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13. ABSTRACT (Maximum 200 words)

New algorithm has been developed for harmonic balance analysis. A robust simulation tool that combined this novel modified harmonic-balance circuit analysis technique with a two-valley temperature dependent hydrodynamic transport model device simulator is developed. We have demonstrated that polar-optical phonons dramatically affects the nonlinearity in capacitance of a material near its transverse polar optical vibration frequency. When a high frequency input signal is applied to a frequency multiplier device, polar-optical phonons can enhance the non-linearities inherent in this device, enabling higher amplitude harmonic generation of the signal to yield better output power and output efficiency of the device. The incorporation of polar-optical phonon physics into the Schottky diode abrupt junction model was developed and applied in this work. Simulation of a GaAs-based Schottky diode multipliers was performed to show the dramatic enhancement of output efficiency in the vicinity of the polar-phonon frequency. In our simulation we have utilized a novel modified harmonic-balance circuit analysis technique which allows for the rapid determination of the matched embedding circuit and an optimized multiplier design. However, to practically utilize these novel nonlinear effects related to polar optical vibration within terahertz region, new materials were required with the Schottky diode barrier height to be of the same order as in GaAs, but with a lower transverse polar-phonon frequency. One of the candidates is Bi_2S_3, which has the transverse polar optical frequency on the order of 300 GHz.

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SIMULATION OF TERAHERTZ FREQUENCY SOURCES. POLAR-OPTICAL PHONON ENHANCEMENT OF HARMONIC GENERATION IN SCHOTTKY DIODES

The accurate design and successful implementation of very high frequency nonlinear circuits requires both a detailed understanding of the physical operation of the active devices and of how these nonlinear devices interact with the linear embedding circuit. Our work combines the hydrodynamic device model with a modified harmonic-balance algorithm to provide a fully unified computer-aided design environment for nonlinear microwave and millimeter wave circuits. This is especially valuable given the importance of both the nonlinear device and its embedding circuit in the design of highly nonlinear circuits. Compare to quasi-static equivalent circuit and drift-diffusion model, the hydrodynamic transport model device simulator is more accurately in treating high-field, nonstationary, and hot-electron effects. In addition, the computational time is much reduced over that of the Monte Carlo method.

The modified harmonic-balance method utilizes a novel strategy where maximum-available diode power at second-harmonic frequency is first derived independently. In our algorithm the matched diode is optimized before constraints on embedding impedance and dc bias are specified. This approach allows for the rapid determination of the matched embedding circuit and an optimized multiplier design. The result for a Schottky-diode multiplier study has been compared to that utilized the Accelerated Fixed-Point harmonic-balance algorithms and it shows that this approach can get accurate results with a minimal time of numerical computation. Specifically, our work demonstrated a computationally efficient and accurate physical description as well as a more robust approach for circuit optimization.

We have also developed a robust simulation tool that combined this novel modified harmonic-balance circuit analysis technique with a two-valley temperature dependent hydrodynamic transport model device simulator.

As the trend towards high frequencies applications continue, research into higher frequency sources is needed in order to accommodate for these demands. Schottky Barrier Varactor (SBV) diodes have traditionally been an important frequency multiplication device for high frequency harmonic generation. Polar-optical phonons play a significant role at high frequencies in introducing a frequency dependent permittivity]. We have demonstrated that polar-optical phonons dramatically affects the nonlinearity in capacitance of a material near its transverse polar optical vibration frequency. Specific to multiplier devices, these enhanced nonlinearities can be harnessed to produce higher harmonic generation of very high frequency signals yielding better output power and output efficiency in multiplier circuits. Hence, signals belonging in the terahertz regime (generally defined between 300 GHz and 10 THz) have the distinct ability to take advantage of these enhancements due to polar-optical phonons within the polar crystal. In our research we have demonstrated the influences introduced by polar-optical vibrations and how they can be applied in obtaining higher efficiency in Schottky diodes. The incorporation of polar-optical phonon physics into the Schottky diode abrupt junction model was developed and applied in this work. Simulation of a GaAs-based Schottky diode multipliers was performed to show the dramatic enhancement of output efficiency in the vicinity of the polar-phonon frequency. In our simulation we have utilized a novel modified harmonic-balance circuit analysis technique which allows for the rapid determination of the matched embedding circuit and an optimized multiplier design.

However, it was desirable to find materials with approximately the same forbidden gap as GaAs, where we expect the Schottky diode barrier height to be of the same order as in GaAs, but with a lower transverse polar-phonon frequency. Hence, to practically utilize these novel nonlinear effects related to polar optical vibration within terahertz region, new materials were required. In particular, a special attention has been taken to a new material Bismuth trisulfide (Bi_2S_3). Bismuth trisulfide has been identified as a polar material that has the transverse polar optical frequency on the order of 300 GHz, which is in a range more suited to THz-frequency multiplier applications. As the second requirement, it was desirable to find materials with approximately the same forbidden gap as GaAs, where we expect the Schottky diode barrier height to be of the same order as in GaAs, but with a lower transverse polar-phonon frequency. Bismuth trisulfide has the forbidden gap of the order 1.6 eV . The modified harmonic balance simulation was first utilized to determine the output efficiency of GaAs at its transverse polar-phonon frequency f_{to}. This simulation was performed using the physical parameters from the UVA 6P4 GaAs Schottky Barrier Varactor. It has been observed the significant boost in efficiency beginning at f_{to} peaking at approximately 1.04 and again at 1.12 normalized frequency f/f_{to}. This suggests strong coupling of the displacement field to the polar-optical phonons within the barrier depletion region. The simulator was able to extract power and efficiency values at a wide range of frequencies within a reasonable amount of computational time. From confirmation in the performance enhancement due to polar-optical phonons in GaAs, simulation of the Bi_2S_3 material was then performed to highlight the phonon effect at a lower polar-phonon frequency. The results show that polar-optical phonons do indeed enhance the performance of a Bi_2S_3-based Schottky doubler, such that it is comparable to the performance of the state-of-the-art Schottky doubler with an operating frequency around f_{to}. The results also show a significant drop in efficiency at roughly half the phonon frequency. This is somewhat interesting in that it means that if one pumps the diode with an LO of frequency equal to approximately half that of the phonon frequency then the phonons absorb most of the second harmonic power that is produced.

As research improves for the Bi_2S_3 such that the material quality improves and better doping processes are established, Bi_2S_3 will likely to become more and more attractive as the candidate material for use in Schottky barrier harmonic generation. This motivates further investigation of use of phonon effects and phonon engineering towards the improvement of very high frequency devices and components. Hence, this research reports on simulations for GaAs and Bi_2S_3 materials systems applied towards Schottky diode based harmonic multipliers and demonstrates the general utility of polar-optical phonon effects towards harmonic generation at very high frequencies.

Furthermore, this research provides new design criterion for the use of polar-optical phonons in the enhancement of high-frequency harmonic generation and motivates the future investigation of artificially engineered materials that can provide for polar-optical phonon based tailoring of the frequency-dependent permittivity.

Results from a study on a Bi_2S_3-based Schottky diode multiplier were presented to WOFE-02 as an invited paper to highlight the phonon effect at a lower polar-phonon frequency.

Publications :

1. C. C. Lee, B. L. Gelmont and D. L. Woolard, "An Efficient Technique for the Optimization of Submillimeter-wave Schottky-diode Harmonic Multipliers," *Proc. 11th Int. Symp. on Space Terahertz Technology*, Ann Arbor, USA, May 1-3,2000 , pp.433-443.
2. C. C. Lee, B. L. Gelmont and D. L. Woolard, "Rapid self-matching modeling and optimization technique for submillimeter-wave Schottky-diode harmonic multipliers," *Proc. 45th SPIE's Int. Symp. On Optical Science and Technology: Terahertz and Gigahertz Electronics and Photonics II,* San Diego, CA, USA, 31 July – 2 August, 2000, v. 4111,ed.R.J.Kwu, K. Wu, pp.247-258.
3. B. Gelmont, D. Woolard, S.Chen, and C.-C.Lee, "Polar Optical Phonon Enhancement of Harmonic Generation in Schottky Diodes", Advanced Workshop on Frontiers in Electronics (WOFE-02)
4. B. Gelmont, D. Woolard, and S.Chen, "Polar Optical Phonon Enhancement of Harmonic Generation in Schottky Diodes", International Journal of High Speed Electronics and Systems, accepted for publication.

Patent:

B.Gelmont and D.Woolard , "Polar-Optical Phonon Enhancement of Harmonic Generation in Schottky Diodes", patent disclosure.

Participating scientific personnel.

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