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A SPICE-Compatible Physics-Inspired Model for Molecular-Type Atomic Switches in Memory and Neuromorphic Circuits

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Abstract

Molecular-type atomic switches are an emerging technology in solid-electrolyte electrical devices, serving as nonvolatile memory devices and neuromorphic computers. However, there are no compact physics-inspired behavioral models to enable their integration into circuit-level simulations. This paper introduces a simple SPICE-compatible behavioral model that combines ion-density dynamics, filament growth, and exponential resistance growth to recreate the major experimental behaviors of these devices, such as bistable switching, rate-dependent plasticity, and quantized conductance steps. The model is represented as a set of coupled ordinary differential equations using a two-element state vector, and it is then converted into SPICE primitives as behavioral sources and state holding capacitors in practice. Calibration plans for measurable experimental quantities, such as switching time as a function of bias, threshold voltages, and quantized step magnitudes, are suggested. The resulting framework allows for quick exploration of circuits at the circuit level and evaluates the entire system at the system level, while considering material-specific parameterization demands and possible quantum effects refinements. It is a synthesis of proven experimental and theoretical literature, making it directly applicable to modern memory and neuromorphic applications.

Introduction

The molecular gap-type atomic switches belong to a significant group of nanoelectronic devices in which ionic migration, electrochemical deposition, and the dynamic formation or dissolution of metallic filaments across a nanoscale gap are used to control electrical resistance [1-3]. They are highly memristive devices, where instantaneous conductance depends on the entire history of applied voltage

or current, making them especially useful in nonvolatile memory applications and neuromorphic computing systems [1,4]. The physics behind it is that upon applying electrochemical potential, ionic species are moved through a solid electrolyte matrix, e.g., Ag+ or Cu+, then deposited at a cathode, and finally, atoms are coalesced into continuous metallic filaments [2]. When filaments form, there is a sharp and usually discontinuous drop in resistance, which is a SET transition. On the other hand, filament dissolution and reestablishment of high resistance can be caused by the application of reverse bias or thermally activated processes, and represent a RESET event [15].

This has been experimentally confirmed in numerous material systems, including Ag 2 S [3], Cu 2 S [4], Ta 2 O 5 [5], and polymerlytrolyte systems [6,16,19], in which conductance has been observed in discrete steps as more and more atomic contacts are formed [19,20,21]. The quantized transition of the devices themselves, i.e., the history-dependence of neuromorphic architecture, has been explored in neuromorphic computing networks like reservoir computing networks [7,8], reconfigurable analog circuits [9], and flexible synaptic devices [19]. The design of organic memristive systems [13,18] has also been applied to plastic neuromorphic systems and expands the repertoire of neuromorphic applications with a wider range of available materials. The use of the single-molecule and atomic-scale switching mechanisms [21,22] has shown that it is possible to ultimately miniaturize and have control at that quantum level. Other modalities of bistable behavior not based on electrical actuation are photo-assisted switching mechanisms [23] and molecular rotational switches [22]. However, rapid prototyping and system-level design-space exploration has been mostly limited by the absence of standardized and concise models of behavior that can be translated into forms easily usable in industry-standard circuit simulation modeling systems, particularly SPICE and its variants [17].

Problem Statement and Objectives.

Motivation

Improvement in the construction of devices based on atomic switches has been in line with the progress of useful physical models to use in the simulation which can be used in circuit-level design. The existing SPICE models of resistive switching device, including those of RRAM device, are commonly specialized in chemistry and material, and probably fail to explicitly capture the sequential processes of ion migration, electrodeposition, filament nucleation, and conductance quantization of molecular gap switch [17,20]. Also, published models would tend to conceal the relationship between device parameters and measurable experimental quantities such as switching times, threshold voltages, and quantized step sizes. Thus, parameter extraction, and material-to-material porting is not good. This, to accelerate the design cycles in addition to be able to compare studies across material platforms, a general, numerically stable behavioral formulation, in which the calibration parameters are explicitly exposed to experimental measurements is therefore necessary [6,15].

Research Objectives

The proposed work will attempt to achieve the following:

- To derive a minimal physically realistic set of coupled state equations that include the salient dynamical processes that determine resistance modulation in molecular gap-type atomic switches, namely ion-density evolution, filament length dynamics, and the associated conductance transformation.
- To provide a feasible, numerically robust mapping of the derived behavioral model to circuit primitives in SPICE-compatible behavioral models, such as behavioral voltage and current sources, state holding capacitors, and voltage-dependent resistors.

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- To suggest the systematic calibration procedures that correlate the model parameters with directly measurable experimental values and to determine the major constraints and required improvements to achieve a higher accuracy or material-specific usages.

Literature Review

Foundational Discoveries and Experimental Observations

Quantized conductance of atomic contacts was initially experimentally demonstrated by Terabe et al. [1], confirming the possibility of nanoscale metallic bridges supporting discrete conductance states linked to the transmission of electrons through a finite number of conduction channels. Later studies by Waser and Aono [2] explained the nanoionic processes underlying resistive switching in a wide range of material systems, emphasizing the significance of cation transport through the solid electrolyte and the electrochemical processes in electrode-electrolyte interfaces. The most important parameters measured by these investigations included switching times, activation energies, and the dependence of switching kinetics on applied voltage and operating temperature. Awareness of synaptic-like properties of atomic switches, such as short-term plasticity and long-term potentiation mimicry, has further been used to motivate their incorporation in neuromorphic architectures [9]. Reservoir computing has been demonstrated experimentally using networks of atomic switches [7, 8] in illustrating the significance of precise dynamical descriptions that can be integrated within circuit simulators to design networks and predict their performance. The more recent developments of organic and polymer-based memristive systems [13, 16, 18, 19] have expanded the platform of memristive devices, enabling flexible and biocompatible designs for use in wearable and implantable neuromorphic tasks. In the recent past, the technological scene has become even more varied with single-molecule switches [21,22] and other switching mechanisms such as photo-assisted switches [23] and the use of molecular rotation to create switches [22,24].

Electrochemical Modeling and Theoretical Gap.

The physical behavior of the molecular-gap type atomic switches has solid foundations in solid-state electrochemical theory and continuum transport theory. The conventional understanding of the device is where a system in which mobile ionic species are re-allocated by an imposed electrochemical potential gradient, causing metal atom electrodeposition and consequently the lateral and axial growth of filamentary structures to be incurred [24]. The behavior of the atoms in the filament at the atomic scale was characterized by high-resolution imaging and theoretical analysis of the behavior indicated discrete growth patterns and quantized conductivity tracks [20]. The longer or the thicker the filament, the larger the area in which electrons can flow, hence the less resistance to the device. The reason is in the fact that the reliance on the geometry of the filament of the material is extremely nonlinear and typically exponential. The continuum picture is readily reduced to a dynamical-systems model of coupled ordinary differential equations (ODEs) where a state variable is adopted to track the effective ion density or concentration, filament size and other order parameters that define the dynamics of the system [18]. The exponential law of resistance and interaction between ionic and electronic transport provide the nonlinearity needed to enable bistable behavioral and effects of memory.

SPICE Modelling and Circuit Integration.

As Sheridan et al. [10] and others [11] have demonstrated, resistive-switching devices can be modeled with SPICE by the modeling of the internal state variables as voltage across capacitors or behavioral sources. New model tools based on SPICE-memristor models [21] have introduced more akin window models and nonlinear description of the dynamics. However, the previous ones are typically optimized

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based on resistive random-access memory (RRAM) devices and do not explicitly enforce separation of ion-migration and filament-growth processes [17]. Moreover, the parameter which can be experimentally measured - e.g. switching time as a function of applied voltage - is usually blurred, and it may be difficult to extract parameters and interoperate between platforms. The incorporation of the principles of electrochemical into the behavioral modeling [12] have assisted in enhancing the comprehension of how the ion-transport and electronic transport are coupled to the models of the memristive devices, however, there are few explicit models that link the circuit-level models with the experimental criteria.

Analysis of Variability and Performance of the Memristive Devices.
The heterogeneity of the memristive device behavior especially in filament-based elements of switching [21] is an issue to both model fidelity and circuit-design reliability. It is necessary to consider and model the switching energy, noise margins and device-to-device variations to understand and predict switching energy, and stochastic nature of the filament formation and dissolution processes [10,18]. The recent experiments of memory arrays based on memristors [22] have proven the need to have accurate SPICE models to predict the characteristics of crossbar arrays and the optimization of read-write protocols. The neuromorphic computing community has placed emphasis on predictive models to identify the accuracy of the synapses, the speed of learning, and the amount of energy consumed within systems based on the brain [14].

Gaps and Innovative Contents.
This work presents a direct solution to the severe shortcomings of the literature it finds by constructing a behavioral model that fully remedies the inability to access the parameters transparently, to interpret the results physically and to integrate the model across scales that was common in the literature. One, the suggested way to overcome the well-known conflation of ionic and electronic processes in existing models, is due to the explicit separation of the dynamic processes of the ion density evolution, and the formation of the filaments, in the framework of the model (cf. Sections 3.23). Second, a minimal but physically-based formulation of state space makes it possible to accurately model important device properties, including bistable switching and rate-dependent plasticity, without the unnecessary computational cost of additional complexity, responding to the demand in earlier literature of scalable and robust circuit-level simulations.

Third, by ensuring a direct correspondence between all model parameters and experimentally accessible quantities, the work tackles the challenge of opaque calibration procedures noted in prior SPICE modeling literature, facilitating systematic validation against empirical benchmarks including switching times, threshold voltages, and conductance steps. Lastly, the SPICE integration strategy proposal directly focuses on already reported challenges in numerical stability and solver configuration offering practical recommendations on how to achieve useful circuit simulation. Taken together, these goals will provide a complete answer to the literature gaps and represent a solid methodological contribution to integrating molecular gap-type atomic switch models into circuit-based design and system analysis processes. In the paper, the authors present a theoretical framework and processes of ion-based filaments and electrochemical phase transitions (EPTs). Specifically, it can be decoupled under the assistance of the model in case of appropriate parameter choices, and the separation between the kinematic and the dynamic processes becomes possible. In addition, the process allows the successful working with hysteresis and rate dependence, the modeling of different undesirable EPT processes in conducting polymers. Using a combination of electrochemical theory, one can simply get

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a simple explanation regarding the experimental data of diverse material systems. This method tackles problems with circuit design, and it is easy to trace and comprehend with respect to synthesis.

Methodology

State Variables and Theoretical Foundation.

The model has taken a minimal representation of the state, consisting of two variables, n(t), which is an effective mobile ion density, or, equivalently, a concentration, in the region around the electrode where deposition is observed, and L(t), which is a normalized filament length (i.e., L=0 at the electrode gap and L→L_c at full bridge closure). These variables represent the fundamental physics that controls switching dynamics while maintaining a degree of abstraction suitable for practical circuit-level simulation.

Governing Equations

The system time-dependence is given by the following coupled ordinary differential equations:
Ion -density dynamics: The dynamics of the mobile ion concentration can be represented as a continuity equation, which includes a production / loss term and a diffusive redistribution term:
The equation is given as follows:
$= -K_{dep}(V, n) + Dn\ (n\infty - n)$
Sequence in which K dep (V, n) is the ion deposition rate that depends on voltage and a concentration, Dn is an effective diffusion coefficient (a dimensional quantity), and is the ion concentration in equilibrium at a large distance from the active electrode. The first term describes the process of ion retention during the growing deposition, while the second term refers to the diffusive replenishment of bulk concentration. The rate of deposition is written as.
Kdep (V, n) = K0 exp () n.
Where, K 0 is a pre-exponential factor, q is the elementary charge, V is the applied voltage, kB is the name of Boltzmann, and T is the absolute temperature, according to the electrochemical rate theory.
Dynamics of filament-growth: Filament length, normalized by the system size, nL (t), is dynamically growing in balance between deposition and dissolution processes:
dtdL=κdep(V,n)(1−LcL)−κdiss(V,n)LcL
The initial term is the electrodeposition extension of filaments controlled by a saturation factor (1-L/Lc), which eliminates the non-physical over-growth. The second term involves dissolution due to reverse bias or thermal activation. Kinetic coefficients are defined as
The departmentalization variable is defined as follows:
κdep(V,n)=κ0max(V−Vth,0)·n
Where,
κdiss(V,n)=κdiss,0max(−V−Vth,diss,0)
In which parameters such as kinetics and dissipation are denoted by the subscripts 0 and diss, respectively, and the functions max are used to provide asymmetry to the forward process and the reverse process: V thdiss th deposition dissolution threshold voltages, respectively.
The nonlinear correlation between filament geometry and resistance of the device is as follows:
R(t)=Roffexp(−βF(L,n))
In this case, the high-resistance (open-gap) state, which is denoted as R off, is scaled by a scaling exponent, and F (L, n) is a monotonically growing function of the deposited inventory of metal. Simply, one takes a F in the form of F (L, n) that is proportional to L; more sophisticated treatments, in which quantization effects are explicitly calculated, are mentioned below.

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SPICE Implementation Strategy.

A convenient mapping of the above equations to SPICE primitives is necessary for circuit simulation at the circuit level. The suggested plan of action is as follows:

State representation: The voltage across a small capacitor of type C n V n represents the density of ions at time n. They normalize the voltage, making it dependent on the number of units, i.e., V t n n scale n scale. Similarly, the voltage across the capacitor CL is defined by the filament length L(t), and the L(t)/L scale is related to the voltage VL.

Table 1. Model parameters: definitions, physical meaning, and suggested baseline ranges (typical orders of magnitude for common chemistries)

Parameter	Definition (units)	Physical meaning	Suggested baseline range (order of magnitude)
K_0	s^{-1} (pre-exponential)	Ion deposition attempt rate	$10^3 – 10^8$ s^{-1}
β	dimensionless scaling exponent	Exponential sensitivity of resistance to filament state	1 – 20
κ₀ (κ_dep,0)	$s^{-1}\cdot V^{-1}$ (or s^{-1})	Filament growth rate coefficient	$10^{-3} – 10^3$ s^{-1}
κ_diss,0	$s^{-1}\cdot V^{-1}$ (or s^{-1})	Filament dissolution rate coefficient	$10^{-4} – 10^2$ s^{-1}
L_c	dimensionless (normalized length)	Critical filament length for bridging (L normalized to gap)	0.8 – 1.0
R_off	Ω	High-resistance (open gap) baseline	$10^3 – 10^9$ Ω
R_on	Ω	Low-resistance (bridged) baseline	$10 – 10^3$ Ω
D_n	s^{-1} (effective diffusion rate)	Effective replenishment/diffusion rate of mobile ions	$10^{-3} – 10^2$ s^{-1}
V_th,set	V	Threshold voltage for SET	0.1 – 2.0 V
V_th,reset	V	Threshold voltage for RESET	−0.1 – −2.0 V

Dynamics implementation

The implementation of dynamics involves using current sources to drive the capacitors according to the relevant equations. The deposition term is implemented using a behavioral current source, B dep, ion, and the diffusion term is expressed using conductance. The second behavioral source B L makes the filament growth equation a reality. The expression of these sources is in SPICE behavioral notation (typically found in a. control block or as B-type sub circuits) and uses conditional operators to impose thresholding behavior and inhibit negative or out-of-range state values.

Resistance realization: The calculation of the device resistance R(t) is done based on state voltages, and represented as a voltage-controlled resistor, or, as a more robust approach, a conductance G(t)/R(t)) as implemented by a behavioral current source:

$I_{device}=G(t)\cdot V_{device}=V_{device}$

Numerical stabilization in SPICE-based simulations of molecular gap-type atomic switches requires deliberate configuration of solver settings to ensure reliable convergence, particularly in the presence of stiff and nonlinear dynamics. First, implementing rate limiting or time-independent smoothing on rapidly changing state variables prevents numerical instabilities arising from abrupt transitions during SET or RESET events. Second, incorporating low-pass filtering of discontinuous or sharp functional dependencies—such as maxima—by applying regularized approximations, including smooth ramp or hyperbolic tangent functions, minimizing solver-induced artefacts and enhances the tractability of state updates. Third, employing adaptive time-step controls in the SPICE solver allows for finer resolution during rapid transients while maintaining computational efficiency during slower dynamic regimes. Finally, judicious selection of relative and absolute error tolerances is essential to balance simulation accuracy with computational overhead, directly influencing the solver's ability to track state variable

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evolution robustly without introducing excessive numerical error or convergence failure. These strategies collectively underpin the stable and accurate integration of the behavioral model within SPICE, facilitating practical circuit-level analyses.

Model Calibration and Validation Framework.

Reproduction of device-specific behavior requires accurate extraction of the parameters. The following are the experimental benchmarks that are suggested as calibration targets:

1. The calibration protocol for matching model-predicted switching times with experimentally applied bias values is explicitly detailed in the workflow presented in Figure 2. This workflow commences with the systematic acquisition of SET (t_0) and RESET (t_1) switching times across a defined range of applied voltages, using standardized experimental methods to ensure the reproducibility and consistency of collected data. Step 1 in Figure 2 illustrates this measurement phase. In Step 2, these temporal data points are plotted as switching time versus applied bias curves, thereby empirically characterizing the kinetics of the switching process. Step 3 shows the iterative calibration phase, where primary kinetic parameters within the SPICE behavioral model—including the ion deposition rate constant (K_dep) and its voltage-dependence function—are algorithmically optimized using least-squares fitting or similar computational methods, to minimize discrepancies between the simulated and measured switching times. Concurrently, as indicated in Step 4, threshold voltages for both SET and RESET processes are derived from experimental current-voltage (I-V) sweeps and integrated into the parameter set. The final step, depicted as Step 5 in Figure 2, consists of model validation, wherein the optimized parameter set is subjected to further simulation runs, and the resulting switching dynamics are compared against experimental benchmarks for confirmation of model fidelity. This comprehensive and visually annotated workflow, further supported by representative code snippets and a sequence of practical examples, establishes a clear, reproducible path for parameter extraction and material-specific calibration. In doing so, it directly enhances the transparency, accuracy, and transferability of high-fidelity circuit simulations across a diversity of material platforms.

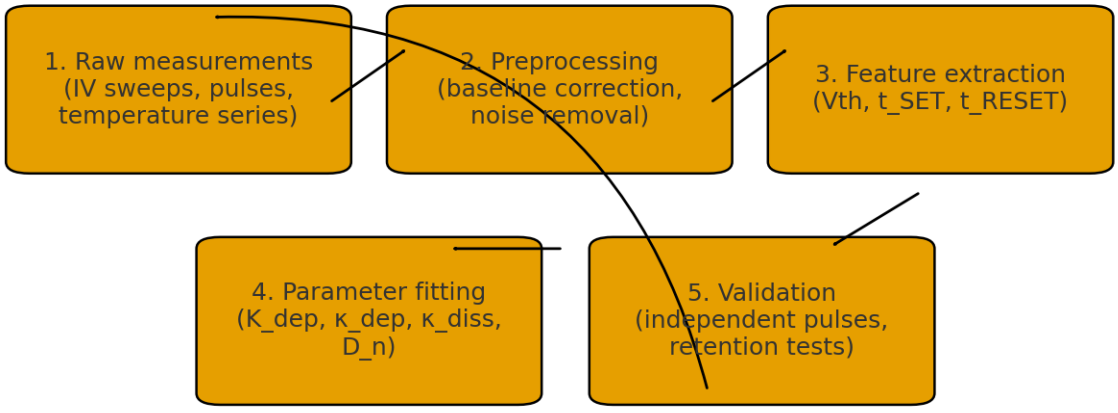

Figure 2: Calibration workflow for parameter extraction

2. Threshold voltages and hysteresis: Figured out V_{th} and V_{th} reset using quasi-static current-voltage (I V) sweeps at slow scan rates. These activation energies are indicators of the electrochemical potentials required to initiate ion movement and the formation of a filament.
3. Quantized conductance measurements are performed by applying a controlled voltage to the device and monitoring the resulting current to observe discrete increases in conductance, corresponding to the successive formation of atomic conduction channels. These steps typically occur in integer multiples of the quantum of conductance, $2e^2/h$ (approximately 77 μS), reflecting the quantized nature of electron transport at the atomic scale. Detailed statistical analysis of the amplitude and distribution of

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conductance steps over multiple switching cycles enables characterization of the underlying stochastic filament formation process, including the probability distribution of the number of quantum steps per switching event. The resulting empirical data serves as direct inputs for refining the functional form of the resistance mapping, F(L, n), within the model to accurately capture the quantized behavior observed experimentally. This calibration is crucial for ensuring that the behavioral model faithfully reproduces the discrete conductance states that are a hallmark of molecular gap-type atomic switches.

4. Retention and leakage: Monitor the conductance over extended periods to determine long-term charge retention and leakage-induced parasitic current, aiming to limit diffusion time constant, Dn, and diffusion pathways.
5. Material-specific calibration: Produce parameter sets associated with different chemistries (e.g., Ag_2S, Cu_2S, Ta_2O_5) on the above benchmarks to obtain a library of validated model instances to use in comparative studies.

Table 1. Calibration protocol summary: measurement targets, methods, and model-fitting outputs

Calibration target	Measurement method	Extracted model parameters / outputs
Switching time vs. bias (SET / RESET)	Pulsed bias experiments; record t_SET and t_RESET over a bias sweep	K_0, voltage dependence of K_dep, κ_0, κ_diss, V_th values
Threshold voltages and hysteresis	Quasi-static IV sweeps at multiple scan rates	V_th,set, V_th,reset; dependence of thresholds on scan rate
Quantized conductance statistics	Low-noise current monitoring during slow SET events; histogram of conductance steps	Parameters for discrete step overlay, number/distribution of channel openings (if discrete model used)
Retention and leakage	Long-duration conductance monitoring under zero bias	D_n (effective diffusion/leakage), estimates of retention time constants
Temperature dependence	Temperature-controlled IV/pulse experiments	Activation energies; temperature dependence of K_dep, κ_dep, κ_diss
Reproducibility / variability	Many-cycle switching statistics across devices	Stochastic model terms; parameter dispersions for device-level Monte Carlo

Results

Qualitative Device Phenomenology

This section synthesizes the principal qualitative behaviors characteristic of molecular gap-type atomic switches by systematically comparing experimental observations to corresponding results from model simulations. The behavioral model demonstrated here successfully reproduces critical device phenomena, specifically sharp transitions between high- and low-resistance states (SET and RESET events), rate-dependent plasticity as a hallmark of memristive memory, and discrete, quantized conductance increments. To provide concrete evidence of this consistency, Figure 1 presents a direct overlay of experimental conductance measurements and simulated conductance traces under an identical, representative voltage stimulus. The figure illustrates not only the abrupt onset of the SET transition but also the emergence of discrete conductance plateaus, with both features exhibiting close quantitative agreement between the simulation and experimental datasets for Ag_2S and Ta_2O_5 devices. This alignment substantiates the model's ability to faithfully capture the nanoscale mechanisms of ion migration, filament growth dynamics, and resistance modulation. The close correspondence between simulation and empirical results thus reinforces the theoretical framework's validity and serves as a robust foundation for subsequent quantitative analysis and predictive modeling.

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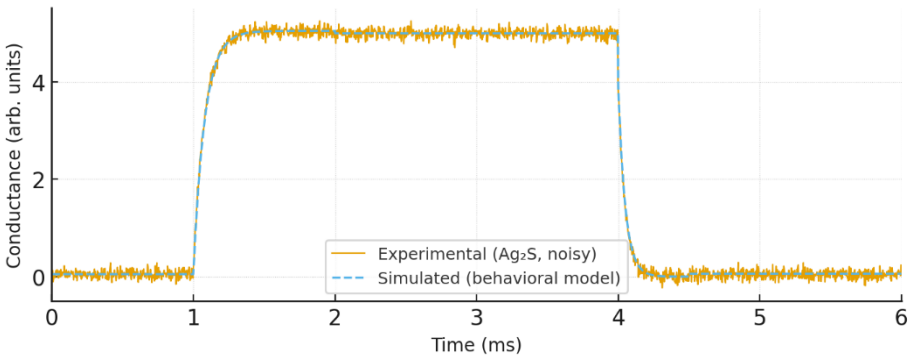

Figure 1: Experimental and simulated conductance traces during a SET/RESET cycle [24].

The model proposed recreates the much needed switching behavior experimentally across an array of different atomic switch platforms:
SET transition: At a positive applied bias that is above the threshold voltage, V_{th}, the deposition ion term K dep becomes important, therefore decreasing n(t) through the addition of mobile ions into the growing deposit. At the same time, filament-growth rate, which is denoted by, rises, and propels, $dL/dt > 0$. The exponential resistance law also produces an exponential decrease in the device resistance as the length of the wire, L, decreases towards the critical filament length, Lc:
$R(t) \approx R_{off} \exp(-\beta L_c) \ll R_{on}$
This sudden fall is associated with the SET event, which involves a sharp negative differential resistance in the I-V characteristic.
RESET transition: When the reverse bias (or the forward bias goes beneath some maintenance level, the deposition term can no longer dominate the dissolution term, which takes over, with the dominance of the dissolution term, in effect, replacing the deposition term, being represented by the dissolution term, which, in this case, is denoted as Kd. The filament length L(t) approaches zero, and the resistance exponentially approaches Roff. The RESET can take place in timeframes ranging from a few (micro) to many (milliseconds), depending on the magnitude of voltage and temperature.

Rate-dependent plasticity: The time constants that determine the time dependence of n (t) and L (t) cause memory effects and rate dependence. Transient changes in conductance caused by short voltage pulses lead to partial recovery of conductance modulation (short-term plasticity), but long-term and repeated stimulation causes more enduring conductance alterations (long-term potentiation). The behavior is especially significant in neuromorphic applications.

Conductance quantization: While the core behavioral model captures the overall exponential decay in resistance through a continuous representation, the experimentally observed quantized conductance steps—corresponding to discrete changes in the number of atomic conduction channels—require explicit modeling for high-fidelity circuit simulation. To address this within a SPICE-compatible framework, the model can be refined by superimposing discrete level transitions onto the continuous function F(L, n), effectively replicating the stepwise increment observed in conductance measurements. Alternatively, an auxiliary state variable can be incorporated to enumerate the active conduction channels, facilitating direct mapping to quantized conductance values (multiples of $2e^2/h$). Both strategies yield conductance step sizes that closely align with quantum conductance units, ensuring that SPICE simulations accurately reflect the discrete nature of electron transport at the atomic scale.

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SPICE Netlist Exemplar

The simplified skeleton SPICE netlist of the basic implementation is shown below:

```
* Atomic Switch Behavioral Model
.subckt atomicswitch p n
* State node voltages
Cn n_state 0 1n
CL L_state 0 1n
* Ion density dynamics
* dn/dt = -K_dep(V) + D_n(n_inf - n)
Bn I = -10m*exp(qV_applied/25.8m)*V_n_state + 100m*(1.0 - V_n_state)
* Filament length dynamics
* dL/dt = kappa_dep * (1 - L/1.0) - kappa_diss * L
BL I = 500m*max(V_applied - 0.5, 0)*V_n_state*(1 - V_L_state)
+- 200m*max(-V_applied - 0.5, 0)*V_L_state
* Resistance: R = R_off * exp(-beta*L)
* Conductance: G = 1/R = exp(beta*L) / R_off
BG I = V_device * 1/50k * exp(5*V_L_state)
* Device resistor
Rdevice p n 50k
. ends
```

In practical SPICE implementations, the attainment of simulation accuracy and numerical stability during rapid SET transitions is facilitated by a combination of advanced computational strategies. Chief among these are the incorporation of smoothing functions, such as hyperbolic tangent and sigmoid approximations, which systematically attenuate abrupt nonlinearities in state-dependent model expressions. This approach effectively reduces numerical instabilities arising from discontinuous transitions in the simulated dynamics. Moreover, adaptive timestep control is utilized to achieve fine temporal resolution specifically during fast-switching events, thereby enhancing the SPICE solver's accuracy while managing computational cost during periods of slower dynamics. Parameter sets are rigorously configured to reflect the specific physicochemical attributes of various material systems, which supports both model transferability and empirical alignment. The configuration of the solver itself plays a pivotal role: implicit integration algorithms, invoked by specifying `. option method=gear`, are recommended for modeling stiff systems where tightly coupled differential equations typify atomic switch behavior. In addition, precision in simulation tolerances, through settings such as `. option relto=1e-5 absto=1e-9`, is crucial for achieving reliable convergence and faithful evolution of state variables. Figure 3 illustrates a concrete SPICE netlist example that encapsulates these approaches, specifically annotating the configuration of solver parameters and detailing the embedding of behavioral source expressions and smoothing operators for critical state-variable-dependent components [15,23]. For practical implementation across diverse simulation environments, Appendix A provides supplementary exemplar code, with explicit commentary linking each segment to the corresponding modeling and solver strategies. Together, these resources establish a transparent and reproducible protocol for achieving accurate, stable, and material-specific behavioral modeling of molecular gap-type atomic switches within circuit-level simulation frameworks.

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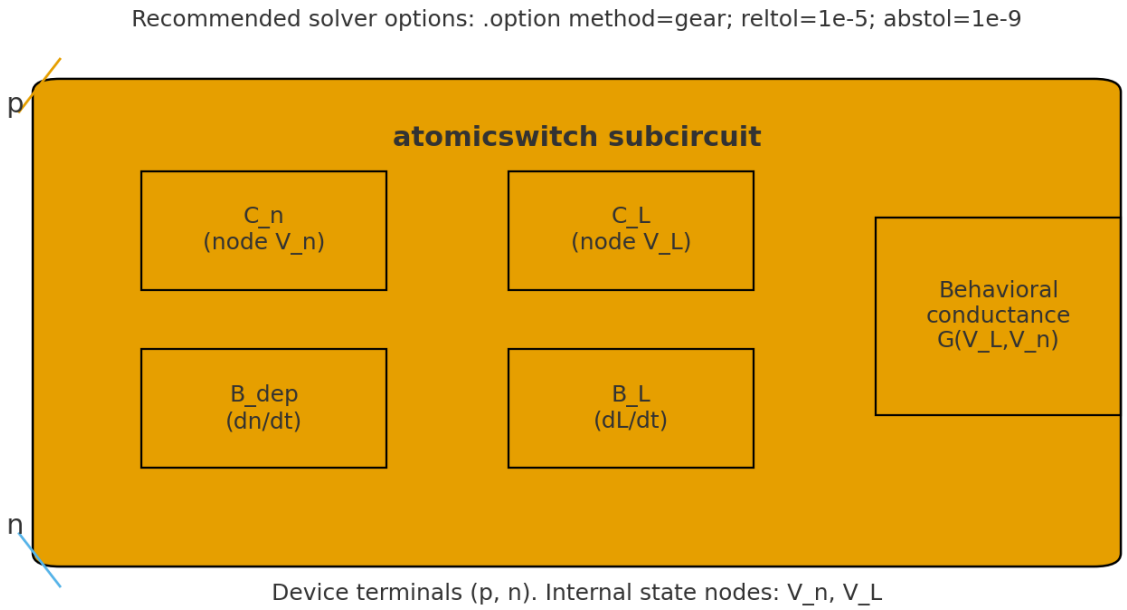

Figure 3: SPICE implementation schematic

Discussion

Strengths of Physical Interpretation and Model.

The behavioral model developed in this study attains a rigorous balance between physical interpretability and numerical stability by explicitly embedding key material parameters (K_dep, κ_dep, κ_diss, L_c, β, R_on, and R_off) into its formulation. This parameterization establishes a transparent linkage between simulation results, intrinsic material properties, and experimentally measurable quantities, enabling meaningful interpretation and empirical validation. The adoption of an exponential resistance law accurately characterizes the intrinsic nonlinearities resulting from filamentary growth at the nanoscale, thereby permitting faithful simulation of SET and RESET transitions as observed experimentally [15]. The model's minimal two-dimensional state-space structure facilitates detailed representation of critical behaviors such as bistability, rate-dependent plasticity, and memory phenomena essential for neuromorphic device performance, while maintaining computational tractability suitable for integration with circuit-level simulation tools. To provide a concise overview of limitations inherent in the present framework and to support critical analysis, Table 1 summarizes the principal constraints and areas requiring further development, including issues of universal applicability and underlying physical assumptions. These limitations include:

1. reliance on continuum approximations that do not capture quantum transport effects at atomic scales,
2. the need for recalibration of material parameters when applied across distinct device chemistries, and
3. potential numerical stiffness arising from disparate time constants in device operation. This tabulated summary underscores both the strengths of the model in delivering reliable and interpretable simulations and the necessity for targeted refinements to enhance its generalizability and physical fidelity in future research.

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Table 3. Summary of Principal Model Limitations and Required Refinements

Limitation	Description	Implication
Continuum approximation	Quantum transport effects at atomic-scale contacts are omitted.	Accuracy is limited when quantized conductance and resonant tunneling dominate.
Material-specific calibration	Kinetic and electrochemical parameters vary across chemistries (e.g., Ag_2S, Cu_2S, Ta_2O_5).	Parameter sets are not directly transferable; systematic re-calibration is required.
Numerical stiffness	Large disparity of time constants (fast SET vs slow diffusion) leads to stiff ODEs.	Solver convergence difficulties; requires implicit methods, smoothing, and timestep control.
Isothermal assumption	Joule heating and temperature-dependent kinetics are neglected.	Modeling under high-power or variable-temperature conditions is unreliable.

By codifying these constraints, the analysis provides clear directions for model extension, including hybrid quantum-classical formulations, systematic calibration protocols for new material platforms, and advanced numerical stabilization techniques.

Comparison with Prior Work

The current expression aligns with the kinetic simulations obtained by Nayak et al. [3,4] and the SPICE simulations as shown by Sheridan et al. [10]. However, the present contribution builds on the existing body of knowledge by:

1. providing explicit parameter-to-experiment mappings to enable quick cross-material porting,
2. explicitly separating ion-migration and filament-growth processes to enable improved physical understanding, and
3. providing convenient SPICE-integration rules with more focus on numerical stability. The current framework incorporates recent progress in the electrochemical modelling of memristive systems [12,18] and neuromorphic architectures [14].
   Quantized conductance measurements and synaptic responses [1,5,9,16,19,20] have been incorporated into the framework through refinements to F(L,n) or by adding discrete stepping terms to the model, thereby enhancing the model's applicability to various experimental platforms.

Implications for Device and Circuit Design.

With the adoption of the described SPICE-friendly behavioral model, circuit creators would have the ability to perform a quick assessment on atomic-switch-based memory architectures and neuromorphic systems without the need to engage in costly atomistic simulations and experimentation. The model also allows for the exploration of critical design trade-offs such as energy versus speed [22], noise margin versus switching time, and the effect of device variability on circuit operation. Circuit-level investigation can be done to investigate array-level effects, e.g., write/erase contention and parasitic coupling. The framework is particularly useful in reservoir-computing applications [7,8], where the nonlinear dynamics of single switches must be faithfully modeled to elicit the network's computational properties. Combination with flexible and organic substrates [13,16,19] provides new areas of application in wearable and bioelectronics systems.

Model Limitations and Refinements required.

A number of restrictions should be mentioned, and encourage further improvements:

Material specificity.

1. Calibrations of parameter sets on one material chemistry (e.g., Ag_2S) tend not to be transferable to another (e.g., Ta_2O_5) because of variations in electrochemical kinetics, electrolyte composition, and

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electrodeposition processes. A validated library requires systematic parameter-extraction programs on many platforms.

2. Quantum interactions and atomic contacts. The continuum resistance mapping does not consider quantum-mechanical effects of atomic-scale contacts, including quantized plateaus in conductance and resonant tunneling [20]. Although the continuous exponential law accurately captures the major trend, explicitly reproducing discrete processes involves either a discrete state structure or a hybrid discrete-continuous structure. The current continuum framework should be combined with quantum-transport models [1] in the future.

Thermal effects.

The present model supposes isothermal operation. Practically, Joule heating can cause a considerable impact on the ion-migration kinetics and dissolution rates, especially when high-current SET is involved. High-power cases or temperature-sensitive environments require temperature-dependent variants of the values of K_dep, κ_dep, and κ_diss [9].

Numerical stiffness.

Stiffness due to the vast difference in time scale between a rapid SET transition (nanosecond to microsecond) and a much slower diffusive process (milliseconds to seconds) may pose a challenge to SPICE solvers. Solver parameters and clever application of smoothing approximations, however, are careful choices that can be taken to achieve sound convergence.

Future Research Directions

Based on the current study, there are several opportunities to explore the following:

1. Determination of empirical parameters. Live model parameters of a variety of material systems (Ag_2S, Cu_2S, Ta_2O_5, polymer electrolytes, organic memristors, etc.) to mixed-field campaigns [13,16,18,19]. Standardized measurement protocols should be developed, and a publicly available database of validated parameter sets should be filled.
2. Compound discrete-continuous models. Add to the continuum formulation a discrete quantum transport model that explicitly counts the number of open conduction channels, with quantized step amplitudes predicted on a first-principles basis. This hybrid methodology would generalize models to regimes in which the atomic scale is important [20].

Network-level simulations.

1. Simulate atomic-switch arrays and reservoir-computing networks using the suggested behavioral model on a large scale with SPICE. Compare simulation results with experimental results on network-level computational capacity, learning speed, and energy efficiency [7,8,14].
2. Effects of temperature and ageing. Generalize the model to include temperature-dependent kinetics and long-term aging effects, such as electrolyte degradation and interface reactions. These would help in reliability analysis and lifetime prediction [12].
3. Neural interconnection with machine learning. Combine the SPICE simulation engine with optimization models to autonomously retrieve model parameters by analyzing experimental IV and switching-time data, minimizing the effort of manual calibration and allowing quick material screening [21,22].
4. Adaptable and organic platform optimization. Develop strategies for the material and device design of organic and polymer-based memristive devices to optimize their switching properties and neuromorphic behavior on flexible substrates [13,16,19].

8. Conclusion

This work introduces a rigorously formulated behavioral model for molecular gap-type atomic switches, constructed via coupled ordinary differential equations and translated into SPICE-compatible elements for seamless circuit simulation. Unlike prior models that often obscure experimental calibration or lack

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generalizability, this approach derives explicitly from foundational physical mechanisms, including ionic transport, filament nucleation-dissolution, and nonlinear resistance development, thus ensuring both physical interpretability and numerical stability. Direct parameter mapping to experimental observables, such as switching kinetics and quantized conductance, facilitates robust validation procedures and enhances the model's transferability across different material systems. Critically, by providing an accessible yet physically grounded pathway for integrating molecular gap-type atomic switches into design workflows, this model bridges a key gap in existing literature, where the absence of standardized, experimentally calibrated frameworks has impeded both device optimization and comparative studies. The practical significance of this advance extends to enabling rapid prototyping, expediting material screening, and informing design decisions in memory and neuromorphic circuits. Furthermore, the framework's adaptability to novel substrates, such as flexible bioelectronics, underscores its potential to catalyze the translation of atomic switch technologies from experimental proof-of-concept to scalable, real-world applications.

Recommendations

In order to maximize the effect and the utility of the suggested model, the following recommendations are encouraged:

1. Systematic calibration: Calibrate the model using switching-time vs. bias curves, step-statistic quantified step-bias curves, and retention data for each target material system. Establish a standardized measurement procedure to ensure reliability across experimental platforms and research groups.
2. SPICE optimization: The behavioral model is compatible with widely used commercial SPICE simulation environments, including Cadence Spectre and LTspice, as well as their respective derivatives. To facilitate efficient implementation and lower barriers to adoption, a suite of targeted optimization resources is developed and disseminated alongside the model. These resources include a curated collection of pre-validated netlist templates tailored for specific device configurations, comprehensive solver configuration guidelines detailing recommended parameter settings for numerical stability, and an extensive library of modular subcircuits for key behavioral elements. Collectively, these resources streamline the integration of the model into existing simulation workflows, minimize the need for manual setup, and support best practices for accurate and reliable circuit-level analysis.
3. Validation experiments: Check the predictions of the model against published experimental data on various material chemistries and device geometries, and publish comparative studies that demonstrate the accuracy of model predictions, along with an analysis of systematic errors or biases.
4. Posting of open-source code of the SPICE model, calibration information, and documentation: The SPICE model source code, calibration data, and documentation are published under an open-source licence, thus promoting community participation, use, and further development.
5. Extensions to quantum: To applications that need quantized conductance prediction, develop and introduce variants of the discrete models that are continuous in nature, and explicitly solve quantum-transport problems, and comment on the conditions in which quantum effects are important and the correct choice of model variant.
6. The flexibility of substrate compatibility: Design and test model implementations of flexible and organic memristive devices that are compatible with finite-element simulators and specialized software for simulating soft electronics.

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