

# DEVICE MODELING AND SIMULATION OF FERROELECTRIC TUNNEL JUNCTION FOR COMPUTING-IN-MEMORY APPLICATION

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## ABSTRACT

For computing-in-memory applications implemented by ferroelectric tunnel junction (FTJ), a multi-pulse FTJ switching model is required. Here, based on the single-pulse nucleation-limited switching (NLS) model, a multi-pulse model capable of calculating the change of ferroelectric polarization under a series of arbitrary waveform pulses at different frequencies is proposed, which shows good agreement with literature-reported experimental results. In addition, the multi-pulse model was adopted in the simulation of an FTJ-based neural network, where it was found that the programming scheme with increasing pulse amplitude could achieve higher recognition accuracy and better FTJ conductance fluctuation tolerance than those with identical pulse or increasing pulse width. This work provides a useful model for further optimization and application of FTJ in neuromorphic computing.

## INTRODUCTION

Various applications based on deep learning have raised higher and higher demand for computing power and data processing capabilities. In the conventional von Neumann architecture, the data computing and storage units are separated [1], and hence most of the energy consumption and delay of the system are spent in memory accessing, which severely limits the data processing speed and leads to the so-called "memory wall" issue. The computing-in-memory (CIM) architecture based on emerging memories such as memristor emerges as a promising computing paradigm to solve this problem [2], [3]. As the fundamental computing unit, memristor with analog resistive switching characteristics plays a vital role in the performance of CIM systems [4]. Thanks to the excellent characteristics of ferroelectric materials, including fast polarization switching speed and stable polarization state, ferroelectric memory has the potential advantages of high speed, low power consumption and non-volatility [5]. In particular, as one type of ferroelectric memory devices, ferroelectric tunnel junction (FTJ) has attracted wide attention because of its ability to realize continuous conductance modulation [6].

Based on the analog resistive switching characteristics of FTJ, an FTJ crossbar array can realize the vector-matrix multiplication operation in one step by

taking the advantage of CIM, which is highly desired for accelerating deep learning algorithms. For the implementation of neural network training and inference, the linearity, symmetry, number of conductance levels, fluctuation and other resistive switching characteristics of the FTJ devices can directly affect the final recognition accuracy [7]. For this purpose, establishing a multi-pulse switching model of FTJ, and studying the influence of its non-ideal characteristics on the array performance are critical for the CIM application of FTJ devices.

The key issue of the FTJ multi-pulse switching model is the polarization reversal of the ferroelectric film. So far, there are two mainstream models which describe the polarization reversal process: Preisach model and nucleation-limited switching (NLS) model [8], [9]. However, neither Preisach model nor NLS model could accurately describe the change of ferroelectric polarization under a series of arbitrary pulses.

In this article, a method is proposed to expand the NLS model to a new multi-pulse model by calculating the cumulative effect of previous pulses. This new multi-pulse model could accurately calculate the polarization changes of ferroelectric materials under arbitrary voltage pulses by dividing an arbitrary voltage waveform into a series of rectangular pulses based on the idea of differentiation. The multi-pulse model could also predict the frequency-dependent characteristics of ferroelectric materials very well. Furthermore, the FTJ multi-pulse switching model was applied in artificial neural network simulation, and the influence of different programming schemes on the classification accuracy was studied.

## DEVICE MODELING

Here it is assumed that  $n$  pulses with the same amplitude  $V$  and a summation of total pulse width  $T_n$  are equivalent to one single pulse with pulse amplitude  $V$  and pulse width  $T_n$ . According to this assumption, the switched fraction of the ferroelectric film under  $n$  voltage pulses with the same amplitude  $V$  is given by:

$$p(n) = p_{NLS}(V, T_n) = p_{NLS}\left(V, \sum_{i=1}^n t_i\right) \#(1)$$

where  $p_{NLS}$  denotes the switched fraction of the ferroelectric film calculated by NLS model,  $t_i$  is the pulse width of the  $i^{\text{th}}$  pulse and  $T_n = \sum_{i=1}^n t_i$ .

Similar to Equation (1), the switched fraction of the

ferroelectric film under  $n+1$  voltage pulses namely  $p(n+1)$  can be derived as follows:

$$p(n+1) = p_{NLS}(V, T_{n+1}) = p_{NLS}(V, T_n + t_{n+1}) \quad (2)$$

where  $T_{n+1}$  denotes the summation of total pulse width of  $n+1$  pulses,  $t_{n+1}$  is the pulse width of the  $(n+1)^{\text{th}}$  pulse and  $T_{n+1} = \sum_{i=1}^{n+1} t_i = T_n + t_{n+1}$ .

Note that this equation of calculating the accumulative effect is only suitable for pulses with same amplitude.

For pulses with different amplitudes, suppose that the value of  $p(n)$  has been obtained. The amplitude of the  $(n+1)^{\text{th}}$  pulse is  $V^*$  and the pulse width is  $t_{n+1}^*$ . In order to calculate  $p(n+1)$ , the accumulative effect of previous pulses namely  $p(n)$  is assumed to be equivalently induced by one single pulse with constant amplitude  $V^*$  and width  $T_n^*$ , thus converting the different amplitudes condition to same amplitude condition.  $T_n^*$  can be derived by solving Equation (1):

$$T_n^* = \text{solve}[p(n) = p_{NLS}(V^*, T_n^*)] \quad (3)$$

Then by substituting  $T_n^*$  into Equation (2),  $p(n+1)$  can be calculated.

$$p(n+1) = p_{NLS}(V^*, T_n^* + t_{n+1}^*) \quad (4)$$

In this way, once  $p(1)$  is known, the evolution of ferroelectric polarization under the pulse sequence can be calculated. Here  $p(1)$  is the fraction of switched volume under the first pulse, which can be directly calculated by NLS model:

$$p(1) = p_{NLS}(V_1, t_1) \quad (5)$$

The overall calculation process is summarized as follows:

$$p(1) = p_{NLS}(V_1, t_1)$$

:

$$p(n) = p_{NLS}(V_n, T_{n-1}^* + t_n)$$

$$T_n^* = \text{solve}[p(n) = p_{NLS}(V_{n+1}, T_n^*)]$$

$$p(n+1) = p_{NLS}(V_{n+1}, T_n^* + t_{n+1})$$

:

where  $V_i$  is the amplitude of the  $i^{\text{th}}$  pulse.

Figure 1(a) shows the fitting results of experimental data (Cu/P(VDF-TrFE)/Cu ferroelectric capacitor) with the NLS model under different electric field strengths [10]. By dividing an arbitrary voltage pulse into short rectangular pulses, each with an approximately constant amplitude, the multi-pulse switching model described above could be utilized, and the simulation results of the polarization change with the external electric field at different frequencies are shown in Figure 1(b). The good fitting between the multi-pulse switching model and the experimental data indicates that the multi-pulse switching model can accurately describe the FTJ switching process.

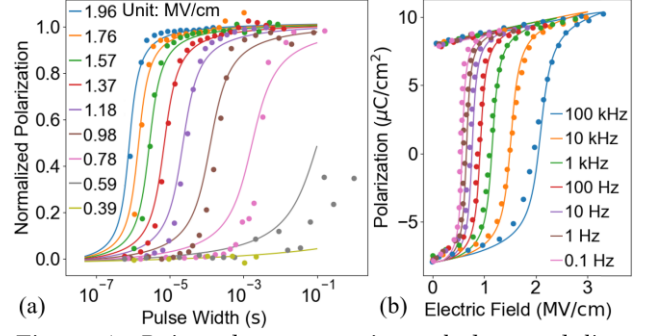


Figure 1: Points denote experimental data and lines denote simulation results. (a) Fitting results of the experimental data with NLS model under different electric field strengths. (b) Polarization vs. electric field at different frequencies calculated by the multi-pulse switching model. The experimental data are extracted from Reference [10].

## SIMULATION RESULTS

### Programming Scheme Simulation Results

Simulations of three different FTJ programming schemes were implemented, using the multi-pulse switching model. The parameters of set and reset pulses and the calculation results of FTJ current density are shown in Figure 2. It can be seen that the programming scheme with increasing pulse amplitude yields the best linearity and symmetry.

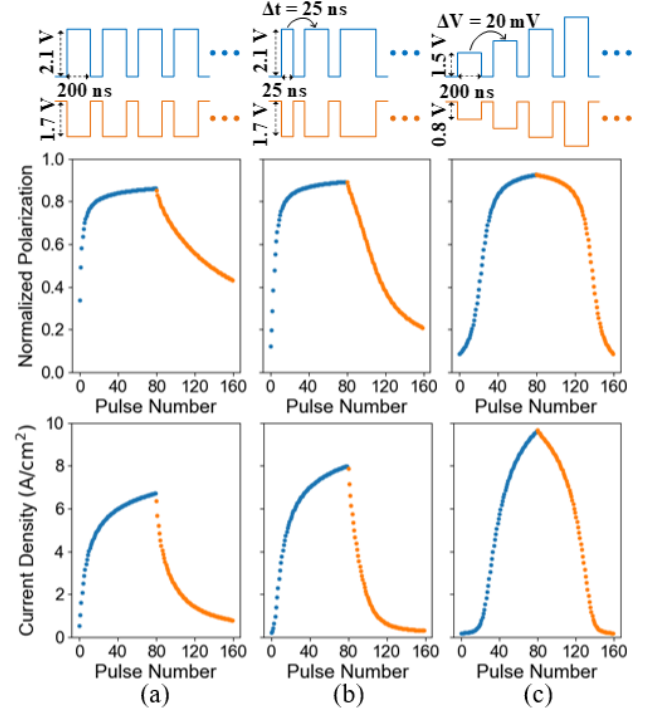


Figure 2: Polarization and current density vs. ordinal number of pulses with different programming schemes: (a) identical pulses; (b) increasing pulse width; (c) increasing pulse amplitude. Pulse amplitudes are reduced in reset

process to improve the linearity and symmetry of FTJ.

### Neural Network Simulation Results

Utilizing the analog switching characteristics of FTJ under different programming schemes in Figure 2, neural network simulations were performed for handwriting digits recognition on the widely used Mixed National Institute of Standards and Technology (MNIST) database. Figure 3(a) illustrates the structure of the simulated multi-layer perceptron of  $784 \times 200 \times 10$ . Differential pairs consisting of two FTJ cells were adopted to realize both positive and negative synaptic weights, and the hidden layer was binarized to simplify the hardware implementation [11]. Device fluctuations were introduced in the training process, by renewing the conductance with a stochastic increment of  $\Delta G \times N(1, \sigma)$  at each time when the weight was updated. The simulation results of recognition accuracy with different programming schemes are shown in Figure 3(b). It can be seen that compared with the other two programming schemes, the programming scheme of increasing amplitude pulses gives the highest recognition accuracy of about 90% and the highest tolerance to conductance fluctuation.

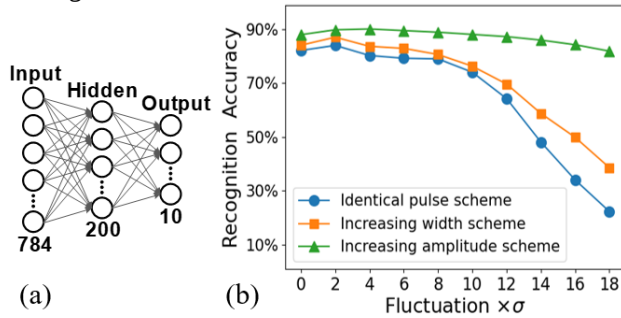


Figure 3: (a) Structure of neural network. (b) Simulation results of recognition accuracy using different pulse programming schemes.  $\sigma$  is the standard deviation, which represents the degree of dispersion of the conductance value drift caused by fluctuation.

### CONCLUSION

To sum up, a comprehensive multi-pulse switching model for FTJ is established, extending the single-pulse NLS model to calculate the change of ferroelectric polarization under a series of arbitrary waveform pulses.

The simulation results of the model were in good agreement with the experimental data at different frequencies. The multi-pulse switching model was further applied to simulations of FTJ-based artificial neural network for MNIST dataset recognition. It was found that using pulses with increasing amplitude achieved the best recognition accuracy up to 90% and the highest tolerance to conductance fluctuation compared with the other two schemes. The developed multi-pulse switching model of FTJ provides a useful guidance for device optimization and also neural network application in the future.

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### REFERENCES

- [1] J. Von Neumann, "First Draft of a Report on the EDVAC," *IEEE Annals of the History of Computing*, vol. 15, no. 4, pp. 27-75, 1993, doi: 10.1109/85.238389.
- [2] Y. Li *et al.*, "Oscillation neuron based on a low-variability threshold switching device for high-performance neuromorphic computing," *Journal of Semiconductors*, vol. 42, no. 6, p. 6, 2021, doi: 10.1088/1674-4926/42/6/064101.
- [3] P. Yao *et al.*, "Fully hardware-implemented memristor convolutional neural network," *Nature*, vol. 577, no. 7792, pp. 641-646, 2020, doi: 10.1038/s41586-020-1942-4.
- [4] M. A. Zidan, J. P. Strachan, and W. D. Lu, "The future of electronics based on memristive systems," *Nature electronics*, vol. 1, no. 1, pp. 22-29, 2018, doi: 10.1038/s41928-017-0006-8.
- [5] R. Guo, W. Lin, X. Yan, T. Venkatesan, and J. Chen, "Ferroic tunnel junctions and their application in neuromorphic networks," *Applied Physics Reviews*, vol. 7, no. 1, p. 011304, 2020, doi: 10.1063/1.5120565.
- [6] A. Chanthbouala *et al.*, "A ferroelectric memristor," *Nature materials*, vol. 11, no. 10, pp. 860-864, 2012, doi: 10.1038/nmat3415.
- [7] Y. Xi *et al.*, "In-Memory Learning With Analog Resistive Switching Memory: A Review and Perspective," *Proceedings of the IEEE*, vol. 109, no. 1, pp. 14-42, 2020, doi: 10.1109/JPROC.2020.3004543.
- [8] G. Bertotti and I. D. Mayergoyz, *The Science of Hysteresis: Mathematical modeling and applications*. Academic Press, 2006.
- [9] A. K. Tagantsev, I. Stolichnov, N. Setter, J. S. Cross, and M. Tsukada, "Non-Kolmogorov-Avrami switching kinetics in ferroelectric thin films," *Physical Review B*, vol. 66, no. 21, p. 214109, 2002, doi: 10.1103/PhysRevB.66.214109.
- [10] W. J. Hu *et al.*, "Universal ferroelectric switching dynamics of vinylidene fluoride-trifluoroethylene copolymer films," *Scientific reports*, vol. 4, no. 1, pp. 1-8, 2014, doi: 10.1038/srep04772.
- [11] H. Wu *et al.*, "Device and circuit optimization of RRAM for neuromorphic computing," in *2017 IEEE International Electron Devices Meeting (IEDM)*, 2017: IEEE, pp. 11.5. 1-11.5. 4, doi: 10.1109/IEDM.2017.8268372.