

Mechanism of Negative Bias Illumination Stress in InGaZn Oxide TFTs

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1. Abstract

Negative Bias Illumination Stress instability in amorphous IGZO thin film transistors is consistently explained by a new model of the photo-excitation of electrons from states of In-O-Zn bridge bonds lying in the lower part of the band gap.

2. Introduction

Amorphous InGaZnO oxide has recently replaced hydrogenated amorphous silicon (a-Si:H) as the main thin film transistor display material due to its high electron mobility [1]. Its high mobility arises from its disorder-insensitive s-like conduction band minimum (Fig 1). However, it does suffer from a negative bias illumination stress (NBIS) instability [2] which limits its performance as an OLED driver. NBIS is like a persistent photoconductivity, and is thought to arise from excitation of electrons from states in the lower band gap to the conduction band (Fig 2). These gap states are seen by hard x-ray photoemission [3].

Various models for NBIS have been proposed, but each has weaknesses. The most common is that it is due to O vacancies [4]. The O vacancy is easy to form in oxides, is consistent with an O deficiency, and the O vacancy has a negative U giving an energy barrier to electron recombination and the persistent photoconductivity. However, vacancy states lie higher up in the band gap than is observed.

The O interstitial has also been proposed [5]. This gives gap states in the correct energy range, it can have an energy barrier towards recombination, but it is an O excess defect, contrary to experiment.

A deep/shallow instability of a single H atom has also been proposed [6], but it is not an O deficiency defect.

3. Results

We now consider the properties of hydrogen in a-IGZO. Hydrogen atoms are well-known shallow donors in ZnO and oxides like a-IGZO. IGZO thin films can be made with very high resistance, so the H must be compensated.

The hydrogen content of a-IGZO was found by SIMS to be $10^{20} - 10^{21} \text{ cm}^{-3}$ [7]. This compares to a photo-excited electron density of 10^{18} cm^{-3} and a subgap state density of 10^{21} cm^{-3} . In comparison, the maximum hydrogen solubility of c-ZnO is much lower [8], of order 10^{14} cm^{-3} .

The simplest form of compensation is if hydrogen exists in pairs at an O vacancy. This configuration is shown in Fig. 3 for ZnO. For V_O [9], there are four metal sp^3 orbital directed into the vacancy. In the V_O^{2+} configuration, these

are empty. In this case 2H forms an H_2 molecule inside the vacancy. For the neutral V_O^0 , the hydrogens form two bridge bonds between pairs of sp^3 orbitals, Fig 3(b).

A similar behavior is found in IGZO. Fig 4 shows a random network model of amorphous InGaZn oxide generated by density functional molecular dynamics. O vacancies are created in the network and their formation energy is calculated, and compared to O vacancies in crystalline InGaZnO. It is found that the O vacancy formation energy is 0.5 to 1.0 eV less in a-InGaZnO. Fig 5 shows H bridging sites at an O vacancy in a-IGZO, and Fig 6 shows their PDOS. The H bridge gives a state in the lower gap at +0.6 eV, and also one at -7 eV below the valence band. Overall, H is in an anion state, H^- .

The formation energy of the $V_O/2H$ configuration in c-IGZO or c-ZnO is quite high, so the H concentration of in c-ZnO is quite low (10^{14} cm^{-3}). However, because of disorder and the lower density of the amorphous phase, the formation energy of $V_O/2H$ is lower in a-IGZO by 1.0 to 1.5 eV, and thus the H content is greatly increased. This is shown in the formation energy diagrams, Fig 8(a,b). Fig 8(b) also shows that the energy of neutral or 2+ state is always lower than the +1 single hydrogen doping state. Thus, a relatively large amount of H can enter a-IGZO in a paired compensated (non-doping) configuration. This is passive in its ground state, but the system is vulnerable to reaction or photo-excitation like Si-H bonds in Si-based systems.

We see that this model fulfils the following criteria;

- It is O deficient, so O plasmas can remove the defect.
- It gives gap states in the correct energy range as in XPS.
- It has an energy barrier to carrier recombination,
- It has a low formation energy and hence high density
- The bridging bonds are seen in IR spectra[10].

4 Summary

A relatively large density of hydrogen can exist in a-IGZO and typically exists in a compensated form but it can lead to instabilities like NBIS.

References

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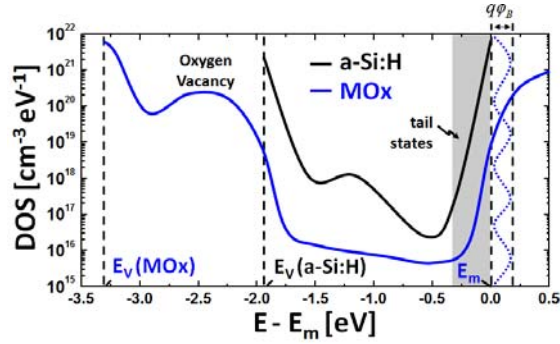


Fig. 1 Density of states of a-IGZO compared to a-Si:H. Note the lower density of tail states at 0 eV.

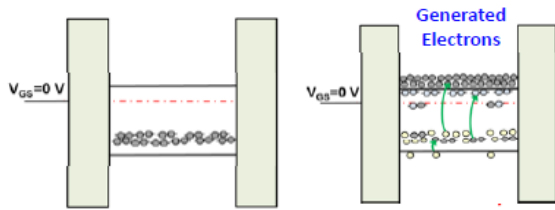


Fig. 2. Photo-excitation of electrons from states in lower gap to conduction band causing conductivity and NBIS.

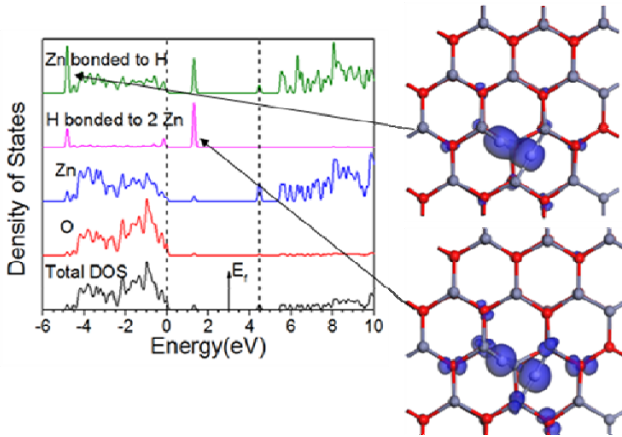


Fig. 3. Local orbitals and the partial density of states of the bridging H states giving states for the case of 2H in ZnO. Note the filled gap state at +0.8 eV responsible for NBIS.

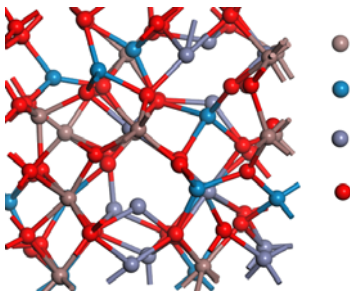


Fig. 4. Molecular dynamics generated random network of IGZO. Red =O, Grey =Zn, Blue = Ga, brown = Ga.

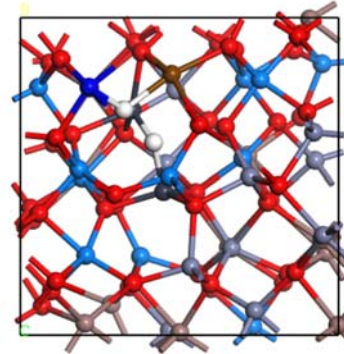


Fig. 5. O vacancy with two H bridging sites in a-IGZO. H= white..

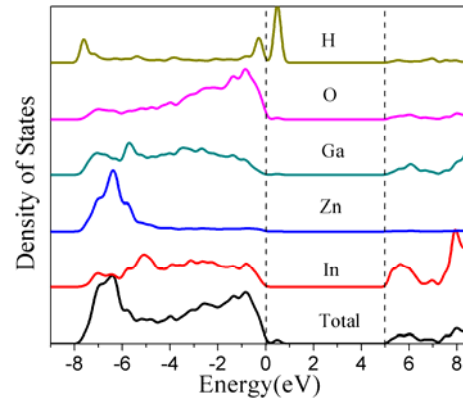


Fig. 6. Partial density of states with the bridging H sites giving states in lower band gap. Note the filled gap state at 0.5 eV.

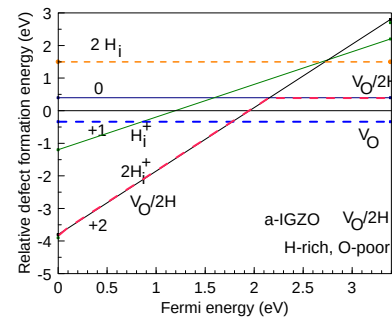
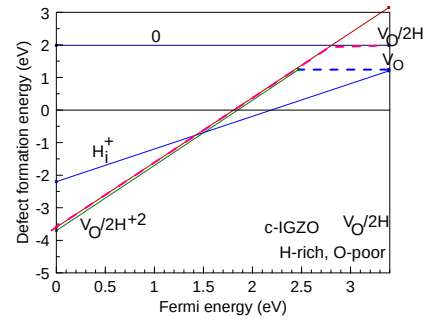


Fig. 7. Defect formation energy vs E_F for c-IGZO and a-IGZO, showing much lower formation energy of 2H/ V_O configuration in a-IGZO, which leads to more H in the amorphous phase.