ZINC OXIDE:

NEW INSIGHTS INTO A MATERIAL FOR ALL AGES

BY

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BSc. Chemical Engineering

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Certificate of authorship/originality

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Amir Moezzi

11/10/2012

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Antoine Laurent Lavoisier (1743-1794), "father of modern chemistry", in 1789 for the first time suggested that "Flowers of zinc" be named "zinc oxide" reflecting the elements in the nomenclature of compound.

"We think only through the medium of words. Languages are true analytical methods. Algebra, which is adapted to its purpose in every species of expression, in the most simple, most exact, and best manner possible, is at the same time a language and an analytical method. The art of reasoning is nothing more than a language well arranged."

Antoine Laurent Lavoisier, Traité Élémentaire de Chimie, 1789

Adopted from translation by Robert Kerr, 1790

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Abbreviations

- α_L = coefficient of expansion
- λ = thermal conductivity value

 $Ac = acetate (CH_3CO_2)$

- ASTM = American Society for Testing and Materials
- a.m.u = atomic mass unit
- BAW = bulk acoustic wave
- BET = Brunauer, Emmett and Teller
- BZA = basic zinc acetate
- BZC = basic zinc carbonate
- BZCl = basic zinc chloride
- BZN = basic zinc nitrate
- BZS = basic zinc sulphate
- CHM = composite hydroxide mediated
- C_p° = specific heat capacity
- CP-MAS = cross polarisation magic angle spinning
- cr = crystalline
- CRT = cathode ray tube
- CVD = chemical vapor deposition
- D2EHPA = di-2-ethyl hexyl phosphoric acid
- DMS = dilute magnetic semiconductors
- DSC = dust settling chamber
- DTA = Differential thermal analysis
- E_a = apparent activation energy
- EAFD = electric arc furnace dust

EG = ethylene glycol

ENR = epoxidised natural rubber

EPDM = ethylene propylene diene monomer

FID = Free induction decay

FTIR = Fourier transform infrared

FWHM = Full width at half maximum

G = Gibbs free energy

GTL = gas-to-liquid

H = Enthalpy

 $H_2O_2 =$ hydrogen peroxide

HCE = hexachloroethane

HDPE = high density polyethylene

HDS = hydroxy double salts

HVPE = hydride vapor phase deposition

ICP-MS = Inductively coupled plasma mass spectrometry

ISP = imperial smelting process/irregularly-shaped particle

ITO = indium tin oxide

 $K_{\rm atm} =$ equilibrium constant

LDH = layered double hydroxide

LED = light emitting diodes

MBE = molecular beam epitaxy

MBT = mercaptobenzothiazole

MCP = mechano-chemical process

MOCVD = metal organic chemical vapor deposition

MS = mass spectrometry

M.W = molecular weight

 $Na_2S_2O_4 =$ sodium dithionite

 $NaHSO_2 \cdot CH_2O \cdot 2H_2O = sodium$ formaldehyde sulfoxylate

NMR = Nuclear magnetic resonance

OECD = Organisation for Economic Cooperation and Development

PFD = process flow diagram

phr = parts per hundred

PMA = polymer-modified asphalts

PP = polypropylene

ppb = parts per billion

ppm = parts per million

PVC = poly vinyl chloride

PVDF = polyvinylidene fluoride

rpm = revolutions per minute

RT = room temperature

SAW = surface acoustic wave

SRB = sulphate-reducing bacteria

SEM = scanning electron microscopy

SHG = special high grade

s-SBR = solution styrene-butadiene rubber

SVP = seeded vapor phase

T = temperature

TCO = transparent conductive oxides

TE = thermoelectric

TEM = transmission electron microscopy

TG = thermogravimetric

TGA = thermogravimetric analysis

TMTD = tetra-methyl-thiuramdisulphide

- UV = ultra violet
- VLS = vapor-liquid-solid
- VPT = vapor phase transport
- VS = vapor-solid
- w/v = weight to volume
- w/w = weight to weight
- XNBR = carboxylated nitrile rubber
- XRD = X-ray diffraction
- $ZnAc_2 = zinc acetate$
- $Zn(CH_3COO)_2 \cdot 2H_2O = zinc$ acetate dihydrate
- ZDDP = Zinc dialkyldithiophosphate
- $ZnSO_4 \cdot 7H_2O = zinc sulphate heptahydrate$
- ZT = figures-of-merit

Publications and conference presentations associated with this work

- Moezzi, A., "Nano vs. Active Zinc Oxide". Presentation at the International Conference on Nanosciences and Nanotechnology (ICONN), Sydney, Australia, February 2010.
- Moezzi, A., Cortie, M and McDonagh, A. "Aqueous pathways for the formation of zinc oxide nanoparticles". Dalton Transactions 40(18) (2011) 4871-4878.
- Moezzi, A., Cortie, M and McDonagh, A. "Zinc Oxide Particles: Synthesis, Properties and Applications". Chemical Engineering Journal 185-186 (2012) 1-22.

Abstract

Zinc oxide is an important material industrially and scientifically. It has a long history dating back to more than four thousand years ago. It has applications in rubber production, cosmetics, pigments and ceramics. The properties of zinc oxide such as porosity, specific surface area and optical properties change as a result of changing the synthetic method and process conditions. The suitability of ZnO for different applications depends on the properties of the material, which in turn are influenced by synthetic routes.

Knowledge of the processes underpinning the various synthetic techniques is key to understanding the properties of the ZnO end-product. In this work, various synthetic techniques have been investigated that may be amenable to large-scale production. The resultant materials were studied and important insights were obtained. For example, it was found that the precursor materials and method of processing for the production of zinc oxide have important roles in controlling the properties of the product such as specific surface area, crystal morphology, particle size and amount of surface hydroxyl groups embedded in the product.

In single-stage production methods, zinc oxide is precipitated directly from a zinc solution. Influences of reaction temperature, concentration of the reactants and feeding techniques on the properties of the products were determined.

In multi-stage routes, intermediate zinc-bearing materials including zinc peroxide and zinc hydroxy carbonate, sulphate, chloride, nitrate and acetate were synthesised. These intermediate materials were then used as precursors for the formation of zinc oxide particles. Relationships between the properties of the precursor zinc-containing compound and the end-product zinc oxide were studied and unexpected results were obtained. For example, it was shown that specific surface area of the zinc oxide product depends significantly on the precursor material from which it is produced. Techniques were investigated that can produce multiple important zinc-bearing compounds and it was found that it could be engineered by selection of the appropriate precursors and process conditions.