

# Abbreviations, Symbols and nomenclature

## List of Abbreviations

Abbreviation	Full Meaning
ANSTO	Australian Nuclear Science and Technology Organization
BPEO	Best Practicable Environmental Option
DFT	Density Functional Theory
DoE	United States Department of Energy
EPA	Environmental Protection Agency
GGA	Generalised Gradient Approximation
HADES	Harwell Automatic Defect Examination System code
HF	Hartree-Fock
HLW	High Level Waste
ILW	Intermediate Level Waste
IT-SOFC	Intermediate Temperature SOFC
LDA	Local Density Approximation
LLW	Low Level Waste
MC	Monte Carlo
MCFC	Molten Carbonate Fuel Cell
MD	Molecular Dynamics
MINATOM	Russian Ministry for Atomic Energy
NRC	Nuclear Regulatory Commission

Abbreviation	Full Meaning
PAFC	Phosphoric Acid Fuel Cell
PEMFC	Proton Exchange Fuel Cell
SOFC	Solid Oxide Fuel Cell
US	United States
UK	United Kingdom
VLLW	Very Low Level Waste
WIPP	Waste Isolation Pilot Plant
YAG	Cubic Yttrium Aluminium Garnet
YAM	Monoclinic Yttrium Aluminium Garnet
YAP	Yttrium Aluminium Perovskite
QMD	Quantum Molecular Dynamics

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## List of Symbols

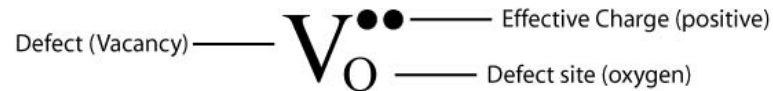
Symbol	Meaning
Å	Angstrom
Bq	Becquerel
Cm	Coulomb meter
N	Newton
m	meter
ppm	parts per million
K	Kelvin
eV	electron volt
$\Delta H_F$	Enthalpy of Formation
$t$	tolerance factor
$R_A$	A cation radius
$R_B$	B cation radius
$R_O$	Oxygen anion radius
$\alpha_D$	Dielectric Polarisability
$[\ ]$	Miller notation for a direction
$\langle \rangle$	Miller notation for a family of directions
$( )$	Miller notation for a plane
$\{ \}$	Miller notation for a family of planes

## Kröger-Vink Nomenclature

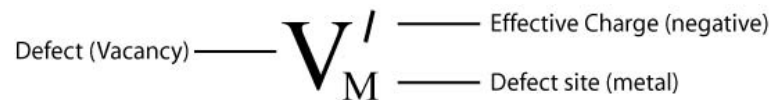
Kröger and Vink proposed a nomenclature to describe defect chemical reactions [3]. The point defects are assumed to be dilute species, with the solid being the solvent. The nomenclature has three constituents; the body, the superscript and the subscript. The body represents the chemistry of the defect itself, ie.  $V$  for a vacancy or  $Mg$  for a magnesium ion. The superscript represents the effective charge of the defect relative to the perfect lattice; an effective positive charge is represented by a dot ( $\bullet$ ), a negative charge by a prime ( $'$ ). The subscript represents the site of

the defect, eg.  $i$  indicates a defect at an interstitial site,  $Mg$  represents a magnesium lattice site.

Assuming a binary metal oxide ( $MO_2$ ), using Kröger-Vink nomenclature, an oxygen vacancy is:



a metal vacancy is:



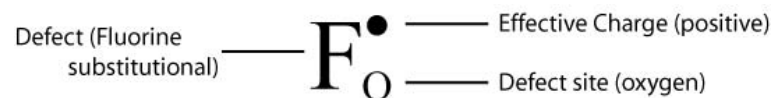
a metal interstitial is:



a cation substitutional is:



an anion substitutional is:



and a metal ion on its lattice site is:

