Design of Rare-Earth Nickelate Memristors

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Rare-earth nickelates (*R*NiO₃) are distorted perovskite oxides that exhibit a charge-transfer insulator-metal transition (IMT) at temperatures dependent on the rare-earth cation size. LaNiO₃ is the exception, remaining metallic at all temperatures. Materials with this thermally driven transition lend themselves memristor applications because they can be switched from high-resistance to low-resistance states via Joule heating. Rare-earth nickelates (RNOs) also span the ideal transition temperature range (400-500 K) and the IMT can be modified by alloying as well as strain state [1]. Previous research in other material systems has found that higher transition temperatures require more energy per operation, but transitions too close to room temperature would require active cooling [2]. This work focuses on the control of RNO material properties for biomimetic neuronal devices.

Our proposed vertical device consists of an LaNiO₃ layer that acts as both a bottom electrode and an epitaxial buffer, an epitaxial RNO switching layer, and metallic top contacts. This structure can be translated to dense crossbar arrays and can be grown on numerous crystalline substrates. However, the different bulk structure of LaNiO₃ (rhombohedral) from the other RNOs and the relevant substrates (orthorhombic) complicates the heteroepitaxial picture. Factors such as biaxial strain alter the NiO₆ octahedral distortions that govern electronic structure, so understanding the substrate/LaNiO₃ and LaNiO₃/RNO interfaces is critical. We have employed both pulsed laser deposition and RF sputtering to grow epitaxial layers and heterostructures. Preliminary studies focus on NdNiO₃, which is more widely studied and easier to stabilize. Both deposition techniques can produce fully-strained, highly-crystalline NdNiO₃ on LaNiO₃ buffer layers. However, crystallinity does not predict electrical behavior, which we find to be highly dependent on deposition conditions even with nominally constant composition and strain state (Fig. 1). These effects are not fully explained by thickness



variation, and we will discuss additional mechanisms underlying this variability. We also measured use material properties to model RNO memristors in LT-SPICE, which provides insight into the necessary electrical behavior as we optimize our thin films.

Figure 1: X-ray diffraction (left) and temperature-dependent resistivity (right) of three NdNiO₃ films grown by sputtering.

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[2] Yi W, Tsang KK, Lam SK, Bai X, Cromwell JA, Flores EA. Nat. Commun. 9, 4661 (2018)

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Supplementary Information