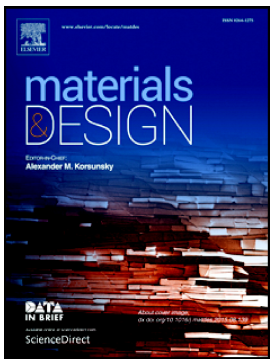

Engineering cationic defects in transparent tin oxide superlattices

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Engineering Cationic Defects in Transparent Tin Oxide Superlattices

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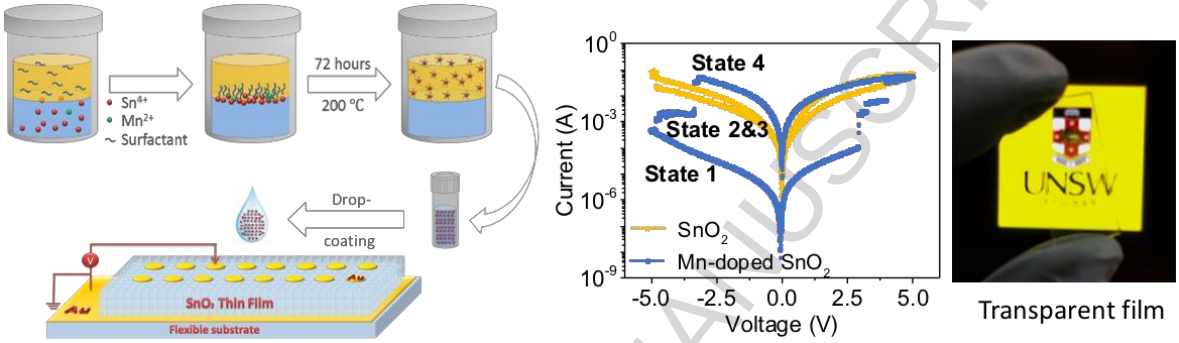
HIGHLIGHTS:

- The formation energy of cationic defects in Mn-doped SnO_2 was studied through density functional theory calculation, and it is found that Mn^{3+} occupies the interstitial sites of SnO_2.
- A liquid-liquid interface approach to fabricate 6.25 mol% and 12.5 mol% Mn-doped SnO_2 nanocrystalline thin films through self-assembly technique at room temperature has been developed.
- Up to 4 nonvolatile resistance states have been achieved via controlling migrations of Mn defects in SnO_2 thin films.

GRAPHICAL ABSTRACT:



ABSTRACT: The lack of understanding in engineering cation defects in metal oxides has impeded the development of high performance, and transparent electronic devices. Through studying the formation energy of various cationic defects in Mn-doped SnO_2 via simulation, we found Mn^{3+} cations occupy the interstitial sites of SnO_2 nanocrystals, and we proved that such defects can be engineered to significantly improve resistive switching performance of tin oxide-based devices. With this finding, a new solution-processed approach has been developed to synthesize Mn-doped SnO_2 nanocrystals with a self-assembly technique for high quality transparent Mn-doped SnO_2 thin film fabrication. Defect migration behavior of the Mn-doped SnO_2 thin film was studied by building a metal-oxide-metal sandwich device. The effects of cationic defects, such as Mn interstitials, on the charge transport behavior were further studied to reveal the underlying mechanism. This study provides new insights into the design and engineering of defects in transparent oxides for high-density data storage applications.

KEYWORDS: nanocrystal growth, self-assembly, tin oxide, liquid liquid interface

1. Introduction

With the increasing demand of flexible, transparent and multifunctional electronic devices, transitional metal oxide thin films have attracted extensive research interests because of their high compatibility with complementary metal-oxide-semiconductor (CMOS) technology.[1-3] Recently, various transparent metal oxides including ZnO[4], SnO_2[5], In_2O_3[6] and TiO_2[7] have been widely explored for applications in thin film transistors[8, 9], non-volatile memories[10, 11], and gas sensors[12, 13]. In applications, manipulation of oxygen vacancies is often considered as one of the most important approaches for tuning the optical and electrical properties of transparent metal oxides.[14, 15] However, the absence of systematic investigations on the role of cationic defects in transparent metal oxides has limited further optimization of their physical properties for practical applications. This is because the modification of the concentration of oxygen vacancies only results in a small range of variation of electrical conductivity and optical transparency.[16] Hence, it is of importance to understand the effects of cationic defects on the electronic and optical properties of transparent metal oxides in order to manipulate the physical properties of metal oxides in innovative ways.