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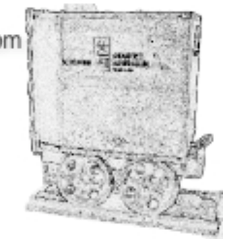

Titanium dioxide (Anatase, Rutile)...

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ANATASE CAS-Reg. No. 1317-70-0
RUTILE CAS-Reg. No. 13463-67-7

Titanium dioxide pigments have surpassed all white pigments, concerning the importance.

There are two different ways to produce titanium dioxide: the **sulfate process** and the **chloride process**. The larest part of TiO_2-pigments is the manufactured by the first method; the **chloride process**, however is getting more and more important. The products sold by **SCHERUHN** follow the **sulfate process**.

After the crystal modification, there is a distinction of the **titanium dioxide pigments** into **anatase** and **rutile**. They exist as **uncoated** and as **chemically coated pigments**, the latter to improve the qualities.

The main part is **chemically refinished**. To increase the **dispersibility** and especially the **photochemical stability**, photochemical inactive substances are employed; **hydroxides** and **oxides** of, for instance, **silicon** and/or aluminum are precipitated on the titanium dioxide.

Recently, the producers have tried to **invent organic after-treatments** for special applications of titanium dioxide pigments. **Dispersibility** and **lustre** are improved enormously.

Chemical properties:

Titanium dioxide is **chemically resistant** against atmospheric influences as well as hydrogen sulfide, sulfur dioxide, oxygen, ammonia etc. It neither oxidizes nor does it reduce. **Hydrofluoric acid** and **hot concentrated sulfuric acid** can attack titanium dioxide. Furthermore, it does neither react exposed to **organic** or **anorganic** acids and bases, nor exposed to solvents or hydrochloric acids. Titanium dioxide is neutral, **extremely temperature resistant** and has **no toxic effects**.

Physical properties:

Titanium dioxide is **polymorphous**. There are three crystal modifications, that even occur naturally:

- **anatase (tetragonal)**
- **brookite (orthorhombic)**
- **rutile (tetragonal)**

Yet, only rutile and anatase modifications have an influence on the production of pigments.

Rutile is the **most stable** modification of titanium dioxide. Anatase and brookite are just the opposite; they are metastable.

Between rutile, anatase and brookite there exist **characteristic differences in the crystal lattice**. All three have in common that each titanium ion is octaedric, surrounded by six oxygen ions. It has a coordinate number of six. To maintain a stoichiometric proportion of 1 : 2 between the titanium- and oxygen, the octaeders in the crystal lattice must be located in a way that each oxygen ion belongs to three octaeders. The difference lies in the local position of the octaeders.

Density:

The **density** is the first quality that ought to be mentioned among the crystal modifications. The rutile lattice has a **higher density** because of the **denser packing**.

- Rutile: 4.2 g/cm³
- Anatase: 3.9 g/cm³

Hardness:

Because of the same reason, the different packings of the lattice pieces and the binding energy, there exists a difference concerning the hardness.

According to Mohs:

- **Rutile: 6.0 - 7.0**
- **Anatase: 5.5 - 6.0**

Particle size and -shape also play an important role concerning **abrasion**, caused by the natural **hardness**.

Refractive Index:

The TiO_2 modifications are **optically anisotropic**, i.e. the optical behavior is characterized by two **refractive indices** (ordinary and extraordinary ray). The refractive indices decrease with an **increasing wavelength**. The average values (for 589 Nm) for anatase and rutile, based on the vacuum, are:

- **Rutile: 2.80**
- **Anatase: 2.55**

Optical properties:

Light scattering power and refractive index:

Titanium dioxide pigments possess a very **high light scattering power**. This is responsible for the **good covering power** of coatings, for the **opacity of plastics** and other pigmented materials as well as for the lightening of colored media.

The high light scattering power is related to a high refractive index, but this is not the final answer to the light scattering power of a pigment. A titanium dioxide crystal seems **transparent**, contrary to a titanium dioxide pigment. In both cases it is the **same chemical** and concerning the lattice structure **completely identical material**. Just the **geometric relations** are different. On one hand, there is a relatively large crystal, on the other hand, there are various particles of an extraordinary fineness. The scattering power depends not only on the refractive index, but also on the **fineness of the particles**.

Light scattering power and particle size:

Rutile crystals are **transparent**. They seem white, when pulverized. The reason is the fast increasing number of **reflecting** surfaces when the particle size is reduced. The disorderly statistic distribution of these surfaces leads, according to the rules of the **regular reflection** to a **diffuse scattering**. This scattering reflection requires that the size of the particles/ the reflecting surface does not fall below a minimum value, which is necessary for the creation of an **even, homogenous wave front**.

The maximum is at a particle diameter of half the wave length of light. This result and the demand for a maximum scattering of the incoming light lead to the best particle size. This is the particle size belonging to this diffusion maximum.

This explanation, however, is only valid for an **undisturbed diffusion** (low concentration of pigment volume) and a **fixed refractive index difference**. For each CPV and for each refractive index difference an optimum of the particle size can be evaluated. The mathematical treatment of the relations among the intensity of diffusion radiation, the refractive index and the particle diameter is part of the **Mie theorem**.

Tone and brightness:

According to the DIN 55 980, the tone of an almost white or uncolored sample is the **low percentage** of color, deflecting the color of the sample from the ideal white. Uncolored can be called the color-place of the light.

When all wavelengths of the visible light are completely reflected by a body, we talk about ideal white. The reflecting spectra of anatase and rutile pigments, however, show lower reflecting values in the blue part of the visible spectrum, when white illuminated. The rutile pigment decreases stronger than the anatase pigment. Therefore the anatase pigment has a lower yellowish hue than the rutile pigment. All other wavelengths imply a higher reflecting spectrum of the rutile pigments compared to the anatase pigments. Therefore, rutile is brighter.

The yellowish hue depends on the TiO_2 pigments as well as the particle size distribution. It **increases** when the **most frequent diameter** of the volume distribution is larger than the best one and it **decreases** when it is smaller than the best diameter.

Yellowish hue and a brightness characterize white coatings; bluish hue and brightness characterize grey coatings. The tone is determined by the **difference** of the reflecting values of the colorimeters **Rx and Rz**. The yellowish hue is defined by the **difference (Rx - Rz)**. The **higher** the (Rx - Rz)- value, the higher is the yellowish hue and the higher is the deflection of the ideal white. A higher (Rz - Rx)- value at greyish coating makes the tone seem more bluish and purer.

Gloss:

Several factors are responsible for gloss of a paint system, like **pigment concentration**, **particle size** and **granulomeric composition** and **degree of dispersion in the binder system**. **Low pigmented** varnishes usually give a **high gloss**. The gloss decreases with an increasing degree of pigmentation. This **loss of gloss** is caused by the **definite size** of the pigments. If the particles are **right underneath** the film surface, they form tiny **elevations** and do not longer **reflect** the light focused, but **diffuse**.

The higher the pigment concentration, the higher is the number of gloss reducing particles.

Furthermore, the gloss is determined by the **pigment particle size**. The particle size distribution of the used pigment also influences the quality. In general: **the finer/smaller the pigment particle diameter, the better the gloss**. The distribution ought to be very dense, too. Yet, agglomerations and flocculates in a varnish can be several times larger than the primary particles, leading to a loss of gloss. Therefore, the pigment **must be completely dispersed** and this condition must be **maintained**. Finally, the **distribution condition** of a pigment, in the layers close to the surface, is **decisive** for the gloss of a titanium dioxide pigment.

Weather resistance:

The phenomena that occur when coatings or plastic coats are exposed to **natural weathering** are various, depending on the chemical qualities of the pigment, the binder and the physical properties of the entire system. Weather resistance means **resistance** against **all meteorologically based influences**.

Anatas is **not** be suitable for outdoor using.

The damages are: loss of gloss, embrittlement, fading, chalking.

Influence of crystal modification, lattice stabilizatuon and after-treatment

The **photoactivity** of various $Ti0_2$- pigments is different. The **anatase** modification has a **higher** one than the **rutile**. To **reduce** the photoactivity of $Ti0_2$- pigments, the particles are either coated, i.e. after-treated, or special substances are implemented in the lattice of the titanium dioxide.

Bibliography:

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- Geächter/Müller: Kunststoffadditive/3. Ausgabe

Our product range:

Please contact us for more information about specific products (link: Contact and inquiries). We are looking forward to provide you with professional advise and a free quote.

It's a matter of course that we are also on your side with professional advise and offer detailed product-specific datasheets as well as further technical documentation.