# Using a Wave Model to Study Light Propagation in Emulsion Layers Containing Realistically Shaped AgX Grains

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# Abstract

The shape and structure of the AgX grains have an important effect on light scattering and absorption in emulsion layers. Most models of light propagation see photons as corpuscles while grains are simplified to spheres. However, for modern emulsions with T-grains this approach is not satisfactory.

It is possible to calculate the light wave propagation in the vicinity of a grain of arbitrary shape from the Maxwell equations of classical electrodynamics, but up until now too great a computing power was required. A new application of multiple-grid algorithms has been developed which drastically cuts the required computation time to 1—2 hours for 1 million grid points when solving the equations for a volume element of  $(2\mu m)$ .<sup>3</sup> The wave model replaces the MIE model in the calculation of the cross-section of extinction, the absorption probability, the angular distribution and cross-section of light scattering on the silver halide grains. Light distribution and internal exposure can be simulated by introducing the layer structure and grain distribution of the real film into the model.

So far area exposures of up to 0.1mm<sup>2</sup> are possible, with an edge exposure to simulate MTF measurements. A method has been developed to remove granularity noise from simulated and measured MTF test scans.

## Introduction

Speed and detail reproduction of photographic materials are influenced in a complex way by film structure and processing parameters. The effective exposure in the emulsion layer (influenced by internal light distribution), the formation of the latent image (light absorption and quantum sensitivity of the individual grain) and the detection and amplification of the latent image (silver development and dye formation) are all important. Computer models can efficiently simulate the influence of film structure on the recorded image. In previous publications<sup>1,2</sup> a computer model of the photographic process was described which simulates latent image formation and detection from a given exposure distribution, resulting in a spatial microdensity distribution for the image which allows the derivation of image quality functions. The three stages of the model—exposure as photon propagation in the emulsion layer and latent image formation, development as latent image detection and reading of the image as image quality measurement by a densitometer or microdensitometer—simulate directly the physial and chemical processes of producing a photographic image.

## Theory

In the first stage of the model, the distribution of incident photons is defined and the photon propagation simulated. The two-dimensional, spatial variant distribution of incident photons covers an area up to  $200\mu \times 500\mu m$ , which may be extended if required by repetitious continuation. Periodic structures such as sine waves may be exposed onto the film. The simulation can be carried out with arbitrary spectral energy distributions from 380—780nm. Absolute photon numbers of up to 106 correspond to absolute exposures between 0.001 and 0.51x s. After simulating a sufficient number of photon paths the spectral distributions of reflection, transmission and absorption are calculated.

When modelling light propagation in an emulsion layer, light scattering and absorption on the individual AgX grains are important. For a single microcrystal the crosssection of extinction, the photon absorption probability, the angular distribution and cross-section of light scattering depend on its shape and structure. These probability functions can only be calculated if simplifying assumptions about the shape of the grains are made (i.e. spherical grains for MIE-scattering). For modern emulsions with T-grains this approach is not satisfactory.

## (i) The Wave Model

In principle, light wave propagation in the vicinity of a grain of arbitrary shape can be calculated from the Maxwell field equations<sup>3</sup> given enough computing power. The basic equations for a stationary electromagnetic wave are

$$curl \mathbf{H} = \mathbf{c}_1 \mathbf{E} \tag{1}$$

$$curl \mathbf{E} = \mathbf{c}_2 \mathbf{H} \tag{2}$$

**E** and **H** are complex vectors whose real parts represent the electric and magnetic fields respectively;  $c_1$  and  $c_2$  are complex constants which contain physical quantities such as wavelength and complex refraction indices. In order to solve the set of coupled differential equations (1) and (2), volume elements (voxels) containing one grain plus an environment of the size of about one wavelength in each direction have to be defined. For the chosen voxel the set of coupled differential equations is then transformed into a set of linear difference equations.

The minimum number of equations needed is governed by the reliability required and the maximum number is limited by the computing power available. For voxels of about  $(2\mu m)^3$  with less than 100 grid points in each direction, about 4.5 million equations are required to achieve a reliability of 85%. To solve such a large set of equations directly (Gauß substitution) would take about 6 months. Classical methods of successive approximations (Jacobi) are also unsuitable, because the set of equations does not fulfill the criterion of convergence.

The set of equations can be solved approximately by optimization. As an auxiliary condition for the optimization it was assumed that at the interface between the grain and gelatin the tangential components of **E** and **H** are continuous and their normal components jump with the refraction index. The convergence of the first approximations is dramatically accelerated and thus computing speed is increased by the novel application of a multiple-grid algorithm.<sup>4</sup> Typically 2 or 3 sub-grids are used in the calculation. The calculation requires 100 Mbyte memory and takes only about 60—100 minutes.

# (ii) Model of the Photographic Process

The wave model can be slotted into the existing model of the photographic process, to replace the MIE model for the calculation of the cross-section of extinction, the absorption probability, the angular distribution and cross-section of light scattering on the silver halide grains.

As previously described,<sup>1,2</sup> light distribution and internal exposure are simulated by introducing the layer structure and grain distribution of the real film into the model. After simulating a sufficient number of photon paths the spectral distributions of reflection, transmission and absorption are

calculated. Further steps in the model are the simulation of latent image formation and detection. The simulation of latent image formation is based on the absolute number of photons absorbed by the individual microcrystals. The number of latent image centres per grain is taken into consideration as well as the quantum efficiency (probability that an absorbed photon contributes to the formation of a latent image centre). The latent image is detected then amplified by chemical development of silver and by dye formation. The factors that govern whether or not a AgX microcrystal is developed are the presence of at least one latent image center and the presence of a sufficiently high number of Ag atoms in at least one of those centers. The size of a fully developed Ag grain is based on the number of Ag<sup>+</sup> ions in the AgX microcrystal, assuming that it develops into a compact silver grain. The results give silver mass as a function of exposure.

#### (iii) Image Quality Measurement

The structure of the final image is determined by the spatial microdensity distribution, the measurement of which requires a scanning microdensitometer. The Monte-Carlo simulation of photon propagation in the developed film provides the microdensity distribution of the recorded image. The optics of the microdensitometer and densitometer are simulated using realistic parameters. For example, sample illumination can be specular or diffuse. Different directional distributions (numerical apertures) and spectral distributions (visual or Status A/M) can be used to detect the transmitted photons. To simulate a CCD microdensitometer, the transmitted photons are registered by an array of pixels.

## (iv) Noise Removal

The spatial microdensity distributions resulting from the simulation (i)–(iii) are distorted by noise because the calculations are carried out for only relatively small areas  $(200\mu m)^2$ . Edge exposures on real films are also scanned by a microdensitometer with a comparably small measuring area  $(2 \times 100)\mu m^2$  and similarly noise removal is also necessary when MTF is calculated from those scans.

When an edge is copied onto a color negative film, its signal usually has a steep slope with sharp bends caused by the adjacency effect as shown in Figure 2 (a). The maximum curvature of the signal (edge image) is comparable to that caused by granularity noise. Therefore smoothing algorithms with a fixed width smoothing window are unsuitable, because they do not differentiate between signal and noise. The MTF values would be lowered considerably if slope and bends of the edge were too vigorously smoothed.

To remove the noise without deterioration of the signal a smoothing filter with a variable window has been developed. This is narrowest at the edge, the position of which is given by the maximum of the first derivative of the signal. The window then gradually increases in width with increasing distance from the edge.

# Results

Figure 1 shows the spatial radiant energy distribution in the environment of a grain as a symmetrical cross-section through its center. The arrow gives the direction of the incident wave. Increasing lightness of the image indicates higher energy levels.



Figure 1: Spatial energy distribution of light scattered by a cubic silver halide grain, pixel size  $2\mu m$ , grain size  $0.53\mu m$ .

The cross-section of extinction calculated for a cubic grain (a =  $0.53\mu$ m, n<sub>Grain</sub> = 2.2, n<sub>Gelatin</sub> = 1.5) from the wave model is Q<sub>ext</sub> =  $0.92 \ 10^{-12}$ m<sup>2</sup>. With MIE theory a value of Q<sub>ext</sub> =  $1.12 \ 10^{-12}$ m<sup>2</sup> was obtained for a sphere of the same volume.

The spatial microdensity distributions resulting from the simulation of the complete photographic process (i) -(iv) are distorted by noise due to the small areas considered. When applied to an edge scan (scanning distance  $\Delta x = 1 \mu m$ , 1024 sampling points) a variable filter window is used in the smoothing algorithm. Away from the edge 400 sampling points can be averaged but in the region around the edge 3 sampling points are used. An edge image and MTF calculated with and without noise removal are shown in Figure 2.



Figure 2. (a) Edge image and (b) MTF with and without smoothing.

## Summary

Newly developed multiple-grid algorithms greatly reduce the computation times needed to calculate approximations of the the light wave propagation in the vicinity of a grain of arbitrary shape from the Maxwell field equations. Rather than the 6 months estimated for conventional numerical methods, computation now takes 1-2 hours for 1 million grid points in a volume element of  $(2\mu m)^3$  layer structure and grain distribution of the real The wave model replaces the MIE model in the calculation of the cross-section of extinction, the absorption proba-bility, the angular distribution and cross-section of light scattering film into on the silver halide grains. After introducing the the model, light distribution and internal exposure can be calculated. Further steps in the model are the simulation of latent image formation and detection plus the measurement of spatial microdensity distribution by microdensitometry.

It is now possible to simulate exposures for areas up to 0.1mm.<sup>2</sup> A novel method of removing granularity from both simulated and measured MTF test scans has been developed.

## References

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