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Defect chemistry of alkaline earth metal (Sr/Ba) titanates



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ABSTRACT

Defect reactions and reaction parameters of SrTiO₃ and BaTiO₃, published in literatures, over the doping range from acceptor to donor, temperature range from room temperature to >1500 K and oxygen partial pressure range of 10⁻²⁵ to 1 bar are summarized in this work, and a Windows® based *DefectChemCal* program is developed. With the program, one can calculate the defect concentrations and the electrical properties of acceptor and donor-doped SrTiO₃ and BaTiO₃, and the validity of the program is demonstrated by comparing the calculation and experimental results.

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Nomenclature

A	acceptor
$A^{\times}$	acceptor atom
A'	acceptor ion with one negative effective charge
A''	acceptor ion with two negative effective charges
$\{A'-V_{\text{O}}\}^{\cdot}$	defect association of acceptor ion and oxygen vacancy
D	donor
$D^{\cdot}$	donor ion
$[D^{\cdot}]$	concentration of donor ions
$D_{V_{\text{O}}}$	diffusion coefficient of oxygen vacancy
e	elementary charge
e'	electron
E_{A}	energy level of acceptor
E_{g}	band gap
E_{S}	energy of Schottky reaction
E_{R}	energy of reaction
Fe_{Ti}'	Fe on Ti site with one negative effective charge
$h^{\cdot}$	hole
K_{A}	equilibrium constant of acceptor ionization reaction
K_{ass}	equilibrium constant of defect association reaction
K_{A}^0	pre-exponential factor of equilibrium constant of acceptor ionization reaction
k_{B}	Boltzmann constant
K_{Fe}	equilibrium constant of Fe ionization reaction
K_{i}	equilibrium constant of band-band reaction
K_{i}^0	pre-exponential factor of equilibrium constant of band-band reaction
K_{Ox}	equilibrium constant of oxidation reaction
K_{Ox}^0	pre-exponential factor of equilibrium constant of oxidation reaction
K_{Red}	equilibrium constant of reduction reaction
K_{Red}^0	pre-exponential factor of equilibrium constant of reduction reaction
K_{S}	equilibrium constant of Schottky reaction
K_{S}^0	pre-exponential factor of equilibrium constant of Schottky reaction
$\text{La}_{\text{Sr}}^{\cdot}$	La on Sr site with one positive effective charge

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