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Oxygen diffusion along dislocations in Sr-doped LaMnO3

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Mixed-valence manganites are very promising candidate materials for resistive-switching devices due to the possibility to generate multilevel resistance states as well as area-dependent switching. This enables their use in future non-volatile memories or novel neuromorphic circuits.
The aim of our work is to gain a deeper understanding of the microscopic mechanisms of resistive switching in mixed valence manganites with the focus on Sr-doped LaMnO3 (La1-xSrxMnO3±δ, LSMO). It is widely accepted that ionic transport, especially oxide-ion transport, plays an important role in the field of resistive switching. Nevertheless, the role played by dislocations (one dimensional lattice defects) in the switching process is unknown. LSMO is unusual amongst the perovskite oxides, since it is the only system to show fast diffusion of oxygen along dislocations. The reasons for this behaviour are however not understood.
To this end, we studied the ionic transport in bulk LSMO as well as along low-tilt grain boundaries (that consist of a periodic array of dislocation) by Molecular Dynamics simulations, employing empirical pair potentials. In particular, the effect of Sr dopants and cation vacancies on oxide-ion transport is examined.

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