Dopability, Intrinsic Conductivity, and Nonstoichiometry of Transparent Conducting Oxides

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In_2O_3 O , -
, W
H,
( ) (“ ”) *H* *n*- W ,
H 2

μ^0

O_2 , W . ., 2 μ_{In},

3 μ

0. 4 V In_2O_3 0.73 O, 3.50 V 3.45 V W

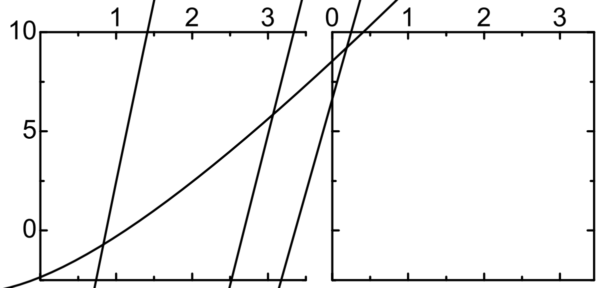
. 24 ( ). W

H_D E_F, μ E_D E_H qE_F $\sum \pm \mu^0$ μ,

E_D E_H , , q .

μ_{In}, μ_{Zn}, μ_{Sn}, μ_{Al},

μ_O ( ) ( )



1100 4 , - V_O

(. 1).

Extrinsic donors do lead to degenerate doping. . 3, Sn_{In} In_2O_3 Al_{Zn} O H E_F M, , , . W 1% In_2O_3, (O_2), . ., (. 2). - (T_a 1073 K) 30 , - $p(O_2) \gtrsim 10^{-6}$ atm, 30 $p(O_2)^{-1/8}$ (. 2). . 3, O_i - - $p(O_2)$, 1 V E_F M . O, 1% - , . 2. W $p(O_2)$, , , V_{Zn} . $p(O_2)^{1/4}$ $p(O_2) \geq$ 10^{-6} atm (. 2), -

($E_F < E_C$). - V_{Zn} E_F N M, . 13,15 , O. O , . ., n $10^{17}\ \mathrm{cm}^{-3}$ (T_g 1423 K) 31 , , . 31 , V_{Zn} , $c(V_{Zn})$ $2 \times 10^{15}\ \mathrm{cm}^{-3}$ $p(O_2)$ 1 atm .

Large equilibrium oxygen deficiency. In_2O_3 O ($\lesssim$1%) O- - 4,8 , , , O , . O - V_O, In_2O_3 O (. 1). In_2O_3, O $2 \times 10^{20}\ \mathrm{cm}^{-3}$ 0.4% O T 1673 K (. 1,), O 1% . 4 O, V_O $4 \times 10^{19}\ \mathrm{cm}^{-3}$ (0.1%) T 1373 K (. 1) - , . 5 . V_O - O - O 8 , $c(V_O)$ $10^{17}\ \mathrm{cm}^{-3}$ O 32 .

Excited O vacancies can lead to (persistent) photoconductivity. V_O O . 14, 16 , V_O^0 , - a_1^2 , . , a_1^0 , , 16 . In_2O_3, M , . ., O 20 , a_1^0 . , F - (V_O) , In_2O_3 O.

Coexistence of coloration and conductivity. - - , In_2O_3 ( ) 4 O ( ) 5 , . O , (. ., - V_O^0 V_O, e), , . V_O^0 V_O, e V_O V_O^2, e , 1.8 1.6 In_2O_3 - ( ), 2.8 2.4 V O 16 . V

, -
V_O (. 1), -
ι In_2O_3 O,
33
In_2O_3. - ι -
10^{17} 10^{19} cm^{-3} [4,5,7] ι ι ι -
ι ι ,