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ABSTRACT
Neuromorphic architectures based on memristive neurons and synapses hold great prospect in achieving highly intelligent and efficient computing systems. Here, we show that a Schottky diode based on Cu-Ta/InGaZnO\(_4\) (IGZO)/TiN structure can exhibit threshold switching behavior after electroforming and in turn be used to implement an artificial neuron with inherently stochastic dynamics. The threshold switching originates from the Cu filament formation and spontaneous Cu–In–O precipitation in IGZO. The nucleation and precipitation of Cu–In–O phase are stochastic in nature, which leads to the stochasticity of the artificial neuron. It is demonstrated that IGZO based stochastic neurons can be used for global minimum computation with random walk algorithm, making it promising for robust neuromorphic computation.

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Memristive neural network has recently emerged as a great candidate for next-generation artificial intelligence (AI) and neuromorphic hardware systems. A neural network typically consists of synaptic and neuronal elements integrated in an architecture with high parallelism and high connectivity. While the artificial synapses define the efficacy of signal transmission and are responsible for memory and learning, the neurons are key elements for spatiotemporal integration of input signals and generation of spikes when meeting certain thresholds. To date, a large number of approaches have been developed to implement artificial synapses, such as nonvolatile memristors, diffusive memristors, synaptic transistors, photonic synapses, etc. However, the exploration for efficient neurons is much more limited. Although several forms of artificial neurons, including the Hodgkin–Huxley neuron, leaky integrate-and-fire (LIF) neurons, and oscillation neurons have been proposed, a scalable neuron with biorealistic stochasticity and CMOS compatibility is still missing. On the other hand, the random walk algorithm based on probabilistic principal component analysis requires the solution of arbitrary segmentation—a global optimization method which can be solved quickly by using the previous solution as the initialization of an iterative matrix solver.

Here, we report a stochastic neuron based on a single Cu-Ta/InGaZnO\(_4\) (IGZO)/TiN device which shows inherent stochastic dynamics and the material systems are CMOS compatible. The Cu-Ta/IGZO/TiN devices exhibit stable Schottky barrier diode (SBD) characteristics before electroforming, which, however, shows threshold switching (TS) in positive voltage polarity after electroforming and in turn be used to implement an artificial neuron with inherently stochastic dynamics. The threshold switching originates from the Cu filament formation and spontaneous Cu–In–O precipitation in IGZO. The nucleation and precipitation of Cu–In–O phase are stochastic in nature, which leads to the stochasticity of the artificial neuron. It is demonstrated that IGZO based stochastic neurons can be used for global minimum computation with random walk algorithm, making it promising for robust neuromorphic computation.
algorithm based on IGZO stochastic neurons. Such stochastic neurons is expected to be helpful for the construction of neuromorphic computing systems with robust neuromorphic computation.

The Cu-Ta/IGZO/TiN devices in this work were fabricated as follows. First, 35 nm thick TiN bottom electrodes were deposited by sputtering and patterned by photolithography and lift-off processes. Subsequently, 30 nm IGZO film was sputtered using an InGaZnO$_4$ target at 100 W with a mixed working gas of Ar/O$_2$ (5:1). Finally, 35 nm thick Cu-Ta (11:1) top electrodes were deposited by DC sputtering and patterned by photolithography and lift-off processes. The devices have a size of $50 \times 50$ $\mu$m$^2$. The electrical measurements were performed using an Agilent B1500A semiconductor parameter analyzer and a B1530A fast measurement unit. The voltage was applied to the Cu-Ta electrode, with the TiN electrode grounded during electrical measurements.

Figure 1(a) shows cross-sectional transmission electron microscopy (TEM) image of the Cu-Ta/IGZO/TiN device along with a structural schematic in the inset. One can see that the IGZO film has an amorphous structure in its pristine state. Initially, the Cu-Ta/IGZO/TiN device shows Schottky barrier diode (SBD) behavior, as can be seen from the representative current–voltage ($I$–$V$) characteristics in Fig. 1(b). The SBD behavior was stable throughout 1000 cyclic DC sweeping. When a forming voltage of 7.5 V was applied onto the device, as shown in the inset of Fig. 1(c), a pronounced hysteresis loop can be observed in the $I$–$V$ plot, and a transition to threshold switching (TS) behavior in the positive voltage region can be clearly observed in all subsequent sweepings [Fig. 1(c)]. Figure 1(d) further shows the threshold switching characteristics in log scale. As the voltage was swept from 0 to 2 V with a current compliance of 7 mA, an abrupt increase in current was observed at about 1.8 V, which is called the threshold voltage ($V_{th}$). This switching event is in agreement with the current-controlled negative differential resistance (NDR) in the inset of Fig. 1(d). During backward sweeping, the device switched to the OFF state at about 1.4 V, which is the hold voltage ($V_{hold}$). However, the device still showed SBD behavior in low voltage region [Fig. 1(c)], with a turn-on voltage of $-0.6$ V. Our experiments have verified the crucial role of the Cu/Ta ratio of about 11:1 in obtaining a stable threshold switching behavior. The devices were found to exhibit bipolar switching behavior that is nonvolatile when the Cu/Ta ratio is higher than 11:1, but will easily get stuck in low resistant states when the Cu/Ta ratio is lower than 11:1.

In order to understand the mechanism of the SBD and TS behaviors in the same Cu-Ta/IGZO/TiN device, high-resolution TEM studies were performed before and after the electroforming process, as shown in Fig. 2. The polarity of the SBD behavior suggests that the Schottky barrier exists at the IGZO/TiN interface, which is consistent with previous studies using a TiN/a-IGZO/Cu structure. When a forming voltage was applied on the top electrodes [in Fig. 2(b)], Cu ions can be generated at the top interface through anodic reactions and subsequently incorporated into the IGZO layer. A Cu filament can thus be formed between the top and bottom electrodes, giving rise to a resistance switching from OFF to ON state [Figs. 1(c), 1(d), and 2(b)]. Given the high current compliance during switching, the Cu incorporated into the filament region must be supersaturated for the IGZO matrix. Previous studies on Cu diffusion mechanisms in IGZO revealed that supersaturated Cu in IGZO tends to form a new Cu–In–O phase at equilibrium, which will decrease the electrical conductivity of
IGZO and thus account for the spontaneous switching back to the OFF state.\textsuperscript{41}

Notably, a thin interfacial layer can be found at the IGZO/TiN interface [Fig. 2(c)], which is expected to be TiO\textsubscript{x},\textsuperscript{22} due to the interfacial reactions between the oxide and the TiN electrode. After forming, an evident increase in the thickness of the interfacial layer from 1.9 to 3.2 nm is observed, after the Cu-Ta/IGZO/TiN device went through a forming process [Fig. 2(d)], which might be ascribed to the electrically induced Joule heating effect that facilitates interfacial reactions at the IGZO/TiN interface. The increased TiO\textsubscript{x} thickness decides that the IGZO film becomes more oxygen deficient, accounting for the increased leakage current that can be observed in the OFF state, as shown in Fig. 2(b),\textsuperscript{41} which in turn leads to significant thermal effects.

It has been reported that the crystallization temperature of IGZO can be reduced when in contact with Ta,\textsuperscript{17} which is present in the Cu-Ta top electrode, and the electrically induced Joule heating provides a local annealing effects around the current path that can promote crystallization. In the present study, although a transition from amorphous to crystalline structure was not directly verified during TEM observation, we have found that the inclusion of Ta is necessary for the threshold switching behavior. Otherwise, the Cu/IGZO/TiN device showed nonvolatile bipolar switching, similar to previous works.\textsuperscript{15,16} As a result, the microstructural change of IGZO contributes to the higher diffusion rate of Cu\textsuperscript{2+} and precipitation of new phases in IGZO as well.\textsuperscript{21} The electroforming process plays an important role in introducing supersaturated Cu in IGZO and also serves as an annealing step when IGZO is in contact with Ta, which eventually results in the threshold switching [Figs. 1(c), 1(d), and 2(b)].

The Cu-Ta/IGZO/TiN devices were in turn used to implement an artificial neuron in this work, where the circuit is shown in Fig. 3(a). A load resistor (\(R_L\)) was connected in series with the IGZO threshold switching device to serve as the synapse for the sake of simplicity, which can represent the equivalent resistance of the corresponding column when the artificial neuron is connected with a memristor array. The Cu-Ta/IGZO/TiN device has an intrinsic 16 pF capacitance that can be used to implement integration dynamics of neurons, as shown in Fig. 3(a). 1 ms wide voltage pulses were generated by an Agilent B1530A fast measurement unit and applied to the circuit, and the output current through the Cu-Ta/IGZO/TiN device was recorded. Previous studies\textsuperscript{15,16} have suggested that a load resistance between \(R_{ON}\) and \(R_{OFF}\) of the threshold switches is appropriate for initiating neuronal oscillations. As a result, \(R_L\) values of 220 and 680 \(\Omega\) were adopted in Fig. 3(b), Figs. 3(c) and 3(d), respectively, with varied input voltage \(V_{DD}\). Since most of the voltage drop is on the Cu-Ta/IGZO/TiN device when it is in the OFF state, the parallel capacitor will be gradually charged and the membrane voltage will be increased. Once the voltage on the capacitor exceeds \(V_{th}\), the Cu-Ta/IGZO/TiN device will be switched to the ON state and a current spike will be generated in the circuit. Due to the small \(R_{ON}\), the capacitor \(C_p\) will be discharged and the Cu-Ta/IGZO/TiN device will be switched back to the OFF state when the membrane voltage drops below \(V_{hold}\). The capacitor charging is a leaky process due to the leakage current in the OFF state of Cu-Ta/IGZO/TiN devices [see Figs. 1(d) and 2(b)]—leaky integrate-and-fire dynamics can be physically implemented using the simple neuronal circuit in Fig. 3(a). Consequently, the transition of the device from stochastic to no spiking can be observed by further decreasing the input voltage to 2.8 V with a load resistance of 220 \(\Omega\), as shown in Fig. 3(b).

Interestingly, the IGZO based artificial neuron shows intrinsic stochasticity. Figures 3(c) and 3(d) shows that the neuron spikes randomly in a given circuit with fixed \(R_L\) and \(V_{DD}\), which is dramatically different from the periodic spiking in a typical oscillation neuron.\textsuperscript{21} Such stochasticity could stem from the precipitation dynamics of the Cu–In–O phase out of IGZO in the previous spiking event, as the nucleation is a stochastic process in nature,\textsuperscript{21} and the amount of Cu-containing phase formed and the Cu concentration left in the conduction channel significantly affects the dynamics in the subsequent integration process. Compared with deterministic neuronal firing, the stochasticity in neuron dynamics is considered more desirable for robust signal encoding and transmission, e.g., applications in population-based neuronal computation and Bayesian inference.\textsuperscript{12,25–27} One can see from Fig. 3 that the number of neuron spikes generally increases as the input basing voltage increases. Besides, all the neuron spikes under fixed input voltages exhibit random behaviors, as can be seen from Figs. 3(e) to 3(f). However, a general trend still holds for the artificial neuron, that is, the spiking rate roughly increases as \(V_{DD}\) increases when \(R_L\) is fixed, as can be seen from Figs. 3(c) to 3(f).
Stochastic neurons can find extensive applications in neuromorphic computing. Here, we show the implementation of a random walk algorithm based on IGZO stochastic neurons for global minimum computation of the function \( f(x) = 2x^2 \cos(32x) \). The following equations are used to obtain the random walks:

\[
u(t + 1) = u(t) + e(t),
\]

where

\[
e(t) = \begin{cases} +1, & N(t + 1) > N(t) \\ -1, & N(t + 1) \leq N(t) \end{cases}.
\]

Here, \( N \) is the number of neuron spikes under various measured conditions within the time step \( t \) (100 \( \mu s \)). To obtain the random walks, four sets of stochastic neuron spiking were measured for 20 time steps, as shown in Figs. 4(a) and 4(b), where \( R_L = 220 \Omega, V_{DD} = 3.4 \text{ V} \) and 4.0 V and \( R_L = 680 \Omega, V_{DD} = 4.3 \text{ V} \) and 4.4 V. It should be noted that the stochasticity of the artificial neuron is irrelevant with the input voltages. Therefore, four sets of random walks can be generated from the neuronal spikes following Eqs. (1) and (2), as shown in Fig. 4(c).

Furthermore, the corresponding \( x \) value for a global minimum of function \( f(x) = 2x^2 \cos(32x) \) can be obtained following the random walk algorithm

1. Initialize the values of \( x \) (in this case 1.2) and the step \( \lambda \) (in this case 0.8).
2. The iteration number \( k \) starts from 1, while the total iteration number \( n \) is 20.
3. Four \( u \) values are obtained from the random walks in \( u(t) \) shown in Fig. 4(c), when \( k < n \). Then, the value of \( x \) is updated following \( x' = x + \lambda u' \) and \( u' \) is the normalized value of \( u \), thus obtaining a set of \( x' \) values.
4. If one of the \( x' \) values can result in \( f(x') < f(x) \), the value of \( k \) will be reset to 1 and \( x \) will be updated to \( x' \). The calculation process will restart from step (2). If \( f(x') > f(x) \), the value of \( k \) will be increased by 1 and set \( \lambda = \lambda/2 \), and the calculation process will restart from step (3).
5. The process will break once the step value of \( \lambda < 10^{-6} \). If not, the calculation process will be repeated from step (1).

Finally, the corresponding \( x \) value for the global minimum solution is achieved (\( x = 1.671 \)), and \( f(x)_{\text{min}} \) of \(-9.312 \) is obtained in the domain \([1.2, 1.8]\) through the random walk algorithm based on the IGZO neurons, showing the potential of stochastic neurons in computing applications.

In summary, we have built a stochastic neuron based on Cu-Ta/IGZO/TiN devices, which exhibit Schottky diode behavior in pristine state. The Cu-Ta/IGZO/TiN devices can undergo a structural and chemical transition during electroforming, leading to threshold switching in the positive voltage direction. Such threshold switching behavior could be attributed to the spontaneous precipitation of Cu–In–O phases when Cu gets supersaturated in IGZO, and the electroforming process effectively plays an important role in introducing supersaturated Cu and serving as an annealing process. The spiking rate of the artificial neuron increases as the input voltage increases in general, however, the spiking event is inherently random, which could originate from the stochasticity during Cu–In–O precipitation. It is demonstrated that the random walk method based on the stochastic neuron can be used in the optimization of numerical functions, showing the potential of stochastic neurons in computing applications.

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