**Hematite (α-Fe2O3)** is one of the most important, stable, non-toxic, nature-friendly and corrosion-resistant metal oxides.

Hematite crystallizes in the rhombohedral lattice system, and it has the same crystal structure as ilmenite and corundum(Al2O3). Hematite and ilmenite form a complete solid solution at temperatures above 950 °C (1,740 °F).

Fe2O3 has many other phases like **beta-Fe2O3, epsilon-Fe2O3** and **gamma-Fe2O3 (maghemite)**. But **alpha-Fe2O3** is the most stable of all the phases.

**Structural Properties:**

**Crystal System:** Hexagonal (trigonal)

**Lattice Parameters:**

\[
\begin{align*}
a = b &= 5.03 \text{ Angstroms} \\
c &= 13.74 \text{ Angstroms} \\
\alpha = \beta &= 90 \text{ degrees} \\
\gamma &= 120 \text{ degrees.}
\end{align*}
\]

I am also attaching a [Crystallographic Information File](fe2o3 alpha hematite.zip).

Alpha-Fe2O3

You can download it and open it using softwares like [Avogadro](https://avogadro初心者手順.com) or [Vesta](http://vesta.cns.gmu.edu/). These are good visualization tools to build and visualize the crystal structures.

**Color:** black to steel or silver-gray, brown to reddish brown, or red.

The following are some of the pictures of the Alpha-Fe2O3 crystal:

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Alpha-Fe2O3 (Cell)

The following is a simulated XRD (X-Ray Diffraction) Pattern for the Alpha-Fe2O3 crystal:
Experimental XRD Pattern of alpha-Fe$_2$O$_3$

The following is a picture of the Density of States for alpha-Fe$_2$O$_3$ calculated using DFT+U (Density Functional Theory+Hubbard Parameter). The plot has been obtained from materialsproject.org.
The following is a calculated electronic band structure found using DFT+U:
Alpha-Fe$_2$O$_3$ Band Structure using DFT+U

**Band Gap**: 2.1-2.3 eV (lies in the visible range)

Therefore, Alpha-Fe$_2$O$_3$ is an *n-type semiconductor*.

**Synthesis**

Synthesis of iron oxides in the nano range for various applications has been an active and challenging area of research during the last two decades. The processes include careful choice of pH, concentration of the reactants, temperature, method of mixing, and rate of oxidation (Domingo et al., 1994). The morphology of the iron oxide particles depends on the competition between several processes like nucleation, growth, aggregation and adsorption of impurities (Cornell and Schwertmann, 1996). However, in many cases it is not possible to precipitate specific iron oxide particles directly in the desired size and shape. Instead, the synthesis must be done by the transformation of another iron oxide precursor particle (Baker et al., 2000). The sensitivity of the preparative method complicates both the reproducibility and scale up of the process. Recently, several colloidal chemical synthetic procedures have been developed to produce mono-disperse nanoparticles of various materials.

**Applications**

Various applications of iron oxides/hydroxides/oxyhydroxides in nano form can be attributed to the difference in behaviour of particles in nano scale as compared to their bulk counterparts. The nano particles usually have much larger surface area due to their smaller size and can reduce the volume required to achieve same effect when used.
**As a colouring and coating material:**

The use of hematite and other iron oxides as natural red ceramic pigments has been practiced since prehistoric times. The iron oxides such as magnetite, hematite, maghemite and goethite are commonly used as pigments for black, red, brown and yellow colours respectively. Predominantly natural red iron oxides are used in primers for steel constructions and cars reducing corrosion problems. World consumption of iron oxide pigments comprises of 63% in synthetic form and 37% from natural resources. The construction sector – roof tiles, paving slabs and other concrete products – accounts for a major chunk of total world consumption. By reducing the particle size to nano range, transparent iron oxide pigments can be obtained. Manufacturing process of transparent iron oxide pigments depend on the control of physical and surface chemistry properties. Particle size is optimized to ensure that minimal light interference occurs thus maximizing transparency. In general particle size from 2 to 10 nm increases transparency 310 times when compared to the bulk form (Elizabeth, 1992). Now a days such transparent iron oxide pigments are preferably used. These have good stability to temperature, the red can resist up to 3000 °C while the yellow, black, green and brown can withstand up to 160 °C. These are strong absorbers of ultraviolet radiation (Sreeram et al., 2006) and mostly used in automotive paints, wood finishes, construction paints, industrial coatings, plastic, nylon, rubber and print ink. The excellent weather fastness, UV absorption properties, high transparency and color strength makes trans-oxide to enrich the colors, increase color shades when combined with organic pigments and dyes.

Nano iron oxides exhibit very different magnetic properties which can be used for soft ferrites and biomedical applications including drug delivery and magnetic resonance imaging. Down to the nanoscale, superparamagnetic iron oxide nanoparticles can only be magnetized in the presence of an external magnetic field, which makes them capable of forming stable colloids in a physio-biological medium. Their superparamagnetic property, together with other intrinsic properties, such as low cytotoxicity, colloidal stability, and bioactive molecule conjugation capability, makes such nanomagnets ideal in both in-vitro and in-vivo biomedical applications.

**Application of Fe2O3 nano powders**

1. Fe2O3 are used as **pigment and coating additives** to aesthetically enhance, strengthen and protect concrete and other materials. For example, iron (III) oxide is used to fill the pores in concrete and reinforce the structure so calcium chloride and magnesium chloride will not easily penetrate the concrete. This extends the longevity of the concrete.

2. Iron Oxide nanopowder (fe2o3) are used as core sand additives to improve sand quality and suppress the incidence of several sand/binder related defects for example lusterous carbon defects, surface carbon pick up in stainless steels, finning veining, piholing and orange peel defect in shell moulding sands etc.

3. Fe2O3 nanopowder also apply to the exothermics, welding rods, offshore drilling muds and colourants in both building products and brown glass beverage bottles.

**Transparent Pigment Used Alpha Non-magnetic Nano Fe2O3 Powders**

1. Nano-iron, with high purity, low impurity content, small particle size, particle size uniformity, high temperature, and good dispersion.

2. Nano-iron is a new nano-materials, can be widely used in coatings, paints, inks, and chemical materials. Because of its small particle size, it has a strong UV absorption, high saturation, high color strength, transparency and other characteristics, and non-toxic, odorless, heat, acid, and therefore use is widespread.
Nano Fe2O3 features:

1. Excellent ultraviolet absorption capacity, high transparency, non-toxic, no color migration.
2. Acid, alkali, light, weather.
3. Heat, water, solvent resistance.
4. Corrosion resistance: a strong corrosion resistance, compared with similar products stronger than doubled its antiseptic properties, can greatly enhance the anti-rust paint.
5. Wear: asbestos, plastic products such as: brake pads, brake pedal, etc. can improve the wear resistance.

Nano Fe2O3 powders Applications

1. Due to the heat resistance of iron-red has, so for a variety of plastics, rubber, ceramics, asbestos products, coloring;
2. For rust, middle and low paint. For cement products, tile coloring;
3. In the fiber of the paste, security coatings, xerography, ink application areas are very extensive.
4. Cosmetics: iron oxide nanoparticles non-toxic and strong ability to absorb ultraviolet resistance, apply cosmetics industry.
5. Powder coating: iron oxide nanoparticles in the temperature 300 ℃ color change.
6. In the medical, biological applications in the field.
7. In catalysis, sensors application.

References:


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