Three-dimensional Fully-coupled Electrical and Thermal Transport Model of Oxide Memristors\textsuperscript{1} XUJIAO GAO, DENIS MAMALUY, PATRICK MICKEL, HAROLD HJALMARSON, BRIAN TIERNEY, MATTHEW MARINELLA, Sandia National Laboratories — Accompanying the spectacular progress in experimental demonstration of oxide-based memristors, there has been significant modeling effort to aid in understanding of switching physics in memristive devices. However, existing models often simplify the treatment of electronic transport and the interplay of electrically and thermally driven processes. In this work, we present a fully-coupled electrical and thermal numerical model that treats the transport of electrons, holes, and vacancies, together with the Joule heating on an equal footing. Namely, we solve simultaneously the five coupled partial differential equations: the time-dependent drift-diffusion equations for electrons, holes, and vacancies, the time-dependent lattice heat equation, and the Poisson equation for all the charged species in three spatial dimensions. This fully coupled model allows us to investigate the microscopic interplay of field drift, Fickian diffusion, Soret effect, and Joule heating, and to facilitate the understanding of physical mechanisms responsible for the SET and RESET switching processes in tantalum oxide memristors.

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