topological optimization and (astonishingly) an equivalent circuit analysis, which will be described in the following. To generate insight into antenna operation beyond the outcome of general purpose CEM solvers, the use of equivalent circuits and other antenna models is motivated shortly. Appropriate models provide a description of port-based parameters, as input impedance or operation frequency. Furthermore, they even enable the determination of polarization, efficiency, and other radiating properties, if an additional far field superposition of fundamental sources (e.g. Huygens sources) is carried out. Compared to the classical full-wave methods mentioned above, for example the equivalent circuit simulation features drastically reduced degrees of freedom, which means that a standard circuit simulator can outperform even high performance full-wave solvers by means of simulation time. As depicted in Fig. 4, modeling the interplay of the antenna with both, sub-THz sources or receivers in the frontend, and the channel describing the environment surrounding the antenna, benefits from both, a simple and insightful antenna representation. On one hand, examples for device-antenna modeling to understand both the THz-generation, as well as desirable operation points, can be found in [60], [61], [62], [63]. Essential system parameters such as, e.g., the equivalent isotropic radiated power (EIRP), can on the other hand be used for channel modeling and system performance evaluation. The physical insight can be increased even further, if dielectric and conductor losses are assigned to the respective antenna parts, such that the effect of each subcircuit on the overall antenna performance is accessible. In this respect, the equivalent circuit model can also be considered as an "epistemic engine" that promotes a deeper understanding into the proper operating mode of chip antennas. As will be shown below, even radiation and near-field coupling can be described and fed into full-wave or ray-tracing solvers.

A thorough overview of different on-chip architectures and utilized structures is presented in [64]. With increasing frequencies above $\approx 100\,\text{GHz}$, the interconnection losses associated with antenna in package or other antenna off-chip solutions increase the attractiveness of on-chip solutions – despite their limitations. These result from the typically lossy and large-permittivity substrates as silicon or indium phosphide for backside radiating antennas, or from a very thin substrate between antenna and on-chip ground for frontside radiating approaches. Here, the electrically small distance

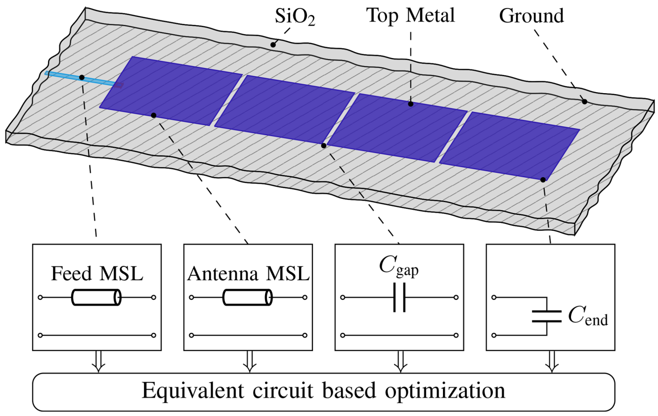


FIGURE 5. Perspective view on an exemplary antenna with the subcircuit models used for equivalent circuit based optimization.

between top- and ground metallization inherently limits both bandwidth and efficiency. With increased manufacturing effort, localized backside etching or large permittivity superstrates and dielectric resonators can partially compensate these limitations. The equivalent circuit modeling described in the following is initially applied to frontside radiating on-chip antennas using an on-chip ground [65]. Generally, the equivalent circuit analysis is a commonly used tool for periodic structures in general [66], even at mm-wave/Sub-THz frequencies [67], [68]. In [69], [70], many design choices and antenna properties of composite right-left handed antennas are derived and predicted from equivalent circuits, however the circuit modeling is not necessarily restricted to antennas. For example, passive reflectors or transmitarrays are described conveniently and insight is generated with and by such circuit models [68], [71].

Given the small distance to the ground plane on-chip, the typically planar antenna implementations are based on classical microstrip antenna designs. For these, prior modeling attempts assigned the radiation mechanism to the so-called radiating edges, as presented in [72], [73]. In detail, it is rather the discontinuity in the microstrip, which radiates [74], [75], than the resulting fringing electric field at the end, however both descriptions enable rough estimations of the resulting radiation [76]. With the approach presented in [77], equivalent circuit elements can be extracted for different local antenna parts, such that the antenna is conveniently described by coupling and cascading subcircuits. The resulting overall equivalent circuit allows for the calculation of current- and voltage distributions, input impedance, radiation efficiency, and even radiated far fields of antennas, as will be shown in the following. An exemplary stripline based antenna with capacitive discontinuities, as initially presented in [78], is depicted in Fig. 5 along with simplified subcircuit models for the different antenna sections. A key motivation for the design of this antenna, which is essentially a modified microstrip patch antenna, was to increase the radiation efficiency by including these discontinuities. With each discontinuity, the antenna length needs to be increased to compensate for its negative phase shift to obtain a constant operation frequency. By proper design, these discontinuities radiate more power than the additional antenna length dissipates, which means the overall radiation efficiency is increased [78]. The actually used subcircuit models include a rather complex frequency dependence, as e.g. skin-effect losses scale roughly according to $\propto \sqrt{f}$ and radiation losses typically follow a $\propto f^2$ behavior. Furthermore, the distinction between shunt- and series elements within the microstrip context allows for the distinction of current- and voltage-driven phenomena, be it reactive, dissipative or radiative. Lastly, the radiating circuit elements can be associated with corresponding far fields, which are calculated either analytically using appropriate greens functions [79], [80], [81], or numerically using full-wave solvers. Given the voltage or current along these radiating elements from the circuit simulation, a far field superposition can be directly carried out yielding not only port parameters, but even far field antenna parameters. A thorough consideration of the far fields allows for definition of coupling conductances, as already carried out in [82]. The coupling (or mutual) conductances can be combined with the radiation conductances of the single radiators into a conductance matrix, which includes the effect of in- or anti-phase radiation on the radiated power. This even enables the consideration of coupling between radiators in one antenna, as well as antenna-to-antenna coupling in total. With this insight, the position of radiators within the antenna can be optimized to achieve either inherent decoupling or in phase radiation, which ultimately yields a structural optimization of the antenna prototype.

With the hemispherical chip antenna measurement setup from [83], the radiated far field of the chip antenna from [77] is recorded. The measured far field is compared to the far field superimposed using fundamental radiation sources and the results from the circuit simulation. Whereas the superposition of fundamental sources only yields the directivity, the mismatch using the input impedance and the radiation efficiency using the separation of dissipative and radiative losses can be obtained from the equivalent circuit resulting in a description of the realized gain. It should be noted that the (expected) overall small gain values result from the small aperture of the on-chip antenna, which has been characterized without any aperture-increasing lens or reflector. The comparison of measurement and circuit model prediction is depicted in Fig. 6, and the agreement is, given the high complexity of on-chip measurements [84] and the simplicity of the circuit, very good. Here, the good agreement is essentially achieved by considering the radiators mutual coupling. The only limitation lies within the on-chip measurement, namely minor interference effects at the on-wafer probe [85] resulting in small undulations along the θ-axis, and a shadowed region caused by the probe [86] for $\theta < 6^\circ$. Finally, this antenna measurement closes the design loop – starting from an antenna concept, which is numerically analyzed with full-wave solvers, resulting in an insightful and simpler circuit representation, to a fabricated prototype, which meets the design specifications.

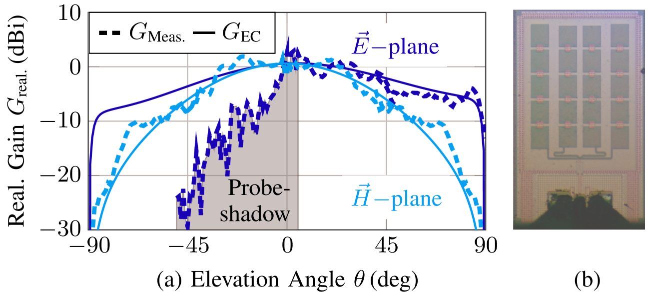


FIGURE 6. Realized gain measurement of the antenna prototype in [77] compared to the estimation of the corresponding equivalent circuit (EC) model in $\vec{E}$- and $\vec{H}$-plane at 290 GHz (a) and micrograph of the antenna prototype (b).

IV. THZ RAY-TRACING SIMULATIONS

Fawad Sheikh, Andreas Prokscha, Thomas Kaiser, Jan Barowski, Christian Schulz, Ilona Rolfes, Johannes M. Eckhardt, Tobias Doeker and Thomas Kürner

A. RADIO CHANNEL MODELS

A new wireless communication system inevitably relies on a well conceived radio channel wherein radio waves carry the signals or information. Radio waves are typically produced by an *antenna*. The undesirable effects caused by these radio channels impact the radio system design. Hence, accurate channel modeling whereby a physical understanding of these channels with their corresponding mathematical modeling is inevitable for improvising the channel behaviour and consequently optimize the system performance. By excluding the effect of the antenna from the channel model results in a *propagation channel* [44], [87]. The aim of these channel models is to efficiently yield accurate coverage predictions on radio wave propagation key statistics namely, CIRs, received signal strengths, angular spreads, delays of direct/indirect paths, electric as well as magnetic field strengths, and interference measures. Typically, the channel model type shows critical reliance on carrier frequency, bandwidth, type of environment and system under consideration. The simplest propagation model for free space radio propagation published in 1946 is the Friis equation [88], with a single unobstructed communication path. However, the Friis model yields useful results only in the *far field* region, being useful for satellite and LoS microwave links. Contrarily, the other NLoS propagation mechanisms such as *reflection*, *scattering*, and *diffraction* collectively termed as *multipath* perform in the absence of LoS links. MPC represents the most serious potential problem in many radio channels, i.e., a source of selective fading and ISI. Adding to it, the wide-band nature further complicates this aspect of channel modeling [89].

In 1956, the classical a priori based simulation approach initially suggested by Turin in a technical report [90] and a classical paper [91] which was then applied to the urban channel [92] marks the foremost work in impulse response modeling of the multipath fading channels. This followed the development of RAKE receiver for multipath channels [93]. Turin's model was later modified by Hashemi [94], [95], Ganesh and Pahlavan [96], Suzuki [97], Saleh and Valenzuela [98], and Rappaport et al. [99]. However, owing to the simplistic nature of this model, some environment related information cannot be incorporated easily without further measurements. Hence, novel simulation models including more site-specific information are developed. Moreover, simulating the propagation channel with ray-tracing can prior to the installation of the wireless system predict its successful operation, and in large part, replace measurements.

B. RAY-TRACING: SUB-GHZ TO LOW-THZ BAND

Ray-tracing, a well known deterministic propagation channel modeling method, from the CEM family among others such as, the finite element method (FEM), the finite-difference time domain (FDTD), the method of moments (MoM), predicts and describes the behaviour of EM waves when they come into contact with physical objects. At lower frequencies, the field of cellular technology, in particular, has greatly benefited from the CEM simulation techniques helping scientists to develop better antennas and communication systems. However, a major drawback of these techniques, in general, is that they require intensive computations along with a detailed description and information of the simulation scenario. Such limitations and restrictions tend to affect the accuracy of their results.

Ray-tracing methods are based on Geometrical Optics (GO) which solve the Maxwell's equations in *high frequency* range. Due to their high frequency approximation, they are not highly dependent on a large computer memory and hence, can solve, complex, 3D, and electrically large problems on modern computers [100]. In contrast, the numerical methods (FEM, FDTD, MoM etc.) are ruled out for very short wavelengths $\leq$5 mm when quantifying the behavior of the EM field in electrically large propagation environments [101]. By far, ray-tracing is highly environment-specific and its accuracy is heavily dependent on the availability of the materials and topographical database utilized in the modeling [102]. Since 1990's, ray-tracing algorithm has been developed based on the theory of GO [103], [104]. The shooting and bouncing ray (SBR) method has an edge over other ray-tracing methods with the advantage of accelerated simulation time [100], [105]. This SBR method, foremost developed for computation of radar cross section (RCS) encompasses three steps, namely, ray launching, ray tracing, and ray reception [100].

For many years, ray-tracing has been at the forefront in channel modeling for outdoor [106]–[110], in-building [111], and indoor [112]–[114] environments in the lower frequency range. Additionally, ray-tracing models for 60 GHz systems have been previously reported in the literature [101], [115], [116]. However, a decade ago, every single commercially available ray-tracing tool failed to respond to the need for THz propagation modeling [11]. The reason being the absence of distinct THz propagation mechanisms such as diffuse scattering (non-specular reflections) caused by rough surfaces [117]. A handful lot from the THz community fulfilled this void by developing the ray-tracing algorithm (RTA) incorporating this critical propagation mechanism [118]–[120]. The attenuation due to surface roughness in a specular direction of reflection can be approximated using the already validated Rayleigh-Rice (R-R) approach [121]. Beckmann-Kirchhoff (B-K) approach, though primarily opted for the diffuse scattering in non-specular direction accounts for diffuse scattering impact in specular direction of reflection as well [118]. Both the aforementioned models employ the average roughness parameter (i.e., the standard deviation height σ_h) and hence, actual random deviations from the 3D surface topography are missing. In our previous works [122]–[124], tailor-made rough surfaces with known statistical parameters of surface roughness are integrated along with their real 3D surface topography to enhance the model further assisting in the comparative study of random and non-random rough surfaces.

When designing very high speed wireless links that offer 100 Gb/s and beyond, high-gain antennas such as horns may be favored particularly for point-to-point THz communications. The horns from measurement setups can be designed using CST MWS simulation software. The 3D radiation patterns of CST MWS designed horn may then be exported for ray-tracer simulations [125]. This implies that *phi*- and *theta*-values for E- and H-planes at defined constant angle spacing or interval can be exported as ASCII data. Since many combinations are possible, in our previous work [123], we have explored the right phi/theta step size which is in good agreement with the measurements. This information can thus, assist in the ray-tracer calibrations at THz band frequencies when employing single antenna or antenna array patterns. Interestingly, horn antennas have a divergent beam (i.e., in their spatial structure unless collimating lenses are used) where the beam spot size gets larger at farther distances. The beam spot diameter from high-gain horn antenna with beam divergence holds a pivotal position for channel modeling in THz communications. For instance, larger beam spot size tends to reduce misalignment losses [17]. Moreover, the increase in beam spot diameter generates unwanted and measurement sophisticated reflections at local scatterers, reflectors or even at the measurement devices, thereby resulting in the so called *ping pong effect* [126].

Previously, a human body model with low complexity is employed to evaluate its influence on channel characterization in blockage situations with the help of ray-tracing simulations. The human is predominantly portrayed as a cylinder shaped model with additional spheres or prisms representing body parts like heads, arms and legs thus enhancing it to resemble the real shape of humans [127], [128], as can be seen in Fig. 7. To some degree, these former approaches are sufficient, however, they may fail to replicate the realistic movements when exploiting mobile THz channels. In our previous work [129], we have employed the quaternion based inertial measurement unit (IMU) data to record human kinematics and the acquired data is then embedded into a male digital twin for simulating

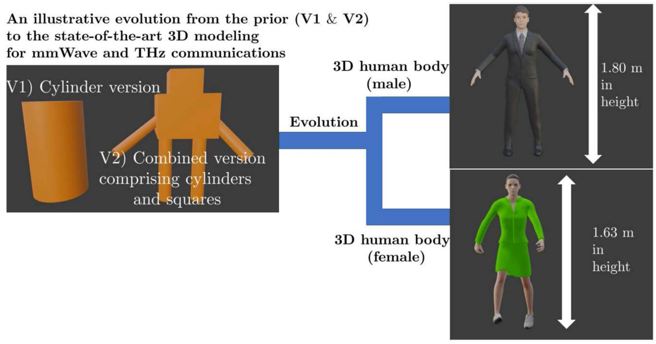


FIGURE 7. Illustration of the evolution of 3D human body models for ray-tracing simulations from previous (left) to novelly introduced, more detailed and gender-related digital twins for 1.80 m male and 1.63 m female (right).

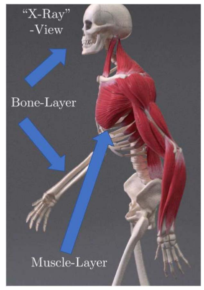


FIGURE 8. Illustration of the bone and muscle layers with the connective tissues on 3D human body model, figure adapted from [133].

real joint movements. This male digital twin represents: i) an accurate 3D human body model with sophisticated details (i.e., hand, fingers, nose and hairs), and ii) its clothing keeping in view the corresponding frequency-dependent dielectric properties of the fabrics, see [130]. In future, the aim is to explore muscle dynamics (*cf.* Fig. 8) employing CEM simulation techniques in supporting the exoskeleton technology further and thus, progressing human capabilities to go beyond previous research.

In fact, the frequencies of THz communications being closer to the frequencies of light, befit deterministic modeling approaches for channel predictions. Considering modern high-performance computing and specialized algorithms, even bigger and complex scenarios can be simulated [131]. The ray-tracing, thus offers results in three aspects for THz communications: First, channel predictions in terms of CIR itself. Second, angular information of the angle of departure (AoD) and of the angle of arrival (AoA) useful for the evaluation of algorithms in device discovery [132]. Third, different types of map predictions [34]. As aforementioned, a prerequisite for ray-tracing is a 3D model of the environment, often called "digital twin," that contains information regarding the material parameters. Fig. 3(b) illustrates the data center and the MPCs of the corresponding setup. The ray-traced MPCs in the data center model depicted in Fig. 3(c) as red crosses together with the PAP of the respective measurement pinpoint that the simulations match very well in terms of angle and delay, whereas the modeling of the amplitude deserves closer attention. In addition, the accuracy of the positioning of the objects is more important than the level of detail for the objects themselves [37].

C. THZ NEAR-FIELD AND MULTI-SCALE SIMULATIONS

Especially when tackling the THz-region with deterministic channel modeling approaches such as ray-tracing, the effort in accurate modeling increases dramatically. In addition to the increasing complexity of geometric models that is needed because of the shorter wavelength, THz communication and sensing systems usually aim at utilizing huge bandwidths demanding wideband material models as well [134]. Therefore, accurate ultra-wideband material characterization [135], i.e. determination of the relative permittivity as well as the material's loss tangent is necessary even before simulations can start. Furthermore, also the dispersion of typical air has to be considered [136].

Once the environment models are available, we can consider the different dimensions and scales that are relevant to the wave propagation within the scenario. On the one hand, there usually are large free space areas that have only minor influence on the transmitted signal, i.e. the propagating ray. In these areas, the wave propagation can be considered as being affected by *large scale* effects such as free space attenuation, dispersion or the interaction (i.e. reflection and transmission) with objects that are large and sufficiently smooth with respect to the wavelength [137]. On the other hand there are plenty of possible wave interactions in the THz-range that affect the wave by *small scale* effects, demanding higher accuracy in the modeling. These may for example be caused by rough surfaces and in-homogeneous media that allow for a relevant penetration and that are not suitable for an average description by e.g. Kirchhoff parameters [138]. In this context also highly deterministic surfaces such as intelligent reflective surfaces (IRS) have to be mentioned [139]. Furthermore, scattering from small objects, complex diffracting objects, and all interactions that have to be considered by near-field methods have to be investigated on a *smaller scale* that is more detailed.

Near-field methods are usually needed in simulations used in THz imaging or when it comes to extremely large radiating (actively or passively like IRS) structures that cause very large Fraunhofer distances [140]. Since an efficient simulation is not possible anymore, if the high level of detail from these small scale regions is transferred to the large scale domain as well, a differentiation of the total simulation domain into several sub-domains that are considered either by large or small scale methods is necessary [141]. Therefore a decoupling of these sub-domains is of high importance and can be realized offline based on precalculated results or online with detailed but efficient simulation methods, such as physical optics (PO) [142], [143], [144]. The interfaces between these domains are a research objective on its own and can be related to full-wave near field methods, dominant mode considerations, or even far field quantities such as (bistatic) RCS and gain.

However, the aforementioned scenarios have in common that plane wave assumptions usually do not hold anymore, making things complex and interesting at the same time. In these scenarios the curvature of the wavefront and the amplitude distribution are of high importance. Due to the short wavelength and the according large free space path loss, electrical large apertures that result in strongly focused fields and beams are very common in the upper mmWave and THz regions [145]. Therefore, full wave methods such as FDTD [146] may be employed for detailed analysis. Of course, the needed volume discretization quickly exceeds computationally efficient scales. Surface related methods such as the MoM [147] may be used for large scattering structures but not for complete scenarios, as well. In the end, asymptotic methods like the PO still offer the opportunity to relax far field assumptions [148], [149], while calculating the propagation channel on explicitly a predefined path. In contrast to MoM (solving an inverse model), a forward model is employed in PO, that allows to tune the granularity of the simulation by manually selecting the propagation paths *a priori*. By suitable extensions [150], PO also offers the opportunity to incorporate sub-surface features and multi-layer dielectrics.

An elegant method to describe these focused fields and propagation scenarios that rely on few dominant modes (i.e. beams) are complex source beams (CSB), sometimes also called complex origin beams. A CSB describes a Gaussian beam [151], [152], as it is used in an optical system. The compact mathematical formulation is based on the well known scalar Green's function of free space [153] in 3-dimensional space

$$G(\vec{r}, \vec{r}_0) = \frac{\exp(-jk|\vec{r} - \vec{r}_0|)}{4\pi|\vec{r} - \vec{r}_0|} \tag{1}$$

with k being the wavenumber, $\vec{r}_0$ the wave's origin and $\vec{r}$ the considered point. In order to describe a Gaussian beam, additional information on the direction and the beam-waist, i.e. the opening angle of the beam is needed. This is included by transforming the origin point $\vec{r}_0$ from $\mathbb{R}^3$ to $\mathbb{C}^3$, whereas the imaginary part of $\underline{\vec{r}}_0$ yields this information. Using the Gaussian beam waist w_0, the Rayleigh distance of the beam is given by

$$z_R = \frac{kw_0^2}{2}. \tag{2}$$

Thus a Gaussian beam of width w_0 originating in $\vec{v} = (x_0, y_0, z_0)^{\mathrm{T}}$ steering into the direction $\vec{u} = (u_x, u_y, u_z)^{\mathrm{T}}$ (with $|\vec{u}| = 1$) can be described by its complex source point

$$\vec{r}_0 = \vec{v} - jz_R\vec{u}, \tag{3}$$

offering a compact and elegant description for focused beams in the near field region of the source. The scalar field magnitude of different CSB for a signal source of 500 GHz is presented in Fig. 9.

With respect to THz-propagation models, these representation comes with the advantage that beam divergence is taken into account at a higher level of detail than classical far field models and is therefore more accurate when it comes to either

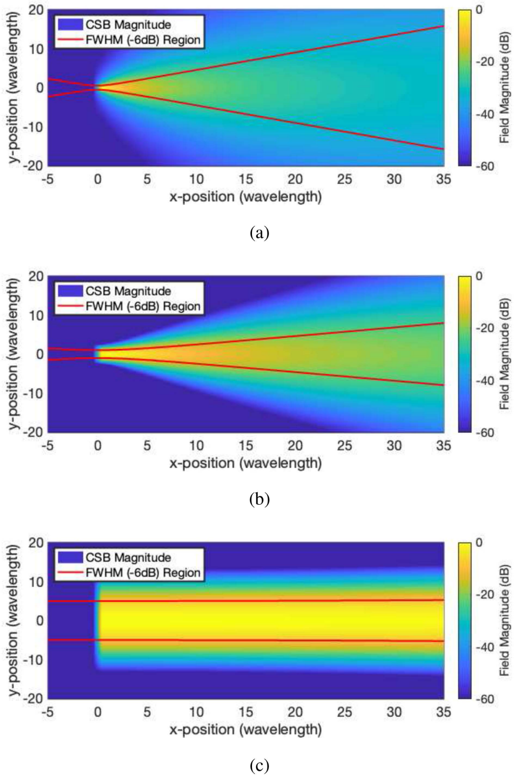


FIGURE 9. Field magnitudes from different complex source beams (CSB) differing by their beam waist parameter: (a) $w_0 = 0.5\lambda$, (b) $w_0 = \lambda$, and (c) $w_0 = 5\lambda$, demonstrating e.g. the ability to describe radiation from extended source areas (e.g. antenna arrays). The beams steer towards the positive *x*-axis, therefore the field magnitude in the negative *x*-halfplane is nearly zero. The red lines indicate the full width half maximum (FWHM) region.

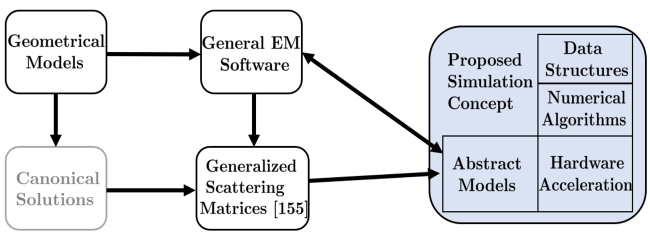


FIGURE 10. A possible concept for a multi-scale THz propagation channel simulator, handling the coupling of several remote domains (i.e. the relations of radiated, incident, and scattered fields in these) by generalized scattering matrices (GSM), figure adapted from [154].

extremely large frequencies, large structures, i.e. high gain structures, or short distances [154]. If one is aiming at multi-scale simulations of the THz regime, taking multiple large- and small-scale domains into account, CSBs provide a compact yet powerful tool, as e.g. basis functions, to describe the fields within and the coupling between several domains. Combining this with generalized scattering matrix representation of the several subdomains and efficient PO based propagation modeling (*cf.* Fig. 10), it offers a set of tools for calculating the calculating the propagation channel throughout the complete simulation environment [155].

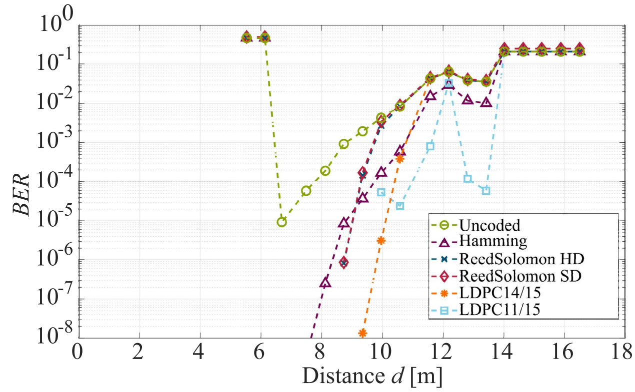


FIGURE 11. BER based on link level simulations in the data center environment for a BPSK transmission with root-raised cosine (RRC) pulse and $B_{ch} = 12.96$ GHz.

D. SYSTEM AND LINK LEVEL SIMULATIONS

The development of novel communication systems is nowadays strongly based on the prediction of the system performance and the testing of algorithms via simulations. A physical layer simulator that is based on a modular block structure enables single-carrier transmissions according to IEEE Std 802.15.3d and multi-carrier transmissions [37]. This way, the influence of the measured and simulated channel and the impact of the configuration parameters on the system can be examined. Fig. 11 shows the BER of a BPSK transmission with root-raised cosine (RRC) pulse for various coding schemes and distances from 0.69 m up to 16.5 m between TX and RX of a top-of-rack scenario in the data center model presented in Section II C. Higher order modulation schemes proved to be challenging due to currently limited TX power. For an increasing number of THz AP, multipath propagation in combination with side lobes of steerable antenna arrays cause ISI or inter-user interference that severely limit the performance. Thus, hardware and algorithm designers have to address side lobe suppression and multiplexing techniques [42].

FUTURE CHALLENGES

Most of the channel measurements in the THz range reported so far in the literature have been performed in static environments. Future applications, for example in railway [157] and automotive environments [158] require measurements in dynamic environments taking mobility into account. This becomes even more important with the advent of joint communications and sensing (JCAS) applications, wherein the communications and radars in automotive applications may operate at THz frequencies. Here, the use of static measurements for the calibration of ray-tracer prior to simulating the dynamic environments might be a promising approach. New technologies like intelligent reflecting surfaces (IRS) and massive MIMO with or without the combination of mobility encompass further challenges in THz measurement, antennas, and simulation research.

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