IEEE Access
Multidisciplinary ⋮ Rapid Review ⋮ Open Access Journal

Received May 27, 2019, accepted June 28, 2019, date of publication July 2, 2019, date of current version July 17, 2019.
Digital Object Identifier 10.1109/ACCESS.2019.2926329

A Physical Model-Based FDTD Field-Circuit Co-Simulation Method for Schottky Diode Rectifiers

HONGZHENG ZENG, YUZHU TANG, XIN DUAN, AND XING CHEN, (Senior Member, IEEE)
College of Electronic and Information engineering, Sichuan University, Chengdu 610065, China
Corresponding author: Xing Chen (xingc@live.cn)

This work was supported in part by the Fund of Ministry of Education of China, under Grant 6141A0202504.

ABSTRACT So far, plenty of microwave power circuits such as microwave diode rectifiers are mainly designed and analyzed by conventional electromagnetic (EM) co-simulation method based on the semiconductor equivalent circuit models. However, the simplified equivalent circuit model may contribute to loss of precision at high frequencies or under high power. Compared with the equivalent circuit model, the semiconductor physical model provides a means for studying the physics of electron transport, and thus, better describes the semiconductor device. This paper explores analyzing microwave diode rectifiers by employing a physical model-based field-circuit co-simulation method. This method combines the physical model-based circuit simulation to the finite-difference time-domain (FDTD)-based field-circuit co-simulation and thus, achieves accurate and effective hybrid full-wave field-circuit co-simulation. For validation, two diode rectifiers working at S- and C-band, respectively, are simulated and analyzed by the proposed method. The simulation result agrees well with measurement and shows higher accuracy than the equivalent circuit model-based simulation.

INDEX TERMS Microwave rectifier, Schottky diode, physical model, filed-circuit co-simulation.

I. INTRODUCTION

It is well-known that, for RF, microwave, and millimeter-wave circuits designing, Electromagnetic (EM) field simulators offer highly accurate results, but this accuracy mostly often comes with slow performance in terms of CPU time and high memory requirements. On the other hand, conventional circuit simulators are fast and highly flexible, but do not account for all field effects. The accuracy strongly depends on the available models and is not always guaranteed [1]. However, the design of modern microwave circuit requires the simulation that includes the relevant electromagnetic interactions between active and passive parts of the whole electronic system. As a result, accurate and efficient hybrid full-wave field-circuit co-simulation is becoming increasingly indispensable.

In general, a microwave circuit could be treated as a hybrid EM field and circuit system and analyzed using either frequency- or time-domain simulators. However, when the circuit under study which employs nonlinear semiconductor devices, time-domain methods enjoy the advantage of allowing for the direct analysis of field-circuit interactions without resorting to harmonic balance or port extraction methods [2]. Nowadays, various extensions to the finite-difference time-domain (FDTD) methods aiming at incorporating device physics/behavior into electromagnetic analysis have been proposed [3]–[10]. The most rigorous one of these schemes is the global-modeling technique, which permits the simultaneous solution of the Maxwell and semiconductor carrier transport equations by regarding them as a strongly coupled nonlinear system of differential equations on the same grid [11]–[13]. Nevertheless, it requires a large amount of computer memory and long simulation time compared with the circuit simulation. Until now, it can only be used to simulate a semiconductor device or, at most, a simple circuit consisting of one semiconductor device and a few other elements. Therefore, in the simulation of actual microwave circuits, to minimize the computational cost, whenever possible, these field-circuit simulators account for device and circuit behavior (as opposed to physics) through their description in terms of equivalent circuit models. Moreover, equivalent circuit models of semiconductor devices are easy to integrate

The associate editor coordinating the review of this manuscript and approving it for publication was Dušan Grujić.

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into circuit simulators. EM co-simulation technology based on the equivalent circuit model has been very popular and widely used in commercial software, such as ADS, AWR, etc [14]–[17].

However, modeling of equivalent circuits depends on the operating conditions and it is difficult to cover all the different situations. In addition, simplified equivalent circuit models lack the means to study the semiconductor transport physics and cannot provide the detailed investigation of the internal physical phenomena occurring in highly nonlinear active devices. The EM co-simulation technology based on equivalent circuit model is difficult to accurately predict circuit performance under high frequency or large signal [18], [19]. Indeed, until now the simulation of microwave rectifiers by the commonly used equivalent circuit model-based EM co-simulation can easily introduce great error. For example, a 2.45 GHz wideband rectifier with an HSMS-2862 diode has been designed and manufactured [14]. The measured results show that the MW-to-dc conversion efficiency increases with the input power and a peak value of 78.3% is obtained on the conditions of 18 dBm power and 900 Ω load, while ADS EM co-simulation results demonstrate that when the power exceeds 16 dBm, the efficiency drops sharply and reduces to less than 60% at 18 dBm. Similarly, a 5.8 GHz microwave rectifier with HSMS-286 Schottky diode is presented [15]. Under the optimum conditions of 19 dBm input power and 190 Ω load, the MW-to-dc conversion efficiency obtained by ADS EM co-simulation is close to 80%, but the corresponding measured efficiency is only 68.1%. Recently, a 2.45 GHz compact microwave rectifier including a HSMS-282 Schottky diode is realized [16]. The MW-to-dc conversion efficiency under different input power is simulated and measured. The comparison between them indicates that with the higher input power and output dc voltage, the nonlinear equivalent circuit model may become not so accurate, resulting in a higher simulation error.

Compared with the widely-used equivalent circuit model-based simulation, the physical model-based simulation could accurately simulate semiconductor devices and provide useful physical mechanisms [19]–[21]. Therefore a circuit simulation method based on physical model is proposed [22], [23]. It utilizes a physical model-based field simulation to analyze the semiconductor devices inside circuits, and incorporates the field simulation into an equivalent-model-based circuit simulation to simulate the circuit. This method is a powerful and effective tool for analyzing semiconductor devices and circuits. Meanwhile, it is capable of depicting useful physical mechanisms. However, those works only involves the research of low frequency electronic circuits' simulation.

In this paper, a physical model-based field-circuit co-simulation method is proposed. This method firstly utilizes the circuit simulation method based on the physical model to reduce error caused by Schottky diode equivalent circuit model. Meanwhile it combines the physical model-based circuit simulation and the FDTD based field-circuit co-simulation to realize the complete analysis of microwave circuit. This method is applied to simulate the two rectifiers of S- and C-band, respectively, and compared with measurements and popular equivalent circuit model-based ADS simulation. The results show that the proposed physical model-based field-circuit co-simulation has higher simulation accuracy than ADS. Thus, it can provide another approach for the design and optimization of the rectifier.

It is worth noting the main purpose of this paper is not to improve the performance of the rectifier itself, but to illustrate the effectiveness and accuracy of this method.

II. THE SIMULATION APPROACH BASED ON THE PHYSICAL MODEL

A. ANALYSIS AND MODELING OF A RECTIFIER SCHOTTKY DIODE

Generally, in the semiconductor simulation, the carrier transport is described by the semi-classical Boltzmann transport equation (BTE). However, finding the exact solution to the BTE is a very hard task. The drift-diffusion model, which is based on the first two moments of the BTE and the Poisson's equation, is easy to solve and has a relatively fast solution speed. It is appropriate for the numerical simulation of diode, triode and long channel MOS device.

1) Poisson Equation:

$$\nabla(\varepsilon\nabla\varphi) = q(p - n + N_t) \tag{1}$$

2) Current Continuity Equation:

$$\partial n/\partial t = q^{-1}\nabla \vec{J}_n + G - R \tag{2}$$

$$\partial p/\partial t = -q^{-1}\nabla \vec{J}_p + G - R \tag{3}$$

3) Drift Diffusion Equation:

$$\vec{J}_n = \mu_n k_b(T\nabla n + n\nabla T) + q\mu_n n\nabla\varphi \tag{4}$$

$$\vec{J}_p = -\mu_p k_b(T\nabla p + p\nabla T) + q\mu_p p\nabla\varphi \tag{5}$$

where ε is the permittivity; φ is the electrostatic potential; N_t, n and p are the doping concentrations, and electron concentrations and hole concentrations, respectively. q is the electronic charge; J_n and J_p are the electron and the hole current density; G and R are carriers generation rate and recombination rate, respectively; T is the temperature; k_b is the Boltzmann constant; μ_n and μ_p are electron mobility rate, hole mobility rate, respectively.

The semiconductor mobility is related to semiconductor materials and may be affected by many factors, such as lattice thermal vibration, ionized impurity scattering, carrier scattering, velocity saturation effect under strong field, etc [20]. Because the rectifier diode operated on strong field, the modified mobility expressed as follows:

4) Field-dependent Mobility Equations:

$$\mu_{n,p}(T) = \mu^0_{n,p} \cdot (T/T_0)^{-\alpha}/[1 + (E/E_c)^{\beta}]^{1/\beta} \tag{6}$$

$$E_c = 2.319V_m/\mu^0_{n,p}[1+0.8\exp(T/600)](T/T_0)^{-\gamma} \tag{7}$$

$$\tau_{n,p}(T) = \tau^0_{n,p}(1 + N_t/N_{n,p})(T/T_0)^{\gamma} \tag{8}$$

where $\mu^0_{n,p}$ is the effective mobility of electrons and holes at ambient temperature; E_c is the critical field; $\tau^0_{n,p}$ are the lifetime of electrons and holes at room temperature; α, β and γ are coefficients.

Boundary values of the carrier densities can be determined from the assumption of thermal equilibrium and zero space charge condition, which holds at a semiconductor device's electrodes. The coupling of the above equations (1)-(8) is used to construct diode physical field equations, however, it is impossible to directly solve such a set of equations by using analytic methods, the finite element method (FEM) is adopted for the solution.

The circuit simulation method based on the physical model needs coupling semiconductor physics simulation into the circuit simulation. For a circuit, its simulation can be simplified to the solution of a system of equations [22], [23]:

$$\begin{cases} f_1(U_1, U_2, \ldots U_k) = 0 \\ f_2(U_1, U_2, \ldots U_k) = 0 \\ \ldots \\ f_k(U_1, U_2, \ldots U_k) = 0 \end{cases} \tag{9}$$

where U is the node voltage and k is the index of the unknown node. Using the Newton–Raphson algorithm, the solution procedure of the nonlinear equations (9) is converted to the iterative equations:

$$U^{n+1} = U^n - J^{-1}(U^n)F(U^n) \tag{10}$$

where J is the Jacobian matrix. For components in a circuit, the branch current is related to the terminal voltage. For linear circuit components such as resistors, capacitors, etc., the relationship is linear and simple, yet for nonlinear components such as diodes, it is nonlinear and complicated. Assuming a diode is located in the j branch and between the (k-1) node and the k node, for an applied voltage, the nonlinear relationship between the diode branch current I_j and terminal voltages U_{k-1} and U_k can be described by:

$$I_j = \psi(U_j) = \psi(U_k, U_{k-1}) \tag{11}$$

By employing the field simulation introduced previously, the branch current I_j can be simulated for given terminal voltages U_{k-1} and U_k.

To obtain the transient response of a circuit, in the iterative matrix equation (10), the diode branch related terms are obtained by the field simulation, while the others are derived from the circuit simulation based on its constitutive equations. In this way, the field simulation and the circuit simulation are integrated into a unified scheme. For more details, please refer to [22], [23].

B. FIELD-CIRCUIT CO-SIMULATION METHOD

In many of the microwave circuit's designs, the whole system can be considered as a hybrid system with both a lumped circuit subsystem and a distributed subsystem. In the proposed field-circuit co-simulation method, the lumped circuit subsystem including a semiconductor is simulated by using the above-mentioned physical model-based circuit method, while the distributed subsystem is simulated by the electromagnetic field FDTD method.

By including an additional current term in Ampere's Law of Maxwell's equations, Maxwell's integral equations are rewritten as [6], [24], [25]:

$$\oint \vec{E} \cdot \vec{dl} = u \int_s \frac{\partial \vec{H}}{\partial t} \cdot \vec{ds} \tag{12}$$

$$\oint \vec{H} \cdot \vec{dl} = \sigma \int_s \vec{E} \cdot \vec{ds} + \varepsilon \int_s \frac{\partial \vec{E}}{\partial t} \cdot \vec{ds} + I_{device} \tag{13}$$

where I_{device} indicates the current due to the lumped circuit subsystem and represents the effects of the lumped circuit subsystem to the distributed subsystem. The partial differential format of Equation (12) and (13) can be solved by the FDTD technique, that is, the lumped subsystem can be included in the simulation of the distributed system. The FDTD simulation employs the CPML (convolution perfectly matched layer) Boundary conditions.

Assuming a circuit including semiconductors is located between the node a and the node b, the port voltage V_{ab} can be deduced from the electric field path integral:

$$V^n_{ab} = \int_a^b E^n \cdot dl \tag{14}$$

Taking the relations between the electric field and voltage, magnetic field and current into account, equation (14) can be deduced in a finite difference format to a constitutive equation which relates the port voltage and current at the current instance of time:

$$I^{n+1}_{EM} = \frac{V^{n+1}_{ab}}{R_{grid}} + I^{n+1}_{device} \tag{15}$$

where R_{grid} is an equivalent resistance determined by the FDTD grid, and I_{EM} is a known current from the FDTD iteration in previous time step. Equation (15) can be interpreted as a circuit branch consisting of a resistor in parallel with a controlled current source, which represents the effects of the distributive subsystem to the lumped circuit subsystem. It can be easily incorporated into a modified nodal formulation of a circuit simulator [24].

The two-part simulation is gradually advanced in time steps, and data is exchanged in each time step to realize field-circuit co-simulation. It should be emphasized that in each time step of the co-simulation, the circuit transient simulation takes the circuit's last state of the previous time step as the initial state of the next time step, including the state of the key semiconductor in the circuit, such as the carrier concentration, semiconductor electrostatic potential and so on. This is particularly critical for the simulation of nonlinear circuits containing semiconductors. The brief simulation process shown illustrated in Fig. 1.

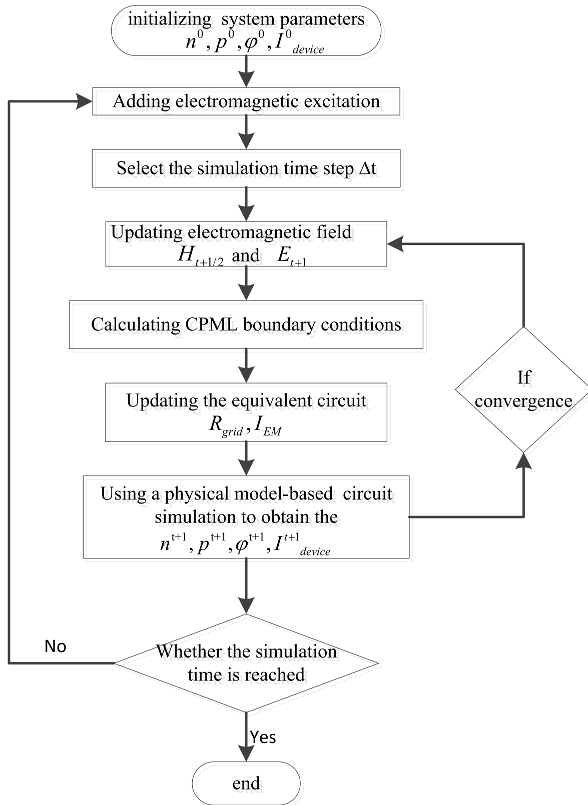

FIGURE 1. The brief simulation flow chart.

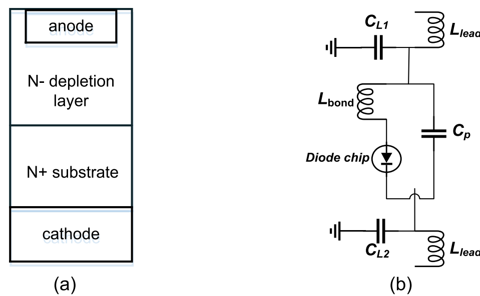

FIGURE 2. The physical parameters of a Schottky diode: (a) One-dimensional geometry of Schottky diode, (b) Package parasitic parameters DC to 6GHz.

III. THE SIMULATION AND ANALYSIS OF A SCHOTTKY DIODE RECTIFIER

A. ANALYSIS AND MODELING OF A RECTIFIER SCHOTTKY DIODE

The structure of a Schottky diode chip is illustrated in Fig. 2(a). We make a one-dimensional assumption for the purpose of simplifying simulation [26]. The lightly doped silicon epitaxial layer is deposited on heavily doped silicon substrate. The epitaxial layer doping concentration is N_d; the highly doped substrate doping concentration is N_{sub}; on top of the epitaxial layer is a Schottky contact with a barrier height ϕ_B and a metal work function ϕ_M; and cathode is Ohmic contact. The depletion layer Length is denoted by L_{epi} and the substrate Length is denoted by L_{sub}. The diode effective cross-sectional area is denoted by A_d.

According to the datasheet for commercial Avago's Schottky diodes, HSMS282B and HSMS286B are selected as the rectifier diodes of 2.45GHz and 5.8GHz, respectively. In high frequency applications, the diode package has to be accurately modeled. Their SOT-323 packages could be modeled as shown in Fig. 2(b), where C_p is the package capacitor and L_{lead} is the lead inductance, C_{L1} and C_{L2} is the lead capacitor, L_{bond} is the welding inductance. Its equivalent circuit could provide package modeling from DC to 6 GHz.

All of the extracted physical parameters are summarized in TABLE 1. The detailed extraction process of diode physical parameters, please refer to [26].

TABLE 1. All physical parameters of two diode.

Parameters \ Diode	HSMS282	HSMS286
ϕ_B	0.629 V	0.568 V
ϕ_M	4.679 V	4.631 V
N_d	5.44×10^{14} m^{-3}	2.91×10^{16} m^{-3}
N_{sub}	2×10^{18} m^{-3}	2×10^{18} m^{-3}
L_{epi}	0.97 um	1.327 um
L_{sub}	1.02 um	1.33 um
A_d	6×10^{-6} cm^2	5.61×10^{-6} cm^2

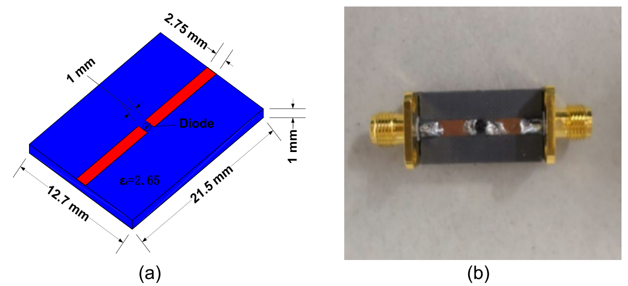

FIGURE 3. (a) Map of the two-port microstrip circuit; (b) Photo of the fabricated circuit.

Next, a two-port circuit was fabricated to extract parasitic parameter of two diodes. A single diode is in the gap of a 50Ω microstrip line, and two port are SMA connectors. The dimensions are marked in Fig. 3(a), and a photo of the fabricated circuit is shown in Fig. 3(b). Employing the aforementioned physical model-based field-circuit co-simulation, the corresponding parasitic parameters of the two diodes are extracted by fitting the simulated scattering parameters to the actual measurement [27].

The measured and fitted scattering parameters amplitude of the HSMS-282b diode and the HSMS-286b diode circuits are shown in Fig. 4 and Fig. 5, respectively. The black circles and squares respectively indicate the |S11| and |S21| of the circuit, and the blue and red curves represent the measured |S11| and |S21|, respectively.

Evidently, the fitted |S11| parameter based on physical model is almost consistent with the measurement, while the

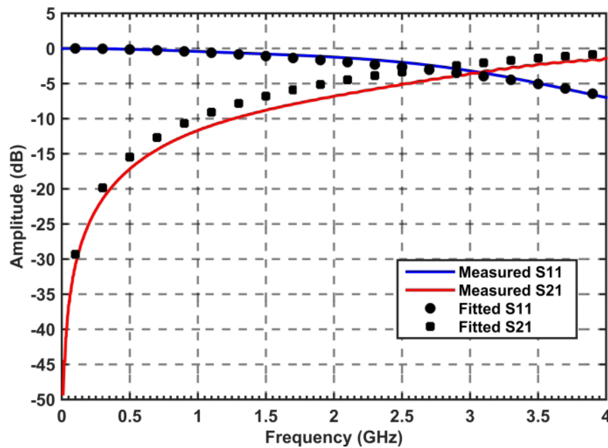

FIGURE 4. Measured and fitted S parameters (HSMS282b diode).

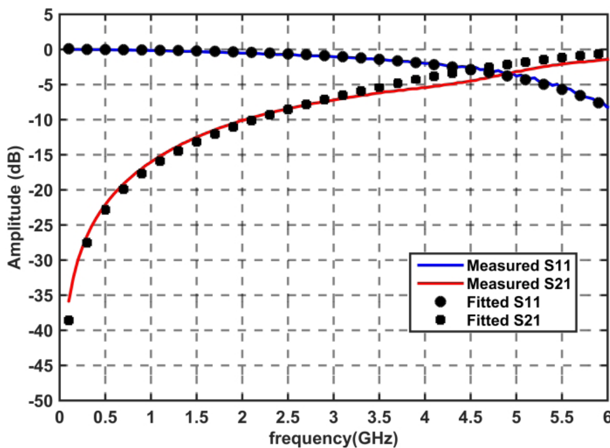

FIGURE 5. Measured and fitted S parameters of (HSMS286b diode).

TABLE 2. Parasitic parameters of diode.

Diode model / Parameters	HSMS282	HSMS286
C_p	0.16 pF	0.2 pF
L_{bond}	0.79 nH	0.525 nH
L_{lead}	0.86 nH	0.98 nH
C_{L1}	0.007 pF	0.02 pF
C_{L2}	0.002 pF	0.08 pF

subtle difference of |S21| parameter may be due to the discontinuity of SMA connectors. The extracted package parasitic parameters are listed in TABLE 2.

Since we have obtained all the necessary physical parameters for the simulation of the HSMS282 and HSMS286 diodes. As samples, the two diode rectifiers working at S- and C-band respectively are designed and manufactured, and simulated by using the above physical model-based field-circuit co-simulation algorithm and ADS.

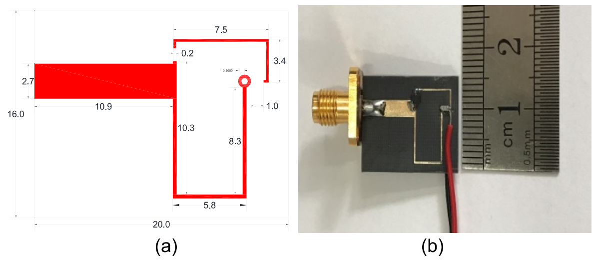

FIGURE 6. (a) Process diagram of the rectifier with HSMS282b; (b) Photo of fabricated rectifier with HSMS282b.

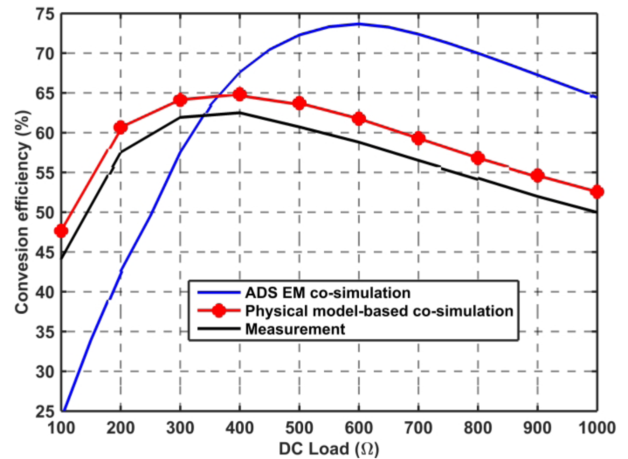

FIGURE 7. Simulated and measured efficiency vs. load (rectifier with HSMS282b).

B. ANALYSIS AND SIMULATION OF A 2.45 GHz SCHOTTKY DIODE RECTIFIER WITH HSMS282b

Utilizing the HSMS-282B diode, a compact microwave rectifier is implemented at frequency 2.45 GHz. The layout of the microwave rectifier is illustrated in Fig. 6(a). The output filter capacitor is 10 pf. The fabricated microwave rectifier is shown in Fig. 6(b). The substrate is F4B-2 (PTFE microfiber glass) with a thickness of 1 mm and a relative dielectric constant of 2.65 and loss tangent is 0.0012. A SMA adapter is connected to the input port of the rectifier. The fabricated rectifier dimension is 20 mm × 16 mm.

In our rectifier measurement, the power source adopts an Agilent vector signal source (DC to 20 GHz) and a solid-state power amplifier (center frequency 2.45 GHz, bandwidth 200 MHz). The voltage meter is used for output DC voltage measurement. An adjustable resistor box is used for the rectifier load. The MW-to-DC conversion efficiency of the rectifying circuit is calculated by the following formula:

$$\eta = \frac{P_{DC}}{P_{MV}} \cdot 100\% = \frac{V_{out}^2}{P_{MV} \cdot R_{load}} \cdot 100\% \qquad (16)$$

where P_{DC} is the DC output power, P_{MV} is the microwave input Power, V_{out} is the output DC voltage and R_{load} is the DC load.

At 20 dBm input power, the simulated and measured MW-to-dc conversion efficiency versus load is displayed

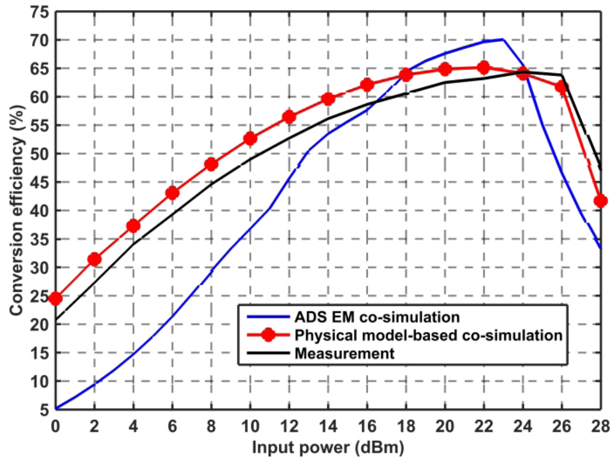

FIGURE 8. Simulated and measured efficiency vs. input power (rectifier with HSMS282b).

in Fig. 7. When the load is 400 Ω, the simulated and measured MW-to-dc conversion efficiency versus input power is displayed in Fig. 8. The ADS EM co-simulation is carried out on both schematic and layout levels. Layout-level simulations are performed using Momentum in ADS. Subsequently, the simulated circuit is brought back to the schematic in order to run co-simulation process.

As can be seen from Fig. 7, the ADS simulation shows that the conversion efficiency increases with the optimal load and reaches the maximum conversion efficiency 73.67% on a condition of 600 Ω. Then with the load continuing to increase, the conversion efficiency gradually decreases. Yet the measurement results show that the optimum load is 400 Ω and the highest efficiency is only 62.5%. In Fig. 8, the efficiency increases with the input power and a peak value 64.34% is obtained at 24 dBm input power. However, the ADS simulation shows that the maximum conversion efficiency reaches the 70% at 23 dBm input power. Overall, there is a large error between ADS simulation and measurement. In contrast, the physical model-based field-circuit co-simulation is almost consistent with the measurement.

C. ANALYSIS AND SIMULATION OF A 5.8 GHZ SCHOTTKY DIODE RECTIFIER WITH HSMS286b

Similar to the previous experiment, to further study the accuracy and applicability of the physical model-based EM co-simulation, we designed and fabricated a 5.8G rectifier based on harmonic harvesting using the HSMS-286b diode, shown in Fig. 9. Similarly, the substrate is F4B-2 (PTFE microfiber glass) with a thickness of 1 mm and a relative dielectric constant of 2.65, shown in Fig. 9 (a). A photograph of the fabricated circuit is shown in Fig. 9 (b). The fabricated rectifier dimension is 20 mm × 30 mm.

At an input power of 19 dBm, the simulated and measured MW-to-dc conversion efficiencies versus load are displayed in Fig. 10. When the load resistance is 300 Ω, the MW-to-dc conversion efficiency under different input power is also simulated by the physical model-based field-circuit

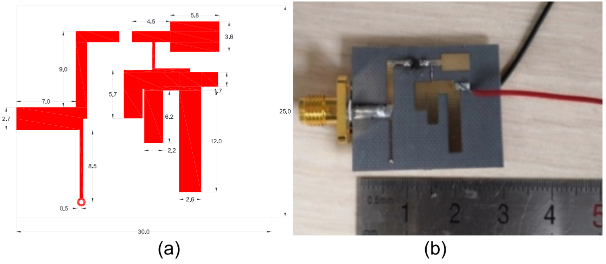

FIGURE 9. (a) Processing diagram of the rectifier with HSMS286b; (b) Photo of the fabricated rectifier with HSMS286b.

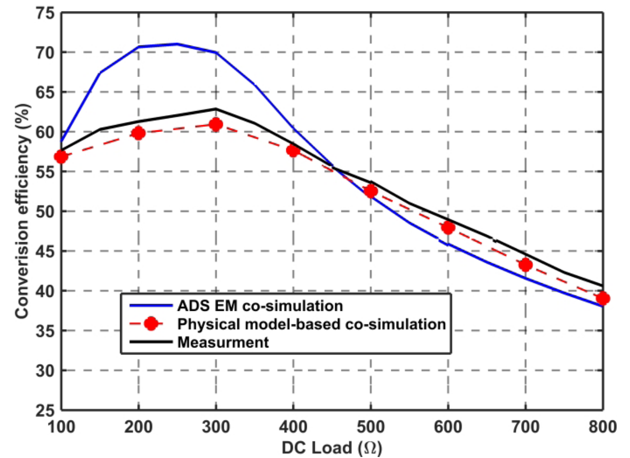

FIGURE 10. Simulated and measured efficiency vs. load (rectifier with HSMS286b).

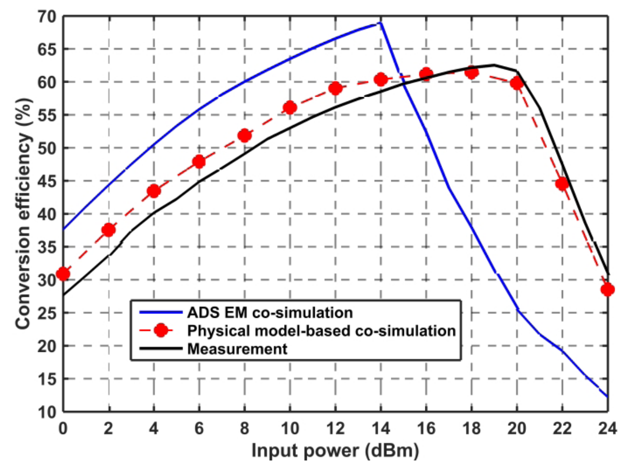

FIGURE 11. Simulated and measured efficiency vs. input power (rectifier with HSMS286b).

co-simulation algorithm and ADS, respectively. The measurement and simulation results are shown in Fig. 11.

From Fig. 10, the ADS simulation displays that the optimum load is 250 Ω and the MW-to-dc conversion efficiency reaches the maximum 71%. However, the measurement demonstrates that the optimum load is 300 ohms and the highest conversion efficiency is only 62.8%. In Fig. 11, the ADS simulation shows that the inflection point of conversion efficiency appears at 14 dBm, yet the measurement

reveal that the actual inflection point of conversion efficiency is 19 dBm. there is still a considerable error between the ADS simulation based on equivalent circuit model and measurement.

Obviously, whether it is a 2.45 GHz or a 5.8 GHz rectifier, the ADS EM co-simulation overpredicts the circuit performance with a higher input power and output DC voltage, This over prediction can be partly due to the variation of the width of the depletion region and carrier concentration, which leads to a varying junction capacitance and series resistance as frequency and power various. This cannot be self-consistently solved by the nonlinear equivalent circuit model of the Schottky diode. In contrast, the physical model-based simulation solves Poisson's equation and the current continuity equation to calculate the displacement and particle current throughout the entire diode. Therefore, it better predicts the circuit performance. Another reason is that when the peak inverse diode voltage reaches maximum, the nonlinear equivalent circuit model of the Schottky diode turns into a saturated condition. While the parameters used in the simulations need to account for phenomena like velocity saturation [28]. That is hard to describe by the equivalent circuit model and becomes a limiting effect of the diode performance especially under large signal conditions. Therefore, the equivalent circuit model-based EM co-simulation can only predict general performance of the rectifier. In contrast, the physical model-based field-circuit co-simulation is almost consistent with the experiment. The maximum error between the physical model-based field-circuit co-simulation and measurement is within 5%.

IV. CONCLSION AND FUTURE WORKS

In this paper, an efficient and accurate physical model-based FDTD field-circuit co-simulation method is proposed to simulate microwave rectifiers. It utilizes the physical model instead of the equivalent circuit model to overcome the problem that the equivalent circuit model of the Schottky diode is not accurate enough under high-power. The physical model-based circuit simulation and the FDTD based field-circuit are combined for co-simulation. The main advantage of this method is that not only it overcomes the inaccuracy of the popular equivalent circuit model-based EM simulation, but also avoids the complexity of global-modeling simulation. The proposed method is employed to analyze two microwave rectifiers in full-wave simulation. Two different Schottky diodes, HSMS-282B and HSMS-286B, are respectively utilized to carry out 2.45 GHz and 5.8 GHz microwave rectification. By comparing the simulated and measured results of the two examples, respectively, the equivalent circuit model-based EM co-simulation is found to be inaccurate. Nevertheless, the physical model-based field-circuit co-simulation can better predict the circuit performance. In this way, it can provide another accurate and effective approach for the design and optimization of the rectifier. Further, it can be applied in the simulation and design of more microwave circuits.

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HONGZHENG ZENG was born in Chongqing, China, in 1989. He received the B.S. degree in electronic information science and technology from the Chongqing University of Posts and Telecommunications, China, in 2011, and the M.S. degree in electronic science and technology from the Chongqing University of Posts and Telecommunications. He is currently pursuing the Ph.D. degree in radio physics with Sichuan University, under the supervision of Prof. X. Chen. He is also an Assistant Electronic Design Engineer with the China Electronics Society. His research interests include computational electromagnetics, hybrid system simulation, microwave power circuit simulation, and multiphysics simulation.

YUZHU TANG was born in Sichuan, China, in 1990. He received the bachelor's degree in communication engineer from the University of Electronic Science and Technology of China, in 2012, and the master's degree in communication and information system from the Chengdu University of Information Engineering, China, in 2017. He is currently pursuing the Ph.D. degree in radio physics with Sichuan University. His research interests include rectifier, antenna, and functional metamaterials.

XIN DUAN was born in Sichuan, China, in 1986. He received the bachelor's degree in electronic information science and technology, and the master's degree in electromagnetic field and microwave technology from Sichuan University, China, in 2008 and 2011, respectively, where he is currently pursuing the Ph.D. degree in radio physics. He was with Huawei Technologies Company Ltd., as a Radio Frequency Engineer, from 2011 to 2013. His research interests include computational electromagnetics, functional metamaterials, and antenna design.

XING CHEN (M'08–SM'09) received the M.S. degree in radio physics and the Ph.D. degree in biomedical engineering from Sichuan University, Sichuan, China, in 1999 and 2004, respectively. In 1991, he joined as a Teaching Staff with the College of Electronics and Information Engineering, Sichuan University, where he is currently a Professor. His research interests include antenna, microwave imaging, global optimization, numerical methods applied in electromagnetics, and parallel computation. He is a Senior Member of the Chinese Institute of Electronics.