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Computational Simulation on the Electrical Conductivity of Gas Sensor Materials by Tight-binding Quantum Chemical Molecular Dynamics Method

○ 朱志剛[1], Chutia Arunabhiram[1], 坪井秀行[1], 古山通久[1], 遠藤明[1], 久保百司[1, 2], Carlos A. Del Carpio[1], 宮本明[1, 3]

[1]Grad. Sch. Eng., Tohoku Univ. (6-6-11-1302 Aoba, Aramaki, Aoba-ku, Sendai 980-8579)
[2]JST-PRESTO (4-1-8 Honcho, Kawaguchi, Saitama 332-0012)
[3]NICHe, Tohoku Univ. (6-6-10 Aoba, Aramaki, Aoba-ku, Sendai 980-8579)

【Introduction】

Metal oxide semiconductor sensors based on SnO_2 are widely used nowadays as efficient gas detection tools. The general principle of SnO_2 gas sensor is proposed to be measuring the change of the electrical conductance in response to surrounding gases. Hence, in the present work, we report the results of electrical conductivity simulation on SnO_2 by means of our original tight-binding quantum chemical molecular dynamics method.

【Method】

The bulk and (110) surface structures of rutile-type SnO_2 were optimized by CASTEP software based on density functional theory (DFT). Our original tight-binding quantum chemical molecular dynamics program, “Colors”, is used to obtain electronic structure and electrical conductivity for a given system is estimated by Monte Carlo method [2].

【Results and discussion】

The experimental lattice constants of bulk rutile-type SnO_2 were well reproduced by CASTEP program. Fig. 1(a) shows calculated partial density of states (PDOS) for bulk SnO_2 using colors program. The most important feature of the calculated bulk PDOS of SnO_2 reported here is the band gap value of 3.62 eV, very close to the experimental value of 3.60 eV. This cannot be reproduced by first-principles method, which is well known to underestimate the band gap. It can be seen from the figure that the top of valence band and the bottom of conduction band are mainly attributed to O 2p and Sn 5s orbitals, respectively. The PDOS for stoichiometric SnO_2 (110) surface obtained by Colors program is shown in Fig. 1(b). It has been reported that the stoichiometric SnO_2(110) surface exhibits surface states within the bulk band-gap region that reduce the surface band gap [2]. As shown in Fig. 1(b), the band gap of stoichiometric SnO_2 (110) surface is 2.2 eV, which is smaller than that of the bulk SnO_2 of 3.62 eV and a new surface state is presented about 0.9 eV above the top of the bulk valence band. It is known that the electrical conductivity of nondoped SnO_2 thin film is in the range of 100-500$\Omega^{-1}cm^{-1}$[3]. Calculated electrical conductivities are $1.5\times10^{-20}\Omega^{-1}cm^{-1}$ for stoichiometric (110) surface and $2\times10^{2}\ \Omega^{-1}cm^{-1}$ for oxygen deficient (110) surface. The good agreement between experimental and theoretical values for oxygen deficient surface gives the substantial evidence that the surface vacancies play an important role in the experimentally observed high conductivity of SnO_2. The conductivity of hydroxyl group and oxygen adsorption on (110) surface will be also presented at the conference.

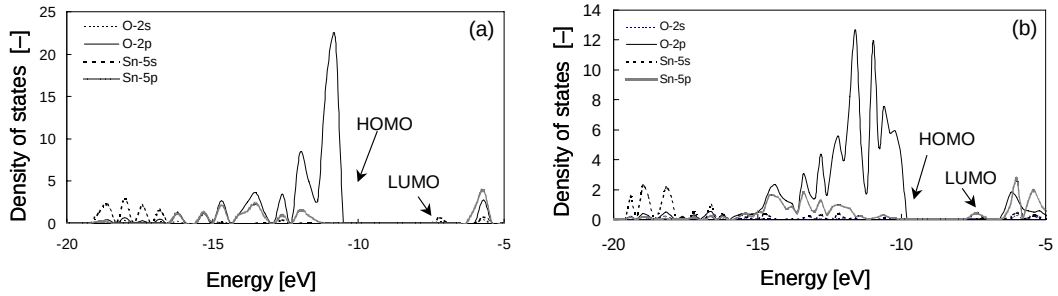

Fig. 1 Partial density of states for (a) bulk and (b) stoichiometric (110) surface of SnO_2

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