Emerging Memory Modeling Challenges

(Invited Paper)

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***Abstract*—Emerging Memory (EM) is a broad class of memory devices leveraging a wide spectrum of physical phenomena and/or material properties, that go beyond the charge storage concept of more conventional NAND and DRAM technologies. Availability of physical models and simulation tools to understand their behavior, predict performance, engineer materials and cell architecture would be extremely useful for their successful development. However, such tools are not always available because of the diversity and complexity of the physical mechanisms. This paper would like to review the main trends of the on-going modeling and simulation activities in the field of EM, trying to point out what are the needs and challenges for the future.**

I. Introduction

As pervasiveness of integrated circuits continues at a restless pace, demand for memory and storage is continuously increasing. Recent applications such as Artificial Intelligence (AI), Virtual/Augmented Reality (VR) or Internet of Things (IoT) are giving an additional boost to memory/storage need. Indeed, last year the memory sector was the largest and fastest growing segment of the total semiconductor market.

Within the memory segment, DRAM and NAND are by far the major players. Interestingly enough, they lie at the opposite ends of the cost/performance trade-off (Fig. 1), leaving a large gap in between for other technologies to be developed with a business sense. Indeed, over time a large number of alternative memory technologies have been proposed to fill this DRAM-NAND performance gap, also with the ambitious goal to provide an easier path for continued scalability that is becoming more and more difficult for conventional technologies. Although some of them already have a long history behind and may have been used for niche application, their large scale adoption is yet to come. That is why they are still referred to as Emerging Memory (EM).

Development of these EM technologies calls also for a large effort in modeling and simulation to speed-up learning and reduce costs. However, many of these EM technologies require non-conventional modeling approaches, rarely available in commercial TCAD tools, that, therefore, are yet in the development phase.

This paper would like to provide an high level overview of the ongoing modeling activities related to EM, focusing on the storage element of the memory cell. We will start in Sect. II by briefly summarizing the working principles of a few types of selected EM, namely Phase Change Memory (PCM), Resistive RAM (RRAM) and Spin Transfer Torque Magnetic RAM (STT-MRAM) that, at the moment, appear to have the greater potential for industrial application. This will help in pointing out the main issues that their modeling must address both in terms of physical models and simulation framework characteristics. These issues are then reported and discussed in more details in Sect. III grouped in categories common to many types of EM, with the ultimate goal to show what has been done and what is yet to be done in the field of EM modeling.

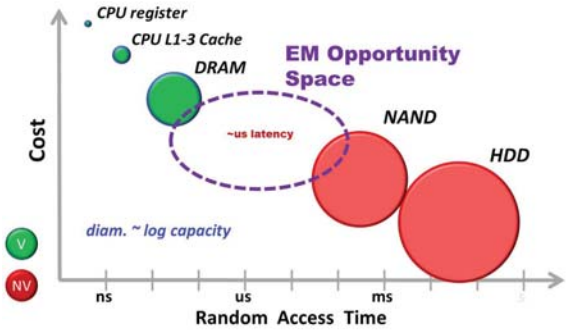

Fig. 1. Cost/performance trade-off and memory hierarchy. The gap in between NAND and DRAM offers an opportunity to EM.

II. Emerging Memory Concepts

A. PCM

PCM storage mechanism is based on the resistivity contrast between the amorphous and crystalline phases of chalcogenide alloys, the most common of which is $Ge_2Sb_2Te_5$ (GST). Amorphization is attained via a high and fast current pulse able to bring the GST above the melting point, and then rapidly quench it down (Fig. 2). Return to the crystalline state is achieved by a lower but longer current pulse raising the temperature in a range where crystal nucleation and growth take place. Notice that nucleation is a stochastic process. In addition to its intrinsically electro-thermal operation, it has been reported recently [1] that, during normal operation, there could be a motion of GST atoms because of high current and temperature, leading to a different alloy composition across the device, which has a fundamental impact on performance and reliability.

B. RRAM

By RRAM we mean a large class of devices whose common feature is the change of their electrical resistance

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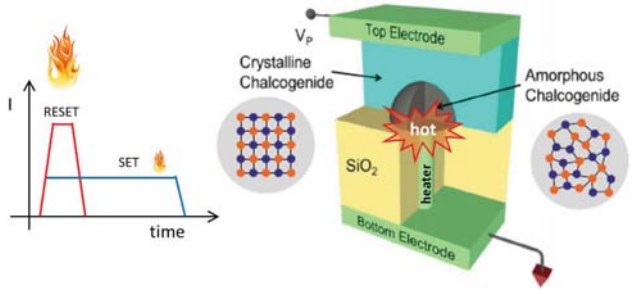

Fig. 2. Schematic PCM operations and device structure. Active region is the amorphous dome surrounding the heater/GST interface that is molten when an high current is flowing through the heater.

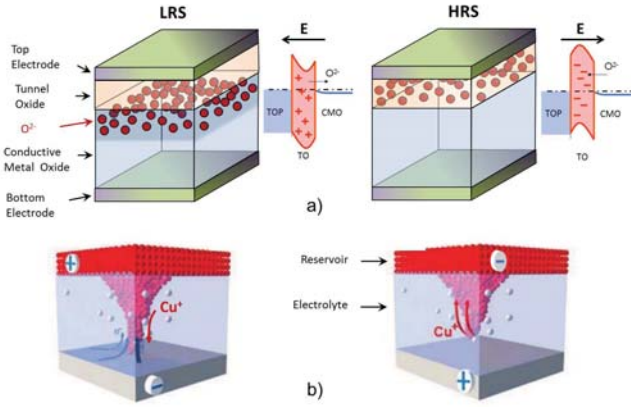

Fig. 3. RRAM schematic with uniform switching (a) or filamentary conduction (b) [2].

(not coming, however, from phase change) upon a properly tailored electrical pulse. A number of mechanisms have been proposed to attain this goal. Some of them feature a uniform switching, where resistance change is coming from the bulk movement of ions/defects changing the barrier height at the active interface (Fig. 3.a). Often, they also imply some field activated chemical reactions to create/remove charged ions/defects. Another class of RRAM is instead based on filamentary conduction (Fig. 3.b). After an initial forming operation that creates the filament, device resistance is modulated by the rupture/reformation of such a filament driven by the electric field. Under one polarity, the field moves the ions along the filament to close the gap with the inert electrode resulting in a low resistance. Reversing the field direction, ions move back creating a gap responsible for the high resistance. Notice that again some chemical reaction is needed to create the moving ions, as well as temperature is crucial to activate ion mobility and reaction rates.

C. STT-MRAM

The latest MRAMs are mostly based on Magnetic Tunnel Junction (MTJ) featuring a large magnetoresistance effect. MTJ are made by two layers of ferromagnetic material separated by a thin insulator (Fig. 4.a). One layer, called the Pinned Layer (PL), has a fixed magnetization. The other, named the

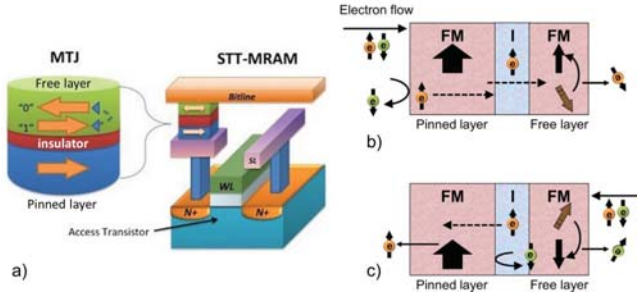

Fig. 4. a) STT-RAM schematic structure. The storage element is the MTJ. Set (b) and reset (c) operation by spin transfer torque [3].

Free Layer (FL), can switch its magnetization from the parallel (P) to the antiparallel (AP) polarization with respect to PL. In the P state, electrons can tunnel more easily through the insulator resulting in a lower resistance in comparison to the AP state. Among the different types of MRAM, STT-MRAM appears to be the most promising [3]. The key advantage is the writing mechanisms controlled in current. This implies a greater localization of the active area respect to magnetic field induced switching, leading to less disturb, smaller/simpler cells, and scalable current/energy consumption. To switch the FL from the AP to the P configuration, electrons flow from the PL to the FL (Fig. 4.b). Only electrons with spin parallel to the PL magnetization are transmitted. Once in the FL, they exert a torque on the FL magnetization tending to rotate its direction. If the current is high enough, the torque is strong enough to switch FL polarization. On the contrary, to drive the MTJ in the AP state, electrons must flow in the opposite direction (Fig. 4.c). Electrons with antiparallel spin are reflected by the PL and 'accumulate' in the FL. Again, if their number is high enough, i.e. if the current is above a critical value, they are able to switch back the FL to the AP polarization.

III. Emerging Memory Modeling Trends

A. Material Modeling

As it can be argued from the previous section, practically all types of EM go beyond the concept of charge storage, as they are rather based on some specific property of the active materials (chalcogenide glasses for PCM, metal oxides/electrolytes for RRAM, magnetic alloys for STT-MRAM). This has put recently a lot of emphasis on the development of new materials with the proper characteristics. In this framework, atomistic simulation (ab-initio, DFT, molecular dynamics, ...) is becoming a fundamental tool to understand material properties, electrical behavior, and for material engineering.

One of the most significant examples of this is the revealed correlation between amorphous chalcogenide atomic structure and crystallization speed in PCM. Indeed, the relatively low set speed (dictated by crystallization) is the main bottleneck limiting a wider adoption of PCM, so far. However, it has been recently shown by several groups through atomistic simulation that the GST amorphous phase, although featuring an overall disordered configuration of the different atoms, may maintain,

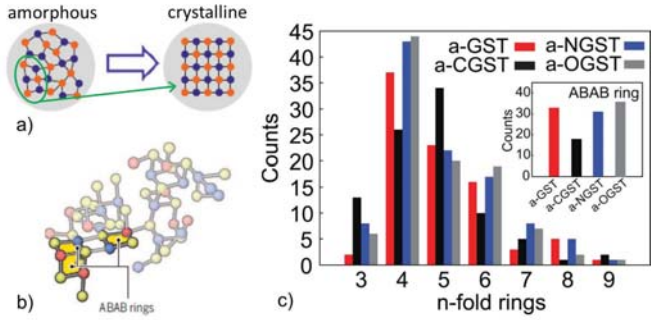

Fig. 5. a) Schematic representation of the crystallization process facilitated by ABAB rings (circled). b) ab-initio simulation of amorphous GST with ABAB rings highlighted [7]. c) calculated ring distribution for different doping [8].

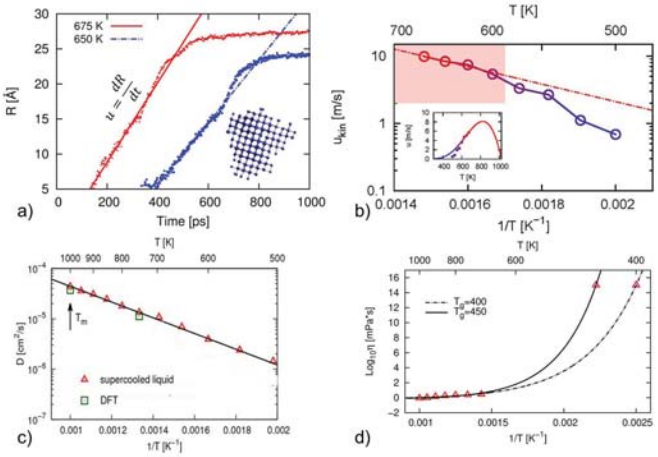

Fig. 6. a) Simulated radius (R) of a crystalline nucleus at two different temperatures. The derivative is the growth velocity u [11]. b) Growth velocity prefactor computed at different temperatures. c) Independent simulation of diffusivity, and d) of viscosity [13].

on a short range, some ordered blocks that resemble the ones of the crystalline phase [4]–[6] (Fig. 5.a). These blocks have been recognized to be the 4-fold rings of type ABAB, where A is Ge or Sb and B is Te (Fig. 5.b). Being similar in the two phases, it is easy to think that these rings act as preferential sites for crystallization. Thus, the larger their number the faster the crystallization is. This suggests a way to improve the set speed by increasing the number of rings, for example, by substituting, at least partially, Ge atoms that can take the tetrahedral configuration unfavorable for ring formation, with other atoms (i.e. doping). Also in this case, atomistic simulation can help in screening the appropriate species by looking at the simulated number of 4-fold rings (Fig. 5.c).

Atomistic simulation helps also to understand the physical origin of a fundamental property of chalcogenide, i.e. the very large difference between the high crystallization speed at moderate temperature (500K-700K), necessary for a fast set operation, and the very low speed at room temperature, necessary for long data retention [9], [10]. Classically, the crystallization process takes place by a combination of formation of stable nuclei with rate $I_{SS} \propto D\ exp(-G_c/K_BT)$ and their growth with velocity $u \propto D(1-exp(-\Delta\mu/k_BT))$, where D is the atom self-diffusivity. These formulae highlight that, in addition to the thermodynamic factors $\Delta\mu$ and $G_c(\Delta\mu)$, representing the energy gain for an atom in joining the crystalline network (facilitated by the ABAB rings), there is also a dynamical factor D linked to atom's mobility. In glasses, D is also related to the viscosity η by the Stokes-Einstein relation (SER) $D \propto T/\eta$. Simulations were done to study independently D, η, nucleation and crystal growth. In large scale atomistic simulations it is possible to observe the actual nucleation and growth of the crystalline phase (Fig. 6.a) from which u can be derived [11], [12]. u turned out to stay at a high value over a broad range of temperatures with a small activation energy [10], [11] (Fig. 6.b). This is consistent with a high D well above what is predicted by SER, as also found with independent simulation [13] (Fig. 6.c). In addition, it was shown that GST is a fragile glass, i.e. η features a sharp increase near T_g that leads to a sudden drop of D explaining the low crystallization speed at room temperature (Fig. 6.d). The root cause of all these effects has been traced back by simulation to the presence of clusters of fast moving atoms around chains of Ge-Ge bonds [14].

Atomistic simulation is also being extensively leveraged in RRAM, finding applications in all aspects of their operations [15]. A few examples are: i) calculation of formation energy determining defect density, also in connection with the process steps such as deposition conditions and annealing; ii) diffusion barriers controlling atom movement (can be used also as input for higher level simulation approaches like KMC); iii) trap levels (Fig. 7.a) and associated density of state (DOS) entering the calculation of the device current, either as stepping stone for trap-assisted-tunneling (TAT) [16] or as the basis of more advanced quantum methods, such as NEGF, that naturally take advantage of the underlying atomic structure; iv) analysis of the switching mechanisms and its fast dynamics [17]; etc. A calculation of the trap levels induced by differently charged defects in an HfO_x based RRAM is reported in Fig. 7.a [15]. The origin of the resistance change is explained in Fig. 7.b on the basis of the different overlap of the wave functions of the defect induced states. In the clustered configuration (top), corresponding to the low resistance state (LRS), the degree of overlap is high enough to induce a delocalized state, whereas in the disordered configuration (bottom) the wave functions remain localized around isolated defects that are both spatially and energetically separated.

Likewise, a number of applications of atomistic simulation to STT-MRAM have been reported in literature. A few examples can be found in [18].

B. Structural changes and Multi-physics approach

As it is clear even from the brief description of the previous section, modeling and simulation of almost all EM must couple the standard electro-thermal simulation with some other equations describing the specific phenomena at the basis of that particular technology. For example, PCM must handle the

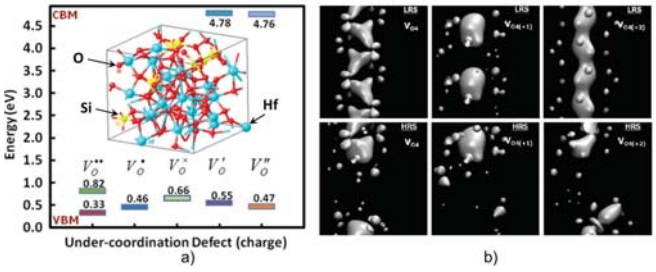

Fig. 7. a) DFT calculated energy levels of electron traps in $Hf_xSi_{1-x}O_2$ for different charge states [15]. b) Charge density iso-surfaces of conductive mid-gap states in HfO_2 corresponding to LRS (top) and HRS (bottom) for different charge states: 0, +1, +2 from left to right [15].

GST phase change that can be treated with several approaches. One is phase field [19], [20] requiring an additional partial differential equation to describe the time evolution of the phase field. Another approach is rate equations between states representing the different GST phases, reducing to a set of additional ordinary differential equations per mesh nodes [21]. Or, in order to account for the randomness of nucleation, Monte Carlo techniques can be adopted [22].

A phenomenon common to many types of EM is mass transport (e.g. GST atoms in PCM, defects/ions in RRAM, etc.). So the coupling with drift-diffusion like equations for each mobile species is mandatory for EM. This also often calls for the inclusion of chemical reactions (e.g. RRAM) providing the generation-recombination terms for the mass transport equations. Moreover, STT-MRAM modeling is based on the Landau-Lifshitz-Gilbert-Slonczeewski equation [23] that represents an additional challenge for the need to describe also spin currents and to adopt specific solutions to guarantee numerical convergence [24].

Given the large variety of involved phenomena and possible simulation approaches no general tool is available. Rather, specific solutions for a given memory type have been reported in literature. For example, we have developed a comprehensive PCM model (Fig. 8.a) that is able to describe the cell I-V in both the crystalline and amorphous states (including amorphous threshold switching), as well as crystallization dynamics and composition change due to mass transport [1], [25]. We also worked out a multi-physics Copper-based RRAM simulation environment [26]. A typical block diagram of a RRAM model of this kind is shown in Fig. 8.b, pointing out again the tight interaction between the multiple physical phenomena. As a consequence, an open framework allowing the user to add quickly new physics is necessary.

In addition, particular attention must be paid to meshing to follow the structural changes present in many EM, a necessity that suggests the need to include some capability, so far typical of process simulation, also into device simulation.

C. Bridging the atomistic and continuous worlds

Several types of RRAM are based on the conduction through a narrow filament made of just a handful of atoms/defects [28].

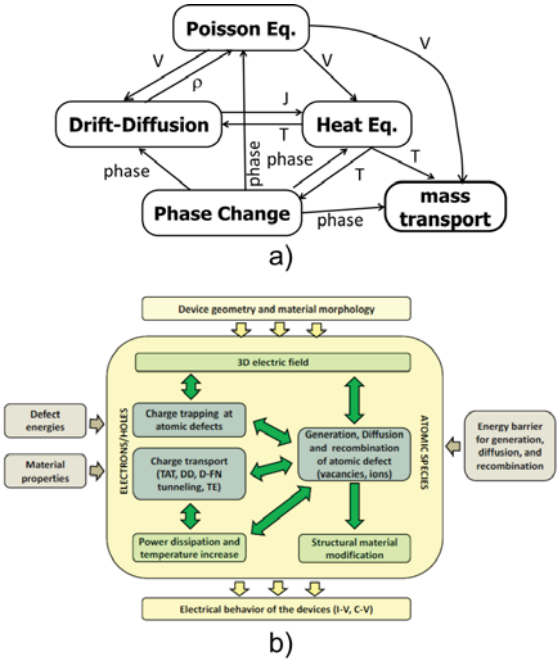

Fig. 8. a) Main blocks of the PCM simulation environment in [1], [25]. b) Typical RRAM modeling platform [27].

Thus, their modeling requires treating those few atoms/defect as discrete particles. Therefore there is the need for robust methods to couple particle based quantities with other finite element method (FEM) equations.

From this point of view, a phenomenon that was given particular attention, since it is at the very base of RRAM electrical characteristics, is trap-assisted-tunneling (TAT) through discrete traps. TAT has been largely investigated, and several physical models are now available (e.g. [16], [29]). However, when the number of traps increases up to forming a continuous filament there is still the problem of when and how to switch the charge transport model from trap-based hopping to a more conventional drift in defect sub-bands. Indeed, difficulties lie in the identification of the physical condition triggering the need for this change, and in its software implementation because of the different type of equations that must be solved, and the corresponding numerical instability due to large conductivity changes.

Moreover, also the coupling with the Fourier equation for the temperature raises some concerns related to the definition of the generated heat power density. The current density J is not well defined in case of conduction through discrete traps, so that the use of the classical Joule heat term $J * E$ is questionable. In this case, it would be better to use directly the energy loss involved in the inelastic TAT process [30], but with the caveat, this time, that the volume in which the energy is released is not known. However, considering that the temperature attained far from the mesh point where the energy is released is rather independent of the release volume, but depends only on the overall power, this last problem is

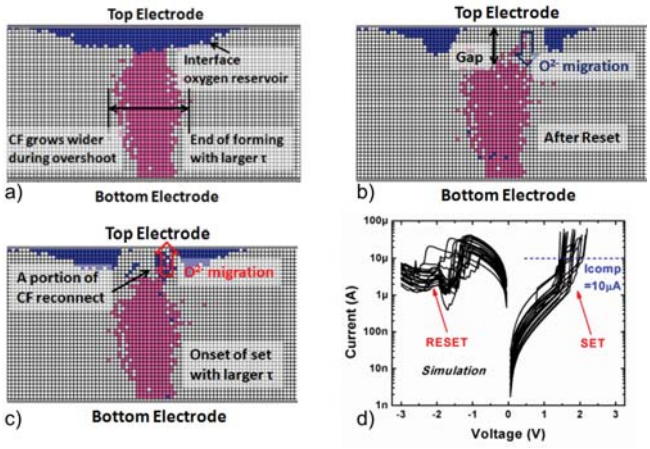

Fig. 9. KMC simulation of (a) forming, (b) reset, and (c) set operations, and (d) cycle-to-cycle I-V variability for a HfO_x RRAM [31].

usually overcome with a proper choice of the mesh spacing.

The Kinetic Monte Carlo method is a common approach to handle the evolution dynamics of discrete particles/events (e.g. [30]–[32]). Each event, like oxygen vacancy/ion creation/annihilation, ion migration, electron hop in and out of a vacancy or an electrode, and so on, is described by its own temperature/field dependent rate. At each time step, dictated by the total rate, an event is randomly chosen and the system updated accordingly. It was shown that this approach accurately captures temporal evolution as a function of the external stimuli, accounting, at the same time, for the intrinsic variability of RRAM operation [31] (Fig. 9).

D. Statistics, noise and fluctuations

Controlling variability in EM is even more important than in conventional memories as many of them have small operational window (e.g. STT-MRAM and RRAM). There are several sources of variability. From intrinsic variability at time zero (geometry, composition, grain boundaries, etc.), to fluctuation in time (RTN) or cycle-to-cycle (e.g. random shape of the filament in RRAM). The conventional approach to handle variability is the Monte Carlo (MC) technique. The aforementioned KMC method is an example, and it has been widely reported in literature. Variability has been also addressed with FEM model by introducing some statistical spreading of some model parameter again with the MC approach [33]. However, MC is too expensive to address the low percentiles of the distribution that are needed. More efficient statistical tools to predict cell distributions and resulting read window budget on a physical basis should be further pursued.

E. Mechanical Stress

In many types of EM, a significant mechanical stress can be attained yet during normal operation. For example, in PCM the high temperature needed to melt GST (≈1000K) induces a large thermal expansion. Also the density change upon phase change (≈7%) is another important source of mechanical stress. In RRAM, the formation of the metallic filament may exert a significant pressure on the surrounding dielectrics. Notice that mechanical stress is a concern for cell reliability. Indeed, it has been linked to void formation after cycling in PCM [34], in a manner much similar to what happens in classical electro-migration in metal interconnect. It has also an effect on the cell operation because, by distorting the atom network, induces a change of the energy barriers governing diffusion and reaction rates. This issue has not been adequately addressed so far (with a few exceptions for PCM [35], [36]), and deserves more attention from the modeling community.

Furthermore, mechanical stress is also generated during the fabrication process because of the intrinsic stress in the as-deposited materials, thermal cycles and etch processes. Its importance is increased in EM because of the many different materials making up the cell stack (e.g. STT-RAM). Such mechanical stress is the cause of structural failure like line collapse and buckling, but also of wafer bowing that is a problem for lithographic and CMP steps. There are TCAD tools to compute process induced mechanical stress at the cell scale, but what is missing is the link to wafer/die warpage. This is another topic that deserves more effort, as it will help to predict the effect of process or layout changes on the process manufacturability.

IV. Conclusion

In this paper, we have tried to portray the current status of the modeling and simulation activities in the fields of EM. We have highlighted a few categories of problems that are bound to become more and more important in the future, and thus may serve as a guide for future developments.

With respect to our previous survey [26], we have seen a great increase in the usage of material modeling based on atomistic simulation. This is for sure an area where to focus more efforts in the future, trying also to increase the integration with the other downstream tools. An open simulation framework allowing users to couple different physical phenomena and to seamlessly bridge continuum and atomistic worlds are still key features to pursue. Definitely, the statistical description of a memory array with all variability sources, and the inclusion of mechanical stress in the modeling framework deserve more attention.

Acknowledgment

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