Numerical Simulation and Spice Modeling of Organic Thin FilmTransistors (OTFTs)

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Abstract: As organic thin film transistors are playing important role in low cost, large area and flexible integrated circuits, there is urgent need of accurate modeling and simulation of these devices with emphasis of compact modeling suitable in integrated circuit simulation using Spice like simulators. This paper presents a 2D numerical simulation of pentacene based organic thin film transistors. Also a spice model extraction methodology of OTFTs base on Silvaco's UOTFT model is presented for circuit simulation. The numerically simulated results are in good agreement with OTFT spice modeling results. The Organic TFT model is extracted from the numerically simulated data and further it is used in circuit simulation of CMOS like hybrid inverter and five stage ring oscillator circuit realized from hybrid inverter. In the hybrid inverter circuit an amorphous silicon TFT is used in place of the NMOS devices and a Pentacene based TFT is used in place of the PMOS devices. Circuit simulation results proves the applicability of the model in circuit design of organic thin film based transistors.

Keywords: Numerical simulation, OTFTs, Spice modeling, Hybrid inverter, Ring oscillator.

INTRODUCTION

In recent years organic electronics has drawn considerable attention of the researchers with organic thin film transistors (OTFTs) as key components for active matrix displays, radio frequency identification tags, and many other small scale integrated circuits. In fact organic electronics is becoming an important research topic both in academia and industry. There is a wide range of applications of these devices in large area displays, sensor arrays, and photovoltaics etc. as discussed in [1-38]. The major advantages of organic semiconductor materials for electronic devices are flexibility, low cost, and applicability of low temperature processing [1, 29]. This will give the opportunity of fabricating mechanically flexible devices on flexible substrates at low cost and low temperature. In organic devices, OLED technology is becoming mature. This accelerated progress has benefited from strong science and technology advances in all areas of OLED technology including materials, devices, and process engineering. Whereas flat panel flexible displays present a large market opportunity for OLEDs, this requires flexible driving electronics. OTFTs are best candidates for this application and for the advancement and commercialization of this flexible display technology [5]. Organic thin-film field-effect transistors (OTFT's) have found application in recent years in low-cost, large-area electronics. OTFT's are flexible and can be fabricated at lower temperatures compared to other thin-film devices making them attractive for large-area applications. Among many organic materials, pentacene-based OTFTs have been extensively tested and so far have exhibited highest mobility for hole transport [30-34]. Field-effect transistors (FETs) using organic materials have generally low-speed due to their low-mobility [35, 36], relatively high operation voltage [37] on the other hand there are many advantages to OTFTs, such as the flexibility of the plastic fabrication substrate and the potential cost savings to manufacturers that adopt a solution process and/or ink-jet printing process. One of the most widely studied organic semiconductor materials used for OTFTs is pentacene and pentacene-based OTFTs have a typical field effect mobility of around 1 [cm^2/(V sec)]. This is of comparable value to hydrogenated amorphous silicon. OTFTs on lightweight flexible substrates are expected to eventually replace hydrogenated amorphous silicon TFT applications on glass substrates. As need to understand basic device operation, to optimize device structures grows the importance of numerical device simulation and spice model development is rising as well. The organic devices Simulation Program with Integrated Circuit Emphasis (SPICE) is still not mature. Compared to the silicon industry where public models are well defined and commonly used to provide designers with a relative good description of any process, organic devices are still lacking for their complete device models that can fully describe their electrical characteristics. Many studies exist in the

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literature to understand the physics of these devices in order to mathematically describe their behaviours as discussed in [38] and references there in. In this direction Silvaco has done an excellent effort and developed organic thin film transistor model fully dedicated to organic technology which incorporates organic device physics and implemented in its circuit simulator and device modeling software to explore the organic device and technology. In this article an effort has been done to investigate OTFT technology using these models with the help of 2D numerical simulation and spice modeling software UTMOST IV.

This paper presents a finite element based 2D numerical simulation results of pentacene based top contact bottom gate organic field effect transistor using commercially available device simulation software ATLAS^{TM} [40] and demonstrates the use of numerical simulation data for spice model extraction using universal organic thin film transistor (UOTFT) model [41-42] developed by Silvaco Inc. and available in analog circuit simulator SmartSpice [43] and in UTMOST IV [44-45] spice modeling software from Silvaco Inc. Simulation of hybrid inverter consisting of amorphous silicon TFT in place of the NMOS devices and a Pentacene based TFT in place of the PMOS devices and 5 stage ring oscillator is also demonstrated using the extracted spice models of the transistors.

NUMERICAL SIMULATION

Numerical devices simulation of top contact bottom gate pentacene based OTFT has been performed using device simulation software ATLAS^{TM} from Silvaco International. The device structure used for simulation is shown in Figure.**1**. In the device under consideration 50nm thick Pentacene is used as channel with 400nm thick SiO$_2$ as gate oxide. The source and drain consists of Au and heavily doped silicon serves as gate.

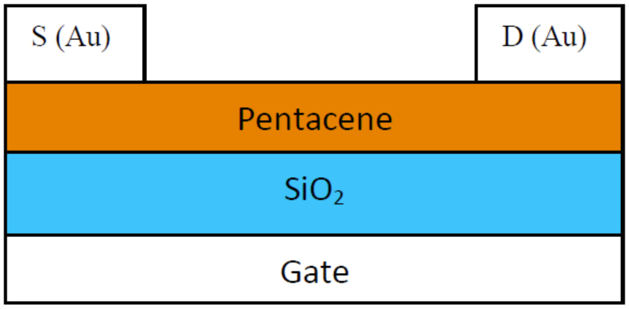


Figure 1: Pentacene based OTFT structure used in numerical simulation.

In order to simulate I-V characteristics of OTFTs, it is important to consider how carrier transport in organic semiconductors is described. In case of OTFT, the space-charge limited current (SCLC) model is successful in explaining the conduction current of organic semiconductors. In the SCLC model, the carriers are self-trapped. In addition, one of the most determinant factors for carrier transport characteristics are the energy distributions of density of states (DOS) within the bandgap. The ATLAS is able to use SCLC model in simulation and the TFT module in ATLAS is able to define these density of state distributions within the band gap. ATLAS predicts the electrical characteristics of the device by solving systems of coupled differential equations and drift diffusion model of charge transport using finite element method. The Poisson's equation and continuity equation for electrons and hole that are a set of coupled, partial differential equations are solved numerically with the help of ATLAS software for obtaining terminal characteristics of the conventional devices. These equations are given below

$$div\left(\varepsilon\nabla_{\Psi}\right) = -\rho \tag{1}$$

$$\frac{\partial n}{\partial t} = \frac{1}{q} div\,\vec{J}_n + G_n - R_n \tag{2}$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} div\,\vec{J}_p + G_p - R_p \tag{3}$$

where ε is the dielectric constant, ψ is the potential, p is hole density, n is electron density, p refers to holes, n refers to electrons, q is the fundamental electronic charge, G is the charge generation rate, R is the charge recombination rate, and J is the current density which is given considering its drift and diffusion components by

$$\vec{J}_n = qn\mu_n \vec{E}_n + qD_n \Delta n \tag{4}$$

$$\vec{J}_p = qp\mu_p \vec{E}_p + qD_p \Delta p \tag{5}$$

where μ is mobility, E is the local electric field, and D is the diffusion coefficient. To account for the trapped charge, Poisson’s equations are modified by adding an additional term Q$_T$, representing trapped charge given in (6). The trapped charge may consist of both donor - like and acceptor-like states across the forbidden energy gap, where the acceptor like states act as electron traps and donor-like states act as hole traps.

$$div\left(\varepsilon\nabla\psi\right)=q\left(n-p-N_D^{+}+N_A^{-}\right)-Q_T \qquad (6)$$

where $Q_T=q\left(N_{tD}^{+}+N_{tA}^{-}\right)$ and $N_{tD}^{+}=density\times F_{tD}$ and $N_{tA}^{-}=density\times F_{tA}$ Here, N_{tD}^{+} and N_{tA}^{-} are ionized density of donor like trap and ionized density of accepter like traps respectively and F_{tD} and F_{tA} are probability of ionization of donor like traps and accepter like traps respectively.

The density of defect states, g (E), is defined as a combination of four components. Two tail bands with an exponentially decreasing function are specified to contain large numbers of defect states at the conduction band (acceptor-like traps) and valence band (donor-like traps) edges, respectively. In addition, two deep-level bands for acceptor-and donor-like defects are defined that are modeled using a Gaussian distribution. The equations describing these terms are given as follows:

$$g_{TA}\left(E\right)=NTA\exp\left[\frac{E-E_c}{WTA}\right] \qquad (7)$$

$$g_{TD}\left(E\right)=NTD\exp\left[\frac{E_V-E}{WTD}\right] \qquad (8)$$

$$g_{GD}\left(E\right)=NGA\exp\left[-\left[\frac{E_V-E}{WGA}\right]^2\right] \qquad (9)$$

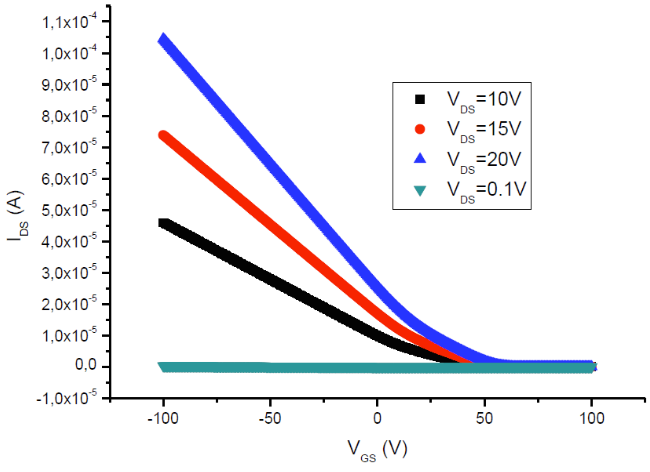
$$g_{GD}\left(E\right)=NGD\exp\left[-\left[\frac{E\ -EGD}{WGD}\right]^2\right] \qquad (10)$$

Where E is the trap energy, E_C is conduction band energy, E_V is valence band energy, and the subscripts T, G , A and D stand for tail, Gaussian (deep level), acceptor and donor states respectively. The exponential distribution of DOS is described by conduction and valence band intercept densities (NTA and NTD), and by its characteristic decay energy (WTA and WTD). For Gaussian distributions, the DOS is described by its total density of states (NGA and NGD), its characteristic decay energy (WGA and WGD), and its peak energy/peak distribution (EGA and EGD).

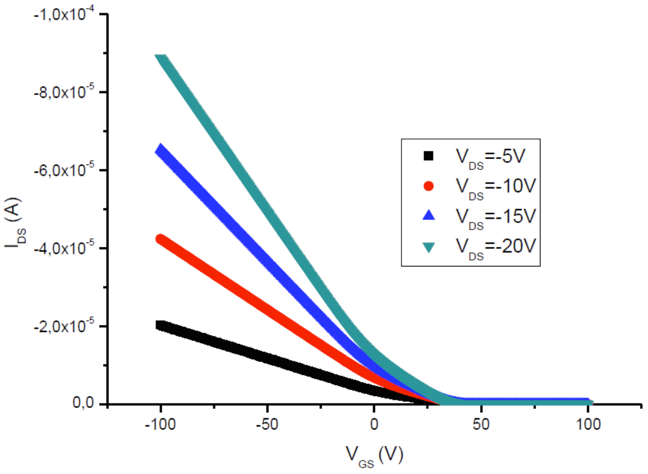
In organic materials at high electric fields the charge transport becomes field dependent. Field dependent mobility effects which is described by Poole-Frenkel mechanism is included in the numerical simulation. The Poole-Frenkel field dependent mobility model used in the simulations is described by equation (11) as in reference [12-13, 41]

$$\mu\left(F\left(x\right),T\right)=\mu_0\exp\left[-\frac{\Delta}{KT_0}+\frac{\delta}{KT_0}\sqrt{F\left(x\right)}\right] \qquad (11)$$

where μ_0 is the zero-field mobility, *F* is the electric field intensity, Δ is activation energy and δ is the characteristic parameter for the field-dependence called Poole-Frenkel factor. The simulated transfer and output characteristics of pentacene OTFT is shown in Figures **2** and **3**.



(**a**)



(**b**)

Figure 2: Transfer characteristics of Pentacene based TFT (**a**) at +ve values of V_{DS} and (**b**) -ve values of V_{DS}.

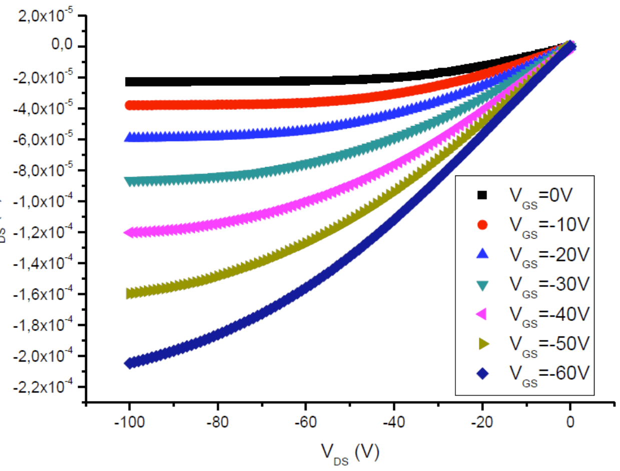


Figure 3: Output characteristics of simulated pentacene OTFT.

Spice Modeling and Application of Spice Model in Hybrid Inverter and Ring Oscillator Simulation.

There is an increasing technological interest in low-frequency application because of the demand for a low-cost circuit. Since amorphous silicon or an organic thin-film transistor (TFT) can be manufactured using low-cost processes, they are adequate for low-cost circuits. However, their mobility is low and their applications are restricted to the low-frequency region. Organic TFTs have been studied for low-cost circuits on glass or flexible substrates [48-57]. Radio frequency identification (RFID) and displays are typical applications of such low-cost circuits. TFT circuits in all NMOS (or PMOS) like topology have a large static power dissipation due to the existence of a direct path from supply to ground. Such power dissipation would prevent these circuits from being used in battery operated portable systems. Thus, the obvious choice is to integrate the a-Si:H n-TFT with pentacene based p-TFT in a complete CMOS structure. This was first shown by Bonse *et al* [58] and CMOS TFT Op-Amps in hybrid TFT technology have been demonstrated in reference [59]. Many TFT models have been reported in past [60-70]. The technology and operation of organic thin film transistors (OTFTs) have a range of peculiar features that require a dedicated compact TFT model. The most important OTFT specific features are: the operation in the carrier accumulation mode, exponential density of states, interface traps and space charge limited carrier transport, nonlinear parasitic resistances, source and drain contacts without junction isolation as well as the characteristic mobility dependence on carrier concentration, electric field and temperature. The universal organic TFT (UOTFT) model has been developed at Silvaco [45] by extending the unified charge control model (UCCM), previously used for a-Si and poly-Si TFTs [66-68], to OTFTs and introducing generic modeling expressions for channel conductivity OTFT [69, 70]. In that way, UOTFT model is suitable for application to a large variety of the OTFT device architectures, material specifications and fabrication technologies [45]. Therefore we have used UOTFT model for spice model extraction of pentacene based OTFT. All the modeling equations can be obtained in [41, 42, 45]. To realize the hybrid inverter circuit we performed a process and device simulation of NMOS a-Si:H TFT and pentacene based PTFT. We converted the TCAD data to UTMOST IV format (from .log file to .uds file), and performed model extraction in

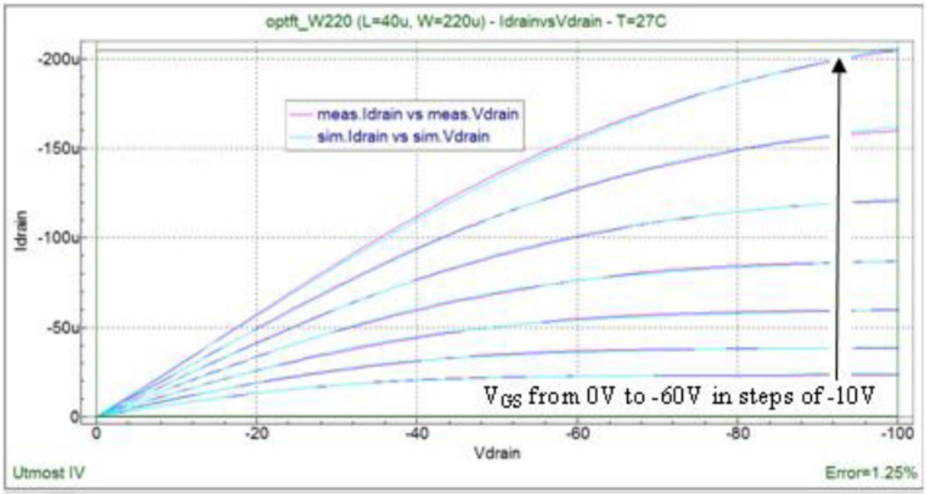


Figure 4: ID-VD characteristics of Pentacene based TFT at V_{GS}=0V to -60V in steps of -10V from bottom to up.

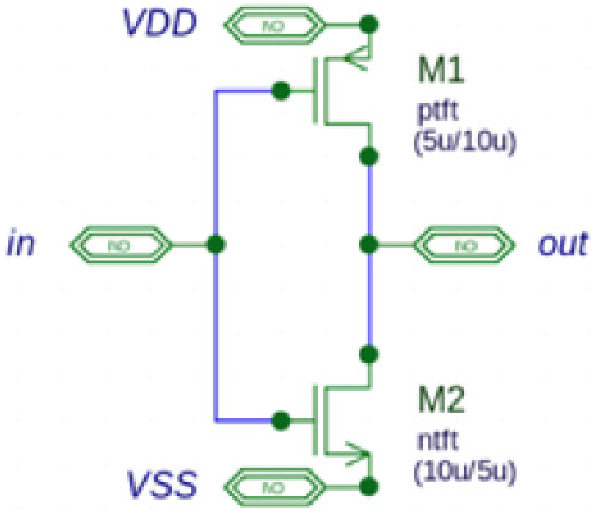


Figure 5: Hybrid inverter schematic.

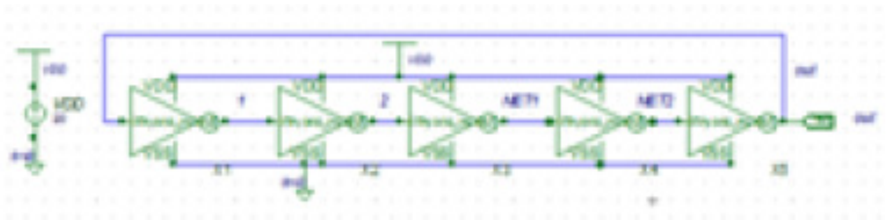


Figure 6: Five-stage ring oscillator using hybrid inverter.

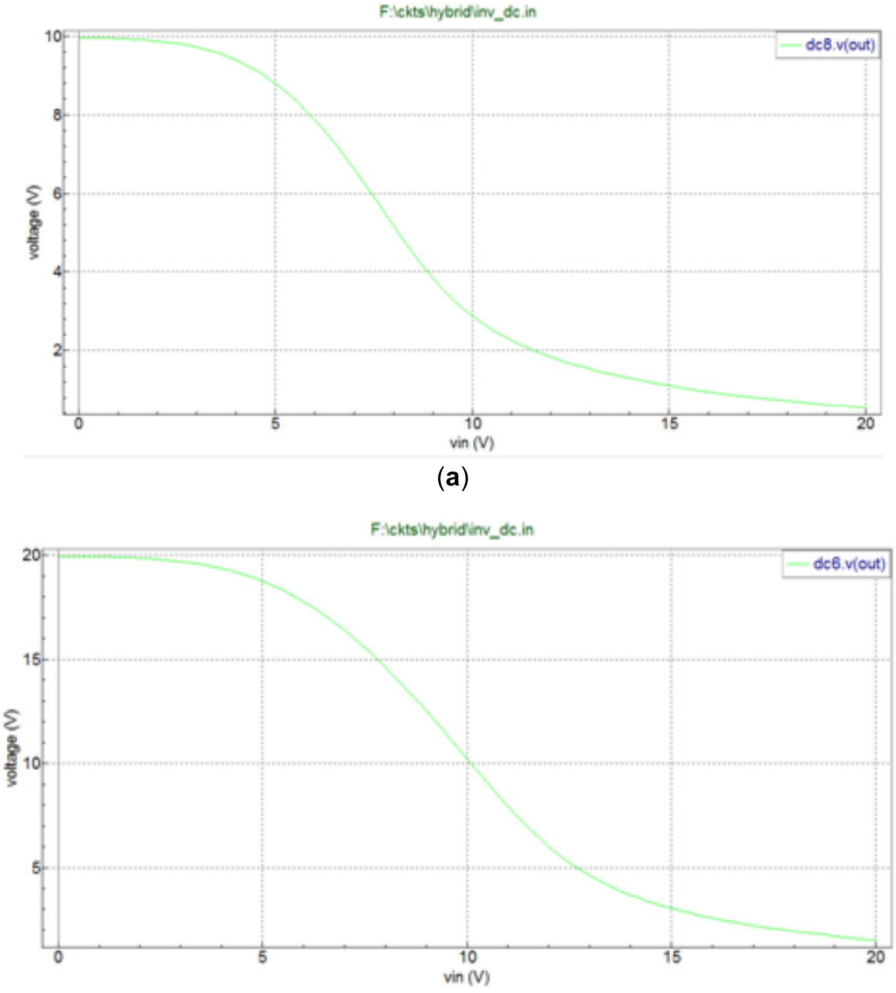
UTMOST IV. For the pentacene based PTFT, a UOTFT model (level=37) was used and for the NMOS a-Si:H TFT an RPI a-Si TFT model (level=35) was used. The detailed explanation of the a-Si TFT and OTFT model extraction methodology can be found [60-61]. Figure **4** illustrates the ID-VD characteristics of the OTFT after optimization in UTMOST IV which is in good agreement with output characteristics of pentacene TFT obtained by numerical simulation. UOTFT model is able to reproduce the same output characteristics of OTFT as obtained from numerical simulation with mismatch error of only 1.25%. For optimization Levenberg-Marquardt algorithm was used in UTMOST IV.

The extracted spice models of the a-Si NTFT and Pentacene based PTFT are then used in the hybrid inverter and the five stage ring oscillator circuits for simulation using Gateway.

The schematics for the hybrid inverter and ring oscillator circuits are shown in Figures **5** and **6**, respectively. The dc simulation characteristics of hybrid inverter is shown in Figure **7**. It is evident that hybrid inverter operates at high voltage (*i.e.* VDD is high at above 10V). The output waveform of the five stage ring oscillator using the hybrid inverter is shown in Figure **8**. From the output characteristics of the ring oscillator it is evident that it operates at relatively high voltage and frequency of oscillation is low, around 0.5 MHz. It can be used for low cast and low frequency applications.

CONCLUSIONS

This paper presented the simulation of pentacene based OTFT by two different approaches, one by means of 2D Numerical simulation using commercially available device simulation software ATLAS^{TM} and in other approach we simulated the OTFT characteristics using UOTFT compact model available in UTMOST-IV software. Simulation results in both the cases are in good agreement. Using the extracted UOTFT model based on numerical simulation data, simulation of a hybrid inverter and 5 stage ring oscillator are successfully demonstrated which gives the confidence to use this model in EDA tools to speed up the design cycle of circuits based on OTFTs.



(**a**)

(**b**)

Figure 7: DC Characteristics of hybrid inverter (**a**) at VDD=10V (**b**) at VDD=20V.

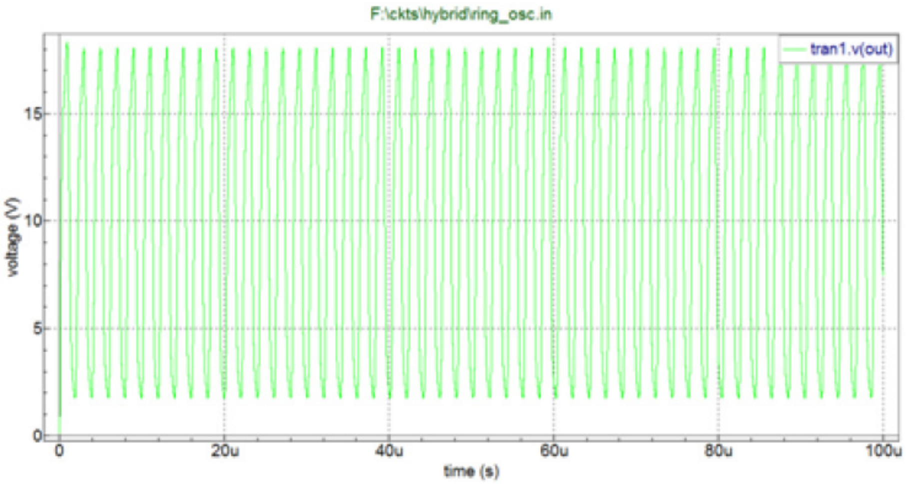


Figure 8: Output of five stage ring oscillator using hybrid inverter.

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