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Correlation between Crystallinity and Formation of Oxygen Vacancies in IGZO
- Comparison between Crystal and Amorphous Using First-Principles Calculations -

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Abstract

We have been investigating the correlation between crystallinity and formation of oxygen vacancy in In-Ga-Zn oxide (IGZO) by experiments and numerical analyses. It is found that by optical and electrical measurements, in c-axis-aligned crystalline (CAAC) -IGZO having high crystallinity without grain boundary, the density of deep defect levels due to oxygen vacancies are significantly reduced. In this study, we obtained theoretical results from first-principles calculation that indicate the formation of oxygen vacancies in IGZO is prevented by improving the crystallinity and oxygen vacancies are increased by lowering the crystallinity.

1. Introduction

In-Ga-Zn oxide (IGZO) was synthesized for the first time in 1985 by Kimizuka et al. [1], and has been widely researched as a semiconductor material. We discovered c-axis-aligned crystalline (CAAC) structure [2] and nano-crystalline (nc) structure [3] in IGZO, and fabricated an FET in which these structures are used for an active layer; thus, we succeeded in fabricating a highly reliable device[4]. In particular, CAAC-IGZO is an entirely novel crystal structure [5] different from single crystal and poly-crystals, in which clear grain boundary is not observed in spite of high layered crystallinity. Advantages of CAAC-IGZO, high crystallinity and no grain boundary, contribute to the high reliability of a CAAC-IGZO FET.

As for an oxide semiconductor (OS), it becomes obvious that various crystal morphologies are formed (Fig. 1) in addition to amorphous and single crystal reported by other research institutions. CAAC and nano-crystal that can be formed at low temperature with high reliability are thought to be particularly advantageous in application to devices for mass production [6].

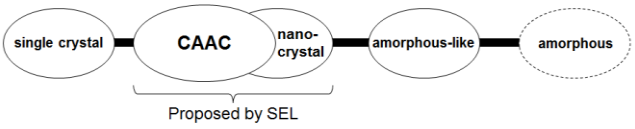

Fig.1 Relationship between single crystal, CAAC, nc, and amorphous OS.

As well as the application to displays which are now mass produced, the application of IGZO FETs to LSI is expected[7], and further improved reliability is required. An example of widely known degradation modes of an IGZO FET is a negative shift of the threshold voltage (negative-bias photodegradation) which is caused when negative bias is applied to the gate electrode under light irradiation. Our previous research revealed that the use of CAAC-IGZO for an active layer of an FET largely reduces the negative-bias photodegradation [4]. A possible cause of the negative-bias photodegradation is deep defect levels due to oxygen vacancies in the band gap in the IGZO thin film.

We quantified deep defect levels due to oxygen vacancies in the IGZO thin film as an absorption coefficient by a constant photocurrent method (CPM), and found that an improvement in crystallinity reduces the absorption coefficient derived from deep defect levels (Fig. 2) [8]. These studies enabled us to assert the effectiveness of CAAC-IGZO with high crystallinity in reducing negative-bias photodegradation also from in terms of physical properties. However, the mutual relationship between crystallinity and formation of oxygen vacancies was not well theoretically discussed. Thus, in this paper, the correlation between the crystallinity of an IGZO film and oxygen vacancies is investigated by experiments and first-principles calculation.

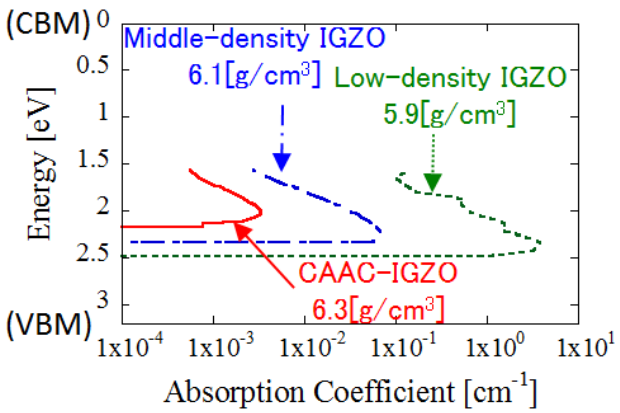

Fig.2 Light absorption due to defect levels measured by CPM in IGZO films [8].

2. Results and Discussion

To investigate the correlation between crystallinity and oxygen vacancies of an IGZO film, an island-shaped single crystal IGZO film was formed to have a low crystallinity region in its side edge. The center portion and the side edge in the film were observed with annular blight field scanning transmission electron microscope (ABF-STEM). The result shows that oxygen vacancies are more likely to be formed in the side edge than in the center portion with high crystallinity (Fig. 3).

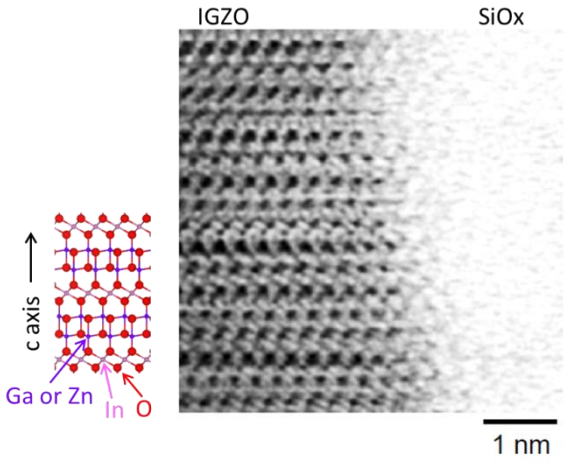

Fig.3 ABF-STEM image of side edge of crystalline IGZO film and crystal model.

In the past study, we compared amorphous IGZO and crystal IGZO in their formation of oxygen vacancies by first-principles calculation. The calculation results indicate that oxygen vacancies are likely to be formed in amorphous than in crystal [9]. However, an energy reference differs between the amorphous model and the crystal model when these models are calculated separately. Therefore, the total energies of the models obtained by first-principles calculation cannot be compared to each other. In this study, we prepared an IGZO complex model to compare the total energies directly. An amorphous model was prepared by melt-quenching method. In the IGZO complex model, the crystal model and the amorphous model were connected in a direction perpendicular to c-axis, and atomic relaxation was performed (Fig. 4). We used VASP software[10].

Variation in total energy in the amorphous model was larger than in the crystal model. Even taking into account this point, oxygen vacancies is more likely to be formed in the amorphous model than in the crystal model. Next, the amount of displacement was estimated to evaluate the ease of atomic relaxation derived from formation of oxygen vacancies. As a result, the amount of displacement is small in the crystal bulk region, while the amount is large in the amorphous region. Atomic relaxation derived from formation of oxygen vacancies in amorphous occurs with high frequency than in crystal, because of disorder of atom arrangement in amorphous. Therefore, it is suggested that oxygen vacancies are likely to be formed in the region where atomic relaxation occurs with high frequency. Details of this calculation will be announced at SSDM 2015.

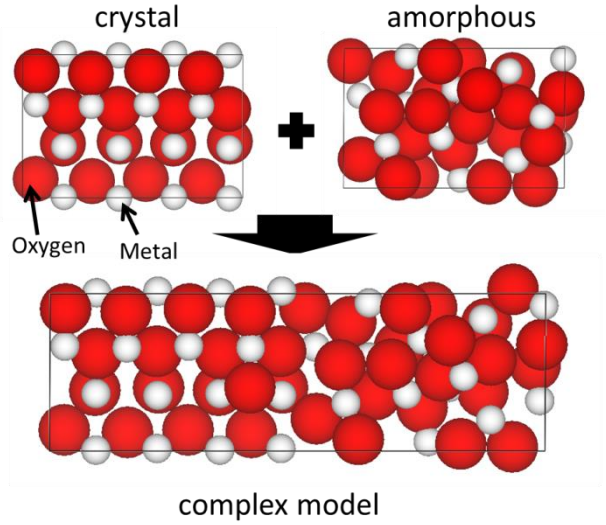

Fig.4 Schematic diagram of IGZO complex model.

3. Conclusions

The relation between formation of oxygen vacancies and crystallinity of IGZO was examined by first-principles calculation based on experimental results. The results show that oxygen vacancies are less likely to be formed in the crystal region than in the amorphous region. The calculated displacement indicates that atomic relaxation derived from formation of oxygen vacancies is less likely to occur in the crystal region than in the amorphous region. Therefore, the CAAC-OS film, which has high density and high crystallinity and in which atomic relaxation is less likely to occur, is suitable for displays, memories, and LSI.

References

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