



What happens to light when it interacts with a particle?

Because the surface of a particle produces an electromagnetic field due to the presence of electrons and since light represents an electromagnetic radiation, light can interact to produce a phenomenon that is described as diffraction. In diffraction, at some distance from the particle in the direction of the incident light, a pattern will develop which is dependent upon the size of the particle and the wavelength of the incident light. From this pattern, information can be obtained which is related to the size of the particle.

Some materials do not transmit light, but they absorb the light energy. In these cases, the substance can be assumed to have an extremely high refractive index as well as a large imaginary component (see Transparent Particles section below). Under these conditions the calculations can be those described by Fraunhofer.

Light can also be reflected from the surface of a particle and the use of such data for particle size measurement would be the subject of a different issue.

A third occurrence of light interacting with a particle is a special case and occurs when the particle is somewhat transparent to the incident light. In this case light can pass through the particle much as it would through a diamond. In the case of a diamond, the light is refracted and produces the well-known glitter; however, light passing through a particle may add to the diffraction pattern for a given particle. This effect will be discussed below.

What is each of the above dependent upon and how do they interact?

As mentioned above, diffraction is solely dependent upon the size of the particle. Reflection has no effect on diffraction but may affect refraction if the surface is sufficiently reflective. The effect on refraction would be to limit the amount of light entering the particle and thus reduce the effect of refraction on a diffraction pattern.



Refraction can have considerable impact on a diffraction pattern, but the magnitude of the effect is highly dependent upon the size and shape of the particle. A sphere will transmit the same refraction pattern regardless of the orientation posed to the incident light. In a measuring system where the spherical particle is constantly changing orientation with respect to the incident light, the pattern is always identical and can give rise to well-defined, reinforced extraneous light information that can distort or interfere with the computation of particle size from the diffraction pattern. (**Figure 1**).





Scattered light is concentrated at one place. Tumbling has no effect.



Fig.1: Secondary peak is Interference (combination) of patterns resulting from light refracted through the sphere and diffracted off the surface.

The impact of the refracted light is also affected strongly by the shape of the particle. Non-spherical particles can also refract light and may produce a pattern that is superimposed on the diffraction pattern as a spherical particle may. However, the effect is somewhat different. Remember that the particles are in motion and will tumble as a result of the motion. Each portion of the particle will



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provide a new and different surface for the light to enter and be refracted. Upon exit from the particle, a new refraction pattern emerges which is superimposed on the diffraction pattern. The reinforcing effects observed with a spherical particle do not occur. The refracted pattern is spread across the diffraction pattern as a somewhat constant pattern and affects the diffraction pattern to much less an extent than it affects a spherical particle. (**Figure 2**)



Fig.2: Note that the secondary peak from the previous slide is greatly diminished. Light transmitted through non-spherical particles is more spread. Thus, Mie calculations are modified to satisfy this difference from perfect spherical particles.



How does one correct for potential errors in the diffraction pattern?

For spherical particles, the well-accepted concepts embodied in a theory developed by Gustave Mie may be used. This compensation is popularly termed "Mie Theory" which describes the effect of spherical particle shapes on light. It includes the aspects of refractive index of the particle in relation to the refractive index of the surrounding medium as well as the scattering efficiency (See footnote for definition) of the transparent particle. If the particles are not transparent (such as in the case of carbon black), Mie compensation for refraction is not required while calculation for scattering efficiency must be included. For Microtrac instruments, materials such as dark pigments, carbon black, and metals are considered to be light absorbing (non-transparent). An appropriate selection in Microtrac software addresses this situation where Fraunhofer calculations can be used.

Transparent particles

Consider only the case of transparent particles. Also consider that the refractive index has two terms that might be considered to act independently of one another to some degree. These two are recognized by the name's real component and imaginary component of refractive index. Each has a particular effect on the compensation in combination with scattering efficiency according to "Mie Theory". The assumption that refractive index has no effect on light scattering (true in the case of carbon black) will reduce Mie Theory to the well-known Fraunhofer diffraction algorithm. Errors can occur in the particle size distribution if Fraunhofer diffraction is applied in situations where the particles are transparent and thus require Mie theory for spherical particles or other compensation for non-spherical particles.

N= m-ik where N is the total refractive index which is a combination of the real component (m) for a substance compared to a vacuum and the imaginary component (ik). The terminology extends from the study of complex numbers. In the case of particle size measurement with particles suspended in a fluid, the value k represents the extinction co-efficient (related to the absorption coefficient of the material and the wavelength), i is $\sqrt{-1}$ and m is the relative refractive index (RI sample/RI fluid each of which has been measured compared to a vacuum). To summarize, pure diffracted light is the desirable information that should be used for particle size measurement. The relative refractive index defines where the exiting light will focus and spread while the imaginary component is an indication of the intensity of the refracted light. If the imaginary component is very low, the intensity of the refracted light will be high.

Thus, for alumina the equation would be N = 1.76/1.33 - ik. The equation can be fulfilled by knowing the value for ik. Unfortunately, such values are NOT readily available in the literature and are difficult to obtain experimentally. Another consideration of the use of the imaginary component is evaluating its influence in calculation of N and the Mie compensation.

Since this discussion is a non-mathematical, explanatory, conceptual approach, mathematical proof of the following is not provided, but the reader is encouraged to study the area as it is fully developed from Maxwell's treatment. Summary of the effects of an RI value and its corresponding imaginary component for a particle is presented below.



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Spherical, Transparent Particles (Figure 1)

- a. When particles are smaller than 1 micron, transparent and not highly light absorbing (e.g. low index glass), the light path through the particle is very short and absorption of the incident light does not occur and the imaginary term can be assumed to be zero. Remaining is the relative refractive index (ratio of RI values), which continues to have an effect on the pattern resulting from light refracting through the particle.
- b. When particles are larger than approximately 10-30 microns, the amount of light transmitted is very low and refraction in general has a very small effect. At sizes much larger than this, the Fraunhofer approximation equations can be used to calculate particle size.
- c. Within the range of approximately 1 10 microns, there can be effects resulting from the absorption of light, but only if the value for k is of the order 0.5 1.0 (high imaginary values). Values considered to be high would include carbon black (0.66i), and metals (imaginary component can be very high, m is very low due to high reflectance: thus, no correction for refraction required and can be treated as Fraunhofer diffraction).

Non-spherical, Transparent Particles (Figure 2)

- a. If the particles are not spherical but are transparent, the compensation (calculation) is not the same as for spherical particles. For non-spherical shapes, particle orientation is constantly changing (Figure 2). The refracted components then produce a combined refraction pattern due to the many orientations presented to the incident light.
- b. The resulting pattern has little definition when combined with the diffraction pattern but still requires some compensation. Since the imaginary component is a minor correction to the relative (real) component, its effect is negligible and can be disregarded. This is shown in Figure 3 where three cases are considered: transparent spherical, transparent non-spherical and absorbing. At the size considered in the diagram, note that a strong resonance feature exists for spherical particles. In comparison, the transparent non- spherical particle having the same size shows extensive reduction of the resonance to the extent that it approaches a completely absorbing particle. In this case, the strict Mie (spherical) calculations should not be used and explains the use of Modified Mie calculations in Microtrac instruments. Also, the refractive component is much less important (but not completely). Since the imaginary component is usually a weak secondary effect compared to the real component, the imaginary component for materials having non-spherical shape, has negligible or insignificant importance.

With what has been discussed, how can the compensation be performed?

From the foregoing, several approaches could be developed regarding the issue of refractive index. In one, the concept can be completely disregarded and Fraunhofer diffraction can be used exclusively, but this may result in extraneous refracted light at wider scatter angles which may in turn result in erroneous reporting of distribution tails particularly at the finer particle portion. Mie scattering for spherical particles may be used in combination with relative and imaginary refractive index values, if both are known. This could be applied to both spherical and non-spherical particles (as supported by **Figure 3**, this may be an unwise choice of calculation options for both types of particle shapes).



Fig.3 : The response of light to a 6 - micron particle having Refractive Index = 1.54. Major peaks (size) are purposely drawn displaced because the patterns are identical for size indication. Note on the right side that non-spherical transparent particle refraction is more similar to an absorbing response than to spherical curve. Microtrac MRB developed special calculations (Modified Mie Theory) that are used to take this effect of non-spheres into consideration.

Usually the imaginary component is not known, and selection of the "correct" value is made empirically by choosing compensation values (both components of refractive index) based upon the "operator's opinion" of the "correct" light scattering particle size distribution. The same empirical approach may be used in the instance when both values are unknown. These latter two approaches exhibit undesirable science and provides opportunities for large errors if the particle size should change, even slightly, because the incorrect (unscientific) selection for the values can lead to under- or overcompensation; particularly in regards to the presence or absence of small amount of distribution fines.

How does Microtrac treat the issue of refractive index?

In consideration of all the above information Microtrac instruments use the following approach described here and shown in **Figure 4**. For spherical, transparent particles, a requirement exists for the index of refraction of the suspending fluid and the particles. The imaginary component does not require consideration because of the above discussion. In the case of NON-SPHERICAL particles, consideration for refraction is made by selection of the RI sample and RI fluid, which determine the proper compensation to make in the calculations (Microtrac proprietary modified-Mie calculations) according to proprietary research and development data. A third option is available for particles that are highly absorbing such as carbon black and toners.



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Fig. 4: Selection of suitable parameters for calculating size distributions with Microtrac analysers.

Summary

The imaginary component of the total refractive index demonstrates little effect on the refraction of light through a particle except in the 1-10 micron region. Even in this region of sizes, the effect is important when the imaginary component is of the order of carbon black (0.66i) or higher (reflective metals). In the case of non-spherical particles refractive index has generally less impact on the calculated particle size distribution but still requires minor compensation from semi-empirically determined data. Under this condition, the imaginary component is of no consequence and can be ignored. In general, the imaginary component can be described as having negligible effect on diffraction light scattering particle size measurement except in highly specific cases, which are rarely encountered.

References:

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