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Mobility of Hydrogen in Oxygen Vacancies in IGZO models with Different Crystallinities

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Abstract

The mobility of hydrogen (H) in oxygen vacancies (V_O) in In-Ga-Zn oxide (IGZO) models with different crystallinities was evaluated by first-principles calculations. In the first-principles molecular dynamics simulations on IGZO models, which contain H in V_O (V_OH), in a temperature range from 600°C to 1000°C, the release of H from V_O was observed in an amorphous IGZO (a-IGZO) model, whereas H was not released in a crystal IGZO (c-IGZO) model. We estimated the activation energy of the release of H from V_O and found that the activation energy in the a-IGZO model was significantly lower than that in the c-IGZO model. This result suggests that the use of an IGZO with high crystallinity is important for forming an IGZO FET with stable electrical characteristics.

1. Introduction

A *c*-axis aligned crystalline In-Ga-Zn oxide (CAAC-IGZO) has been developed in recent years [1]. Moreover, miniaturized CAAC-IGZO FETs have been developed with the aim of application to LSI [2].

Typical examples of defects in an IGZO include hydrogen (H), oxygen vacancies (V_O), and H in V_O (V_OH, also called H_O). The results of first-principles calculations suggest that V_OH may serve as a donor in an IGZO [3]. In forming an IGZO, not only reducing defects but also suppressing diffusion of defects is necessary. An FET needs to have an i-type channel region. When V_OH serving as a donor is diffused from an IGZO under source and drain electrodes of the FET, the I_d-V_g characteristics might shift in the negative direction. This problem is serious particularly in the case of an FET with a channel length of several tens nanometers.

In order to control and suppress defects, it is desirable that an IGZO have high crystallinity. It has been actually revealed that an FET using an IGZO with high crystallinity has small variation in characteristics [4]. Furthermore, calculation reveals that V_O and V_OH are hardly generated in an IGZO with high crystallinity [5,6]. Diffusion of defects is assumed to be reduced in an IGZO with high crystallinity. However, in a miniaturized FET, actual observation of the movement of defects is difficult. In view of the above, in this study, we evaluated the mobility of H in V_OH in IGZOs with different crystallinities by the first-principles calculations.

2. Calculation Method

In the calculation, plane-wave basis first-principles calculation software Vienna ab initio simulation package (VASP) based on density functional theory was used [7]. For the exchange-correlation functional, Perdew-Burke-Ernzerhof generalized gradient approximation was used, and for the pseudopotential, a projector-augmented-wave method was used. Γ-only k-point sampling was used in first-principles molecular dynamics (FPMD) simulations; 2×2×3 (crystal model) and 2×2×2 (amorphous model) Γ-centered k-point grid were used in calculations of activation energies. The cut-off energy was set to 500 eV.

3. Evaluation by FPMD Simulations

First, FPMD simulations were performed on a crystal IGZO (c-IGZO) model and an amorphous IGZO (a-IGZO) model in order to evaluate the mobility of H in V_OH. The a-IGZO model was fabricated by a melt-quenching method such that atoms were randomly arranged (density: 5.8 g/cm^3). Figure 1 shows the c-IGZO model (56 atoms) and the a-IGZO model (84 atoms), which contained V_OH and were used for the calculations. The FPMD simulations were performed on the structures shown in Fig. 1 under conditions of NVT ensemble and temperatures of 600°C, 800°C, and 1000°C for 50 ps.

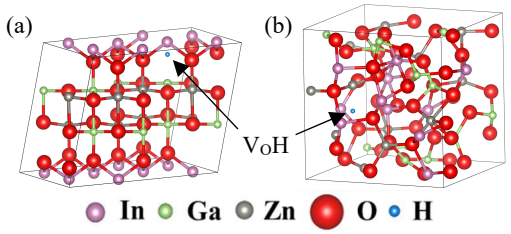

Fig. 1 (a) c-IGZO model and (b) a-IGZO model, which contained V_OH and were used for calculations.

Figure 2 shows trajectories of H atoms in the FPMD simulations. In the c-IGZO model, H existed around V_O and the release of H from V_O was not observed at any temperature. On the contrary, in the a-IGZO model, H was released from V_O after thermal motion for some time. After that, H was bonded to oxygen (O) and diffused. The release of H occurred even at 600°C. These results suggest that H is likely to be released from V_O when crystallinity is low.

4. Estimation of Activation Energy

Then, we estimated the activation energies of the release of H from V_O in the c-IGZO and a-IGZO models using

nudged elastic band (NEB) method. However, since an amorphous structure is random, it is difficult to perform NEB calculation on the amorphous structure. Thus, in this study, we performed NEB calculations on atomic structures of the a-IGZO model before and after the release of H from V_O in the FPMD simulations at 600°C, whereby the activation energies were evaluated. Note that the number of atoms in the c-IGZO model in this calculation was 112.

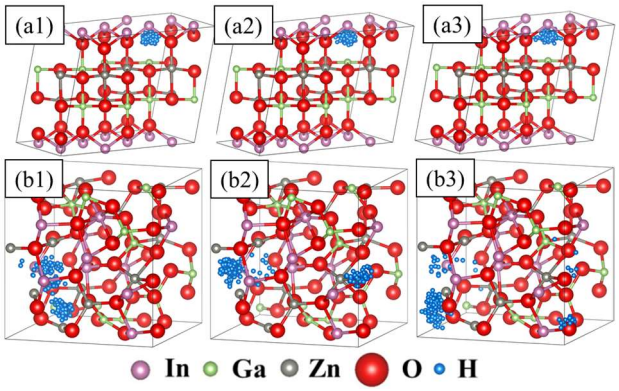

Fig. 2 Trajectories of H in FPMD simulations on c-IGZO model at (a1) 600°C, (a2) 800°C, and (a3) 1000°C, and on a-IGZO model at (b1) 600°C, (b2) 800°C, and (b3) 1000°C. Initial models contained V_OH. Although atoms other than H also moved, only initial atomic arrangement of them is shown here.

Figure 3 shows the total energies and atomic structures on minimum energy path of the release of H from V_O obtained by the NEB calculations. The activation energy of the release of H from V_O in the c-IGZO model was 1.50 eV, and that at a certain point in the random structure of the a-IGZO model was 0.85 eV, which was smaller than that in the c-IGZO model. Table I summarizes the activation energies E_a and the reaction frequencies Γ of the release of H from V_O in the c-IGZO and a-IGZO models [3]. According to the results, the release of H from V_O is likely to occur in the a-IGZO model even at a temperature of 125°C, which is widely used in the reliability test of LSI devices, whereas the release of H is less likely to occur in the c-IGZO model. The release and diffusion of H may cause diffusion of V_OH serving as a donor, which may change the electrical characteristics of an IGZO FET. That is, the results indicate that an IGZO FET using an IGZO with high crystallinity has stable characteristics.

5. Conclusions

In this study, we evaluated the mobility of H in V_O in the IGZO models with different crystallinities. In the FPMD simulations on the c-IGZO model and the a-IGZO model, which contained V_OH, in a temperature range from 600°C to 1000°C, the release of H from V_O occurred in the a-IGZO model, whereas the release did not occur in the c-IGZO model. In addition, the activation energy of the release of H from V_O calculated by the NEB method was significantly lower in the a-IGZO model than in the c-IGZO model. The results suggest that the release of H from V_O is less likely to occur when crystallinity is high, which can suppress variation in the electrical characteristics of an IGZO FET. In view of this, an IGZO with high crystallinity is preferably used for forming an FET with stable electrical characteristics.

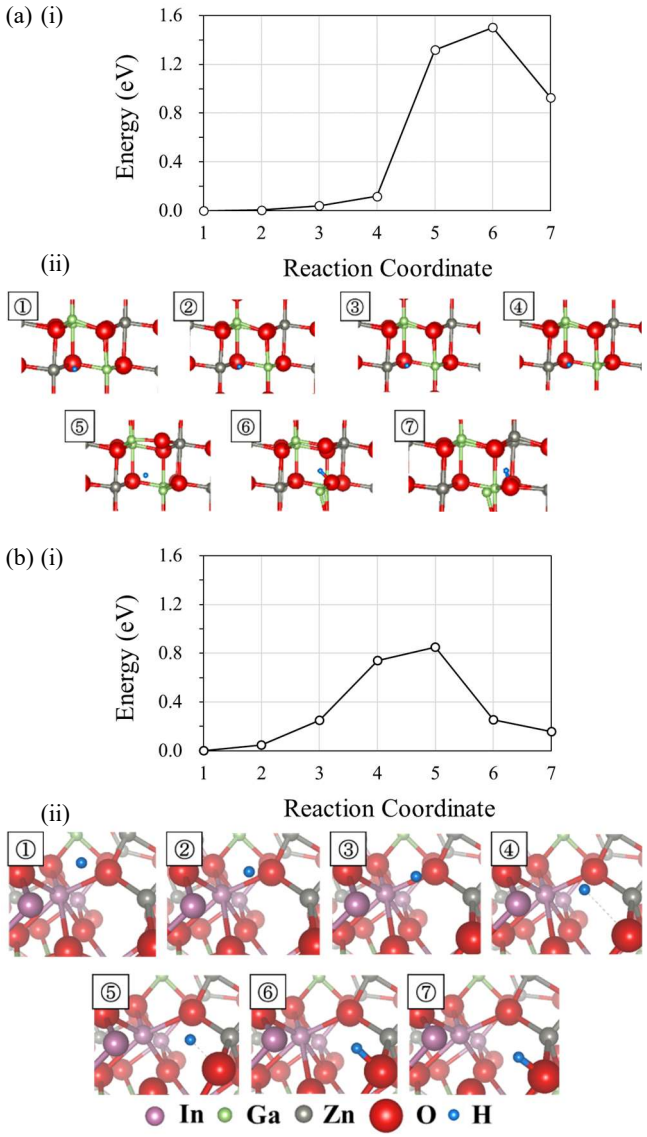

Fig. 3 (i) Total energies and (ii) atomic structures on minimum energy path of release of H from V_O calculated by NEB method in (a) c-IGZO model and (b) a-IGZO model. For clarity, structure images in (b)(ii) are enlarged.

Table I Activation energies E_a and reaction frequencies Γ of release of H from V_O in c-IGZO and a-IGZO models.

	E_a [eV]	Γ (125°C) [s^{-1}]
c-IGZO	1.50	9.62×10^{-7}
a-IGZO	0.85	1.69×10^{2}

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