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“化学を基盤とするヒューマンマテリアル創成”

平成１８年度後期リサーチ・アシスタント報告書

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学年	博士課程　　3　年	
研究題目	第一原理計算による銀 - 硫化銀 - 銀系の電気特性の研究	
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I　研究の成果　（１０００字程度）

（図表も含めて分かりやすく記入のこと）

1. INTRODUCTION

Currently, much attention have been paid to a newly-developed atomic switch based on low-temperature Ag_2S,[1] which is expected to be able to reduce the size of device to nanoscale. Since the working mechanism of the atomic switch is unknown but is speculated to be closely related to the diffusion of mobile Ag ions in low-temperature Ag_2S, we investigated the diffusion of Ag ions in the low-temperature Ag_2S using first-principles calculations.

2. CALCULATION MODEL AND METHOD

In low-temperature Ag_2S, there are two types of Ag ions of equal number in one unit cell: they occupy positions close to ideal octahedral (*O*) and tetrahedral (*T*) positions of the $P2_1/c$ space group. We investigated diffusion pathways and energy barriers for the diffusion from a *T* (*O*) site to its neighboring *T* (*O*) vacancy by performing calculations using a 48-aom (4 unit cells) and a 96-atom (8 unit cells) supercell, respectively. The Nudged Elastic Band (NEB) method in VASP code was adopted. After that, molecular dynamics simulations were carried out using a 96-atom supercell (8 unit cells) using VASP code.

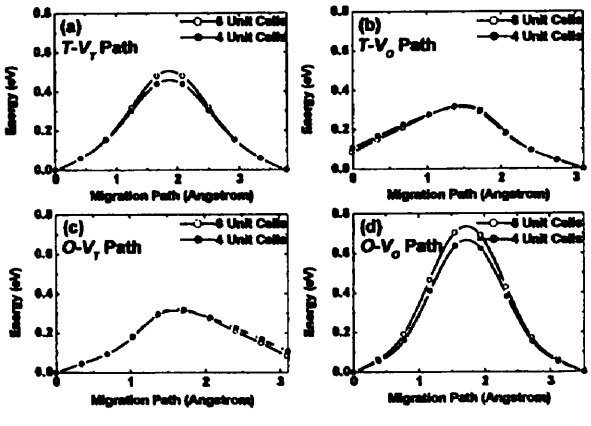

Fig.1. Energy along the migration path from (a) *T* to *T* vacancy; (b) *T* to *O* vacancy; (c) *O* to *T* vacancy; (d) *O* to *O* vacancy.

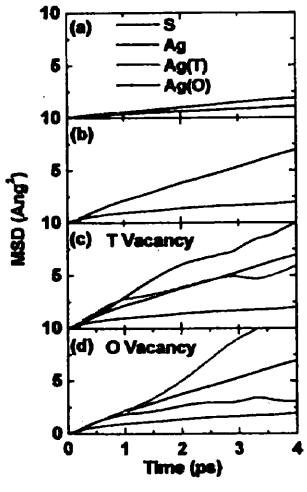

Fig. 2. Mean square displacement (MSD) of Ag and S at (a) 300K and (b) 700K, and those of Ag ions around (c) *T* vacancy and (d) *O* vacancy at 700K.

3. RESULTS AND DISCUSSION

As illustrated in Fig. 1, the diffusion energy barriers of an Ag ion from *T* to *T* vacancy, *T* to *O* vacancy, *O* to *T* vacancy and *O* to *O* vacancy by using 48-atom (96-atom) supercell are 0.461 (0.504), 0.218 (0.228), 0.318 (0.312), and 0.668 (0.734) eV, respectively, which are in good agreement with experimental values of 0.43-0.48 eV.[2] It is apparent that direct diffusions from *T* to *T* and *O* to *O* are not energetically preferable to indirect one from *T* to *O* and *O* to *T*.

Figure 2 plots the mean-square displacements (MSD) of Ag and S ions. Note that the low-temperature was assumed and a *T* and *O* vacancy were introduced in all cases. For atoms far from the vacancy , the MSD is small at 300K indicating no obvious diffusion (see Fig. 2 (a)), while Ag ions diffuse significantly at 700K (see Fig. 2 (b)). On the other hand, as seen from the MSD at T=700K shown in Fig. 2 (c) and (d), the nearest octahedral Ag (Ag(*O*)) ions around a T vacancy diffuse more than the nearest tetrahedral Ag (Ag(*T*)) ions, and the nearest Ag(*T*) ions around a *O* vacancy move more than the nearest Ag(*O*) ions. We also observed diffusions of a tetrahedral Ag ion into neighboring *O* vacancy and an octahedral Ag ion into neighboring *T* vacancy, which is consistent with the pathways of low diffusion energy barriers found in the NEB calculations.

Reference

[1]K. Terabe, T. Hasegawa, T. Nakayama, and M. Aono, Nature **433**, 47 (2005).

[2]R. L. Allen, and W. J. Moore, J. Phys. Chem. **63**, 223 (1959).

氏名　王 中長

II　学術雑誌等に発表した論文（掲載を決定されたものを含む．）

共著の場合，申請者の役割を記載すること．

（著者，題名，掲載誌名，年月，巻号，頁を記入）

学術雑誌と学会等のプロシーディングなどを以下のように区別して記入すること．

（1） 学術論文（査読あり）

（2） 学会等のプロシーディング

（3） その他（総説・本）

List of articles published or being in press during the period of mater degree

Published articles:

[1] Wang Zhongchang, Liu TianMo, Li JiaMing. Fermi energy formulae and numerical calculation of mixed additive semiconductor. Journal of Chongqing University. Vol26,No.11,53(2003). (In Chinese).

[2] Wang ZhongChang, Liu TianMo, Li Jia, Li JiaMing. Additive gas sensitive material of $ZnSnO_3$. Journal of Materials Science and Engineering. 22,5(2004). (In Chinese).

[3] Wang ZhongChang, Liu TianMo, Li Jia, Yu Long, Liu JiaMing. Preparation and its gas sensitive characteristics of nano-sized $ZnSnO_3$. Journal of Ceramic Society. 32,36 (2004). (In Chinese).

[4] Wang ZhongChang, Liu TianMo, Li Jia, Yu Long, Liu JiaMing. Enhanced sensitivity of $ZnSnO_3$ ethanol sensor by titania addition. Material Science and Eng. B. (In press). (In English).

[5] Editor: Liu TianMo, Huang WeiGuang. Co-authors: Wang Zhongchang, Yu Long, Wang Jinxing, Li Jiang. Basis of materials science. Published by mechanical industry. (2004.4). (In Chinese).

Articles in review during doctor course:

[1] Z. C. Wang, T. Kadohira, T. Tada, and S. Watanabe. First-Principles Investigation on Electronic States, Interface Structures and Electric Properties of Ag-Ag_2S-Ag System.

[2] Z. C. Wang, Tingkun Gu, T. Kadohira, T. Tada, and S. Watanabe. Frist-Principles Simulations on Migration of Ag ion in Low-temperature Ag_2S.

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III　学会において申請者が口頭発表もしくはポスター発表した論文
（共同研究者（全員の氏名），題名，発表した学会名，場所，年月を記載）
国内学会および国際学会を区別して記入のこと

Domestic Conference:

[1] Z. C. Wang, T. Kadohira, T. Tada, and S. Watanabe. First-Principles Investigation toward Electronic States, Interface Structure, and Electric Properties of Ag-Ag_2S-Ag System. Fall Meeting of Electrochemical society. Kyoto, Japan. 14/09/2006. (In English)

[2] Z. C. Wang, T. Kadohira, T. Tada, and S. Watanabe. First-Principles Simulations on Migration of Ag Ions in Low-temperature Ag_2S. The 32th Symposium on Solid State Ionics. Kyushu, Japan. 27/11/2006. (In English)

International Conference:

[1] Z. C. Wang, T. Kadohira, T. Tada, and S. Watanabe. First-Principles Study of Electrical Properties of Ag-Ag_2S-Ag System. 3rd International Symposium on Frontier Of Nanochemistry and Nanomaterials. Tokyo, Japan. 3/10/2005. (In English).