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Shape Reconstruction of Partially Overlapping Objects in SEM Images: Application to Silver Halide Microcrystals

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Abstract

A method for shape reconstruction and extraction from objects that have a certain regularity but are observed in a scanning electron microscopy image with some degree of overlap is presented. The proposed algorithm first calculates the curvature at each contour point of the object in the digitised binary image in order to detect the vertexes. Reconstruction of the shape of overlapping objects is then based on geometrical considerations using the information from the vertex co-ordinates. The procedure is independent of the size and orientation of the objects. The method is applied to the shape reconstruction of partially overlapping tabular silver halide microcrystals.

Key words: Shape reconstruction, SEM-images, silver halide microcrystals.

1. INTRODUCTION

Scanning electron microscopy (SEM) is often used to study the shape and size of microscopic objects. E.g. this technique is applied to investigate atmospheric particles and industrial particulate materials such as ceramic powders and microcrystals. In combination with x-ray analysis (SEM-EDX) also the chemical composition of these microparticles can be obtained [1]. This type of studies involves the analysis of a large number of objects (typical between a few hundred to a few thousand) in order to obtain statistical valid results for the size, shape (and composition) distribution, so that automation of the procedure is often required.

In order to analyse the particle with SEM they need to be dispersed on a suitable conducting and flat substrate, e.g. by filtration of a suspension on a Nuclepore filter or by evaporating a drop of the suspension on a carbon stub. With carefully controlled sample preparation, agglomeration and overlap between the microparticles can be avoid to some extend but never excluded. Overlap occurs more frequently and is especially problematic with flat shaped objects such as tabular silverhalide microcrystals that have a diameter to thickness ration between 5 and 10. One possibility is to disregard all case of overlapping particles at the expense of an increased measurement time as one has to continue the measurement until the required number of non-overlapping objects have been identified and analysed.

In this article we propose an algorithm that is able to reconstruct the shape of the overlapping object based on geometrical considerations. The article emphasises on the shape reconstruction of silverhalide microcrystals but can be extended to other objects with a more or less regular shape.

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The tabular silverhalide crystals are used in light sensitive photographic emulsions. They are produced in a reactor vessel by the precipitation reaction of Ag^+ with Cl^-, Br^- or I^- ions. Their shape, size and composition is determined by the growth (precipitation) conditions and in turn determine the properties of the photographic material [2]. Knowledge about the size and shape distribution of these microcrystals is important for the optimisation of the precipitation process and for the study of the photographic properties of light sensitive film. Under certain precipitation conditions a limited number of shapes are produced: regular triangles, regular hexagons and truncated triangles. Fig. 1a shows binarized SEM backscattered electron images of some typical crystals. For the shape characterisation and classification of these silver halide crystals methods have been proposed in the literature [3, 4]. However these methods cannot be applied when one or more microcrystals are partially overlapping (Fig. 1b) as is often the case because of the limited control that one can exercise during the sample preparation process.

2. THEORY

In the following we assume that the fact that two or more objects are overlapping each other have been established on the basis of a binary SEM image, e.g. using an approach described in [5]. The algorithm to extract the shape of the individual entities from such an ensemble (a collection of more or less overlapping objects) involves 4 steps. First an ordered 8-connected list of contour coordinates of the ensemble is extracted. In the second step this list is analysed and the vertexes are detected. Having found $\boldsymbol{N}$ vertexes the ensemble is approximated with an $\boldsymbol{N}$-side polygon. In the last two steps hexagonal and triangular (truncated and regular) shapes are reconstructed on the basis the geometrical information obtained from the vertex positions.

Contour extraction

The border following algorithm [6] is used for finding and storing the connected list of contour coordinates of the ensemble of overlapping objects. To illustrate this, assume that point $\boldsymbol{L}$ belongs to the ensemble and the point $\boldsymbol{R}$ not as shown in Fig. 2a. This pair of the points defines one of the "*cracks*" on the border as called in [6]. We consider two other points $\boldsymbol{L_1}$ and $\boldsymbol{R_1}$ which are 4-adjacent to $\boldsymbol{L}$ and $\boldsymbol{R}$ respectively. Then the following rules define the next crack on the border (see Fig. 2b):

$\boldsymbol{L}_{\text{new}} = \boldsymbol{L_1}$, $\boldsymbol{R}_{\text{new}} = \boldsymbol{R_1}$ if $\boldsymbol{L_1}$ belongs to the ensemble and $\boldsymbol{R_1}$ not;
$\boldsymbol{L}_{\text{new}} = \boldsymbol{L}$, $\boldsymbol{R}_{\text{new}} = \boldsymbol{L_1}$ if $\boldsymbol{L_1}$ and $\boldsymbol{R_1}$ do not belong to the ensemble;
$\boldsymbol{L}_{\text{new}} = \boldsymbol{R_1}$, $\boldsymbol{R}_{\text{new}} = \boldsymbol{R}$ if $\boldsymbol{L_1}$ and $\boldsymbol{R_1}$ belong to the ensemble;
$\boldsymbol{L}_{\text{new}} = \boldsymbol{R_1}$, $\boldsymbol{R}_{\text{new}} = \boldsymbol{R}$ if $\boldsymbol{R_1}$ belongs to the ensemble and $\boldsymbol{L_1}$ not.

The algorithm terminates when we come back to the initial pair of points.

Detection of vertexes

Vertex detection is based on the idea than if there is a vertex in a certain point of a contour then the change in tangent direction at that point will be essential. Thus in order to find vertexes, the tangent direction at each point of the contour is calculated and its change monitored.

To estimate the tangent direction, the "median filtered differencing technique" [7] is applied. Let $\{\boldsymbol{p_i}\}$ be an 8-connected list of contour coordinates, then at each point $\boldsymbol{p_i}$ let us define a set of $\boldsymbol{2M}$ difference vectors (Fig. 3a) $\vec{d}(i,i+j)$, $\boldsymbol{j}$=-$\boldsymbol{M}$, ..., -1, 1, ..., $\boldsymbol{M}$, such that

$$\vec{d}(i,i+j) = \begin{cases} \vec{d}(p_{i+j}, p_i), & j = -1,\ldots,-M \\ \vec{d}(p_i, p_{i+j}), & j = 1,\ldots,M \end{cases}.$$

These difference vectors can be represented in polar coordinates and sorted according to their polar angle θ. If θ_k be the angle of the k-th vector in the sorted sequence of 2M vectors, the direction of tangent is estimated as a median of the sequence:

$$\textit{tangent direction} = \frac{1}{2}(\theta_M + \theta_{M+1}).$$

The algorithm effectively selects the median slope of the tangent direction as a function of arc length. The same idea was used for curvature estimation at each point of the contour (Fig. 3b).

It is assumed that point **P** of the contour is a vertex if the tangent direction at that point is larger than a certain limit value $\Delta\Theta$. It might occur that a few consecutive points have a tangent direction larger than $\Delta\Theta$. In that case the middle point in the sequence (the point with the highest tangent direction) is considered to be the vertex point.

Extraction of hexagonal shaped objects

Both hexagonal and truncated triangular objects (silver halide microcrystals) have all vertexes equal to 120°. A regular hexagon has equal sides whereas a truncated triangle has sides of two different lengths. These properties and the parallelity of the opposite sides can be used to reconstruct partially overlapping objects of this category.

The angles between two vertexes of an N-sided polygon are determined with the cosine theorem. If an angle is between α_l and α_u we mark the corresponding vertexes as belonging to a hexagonal object. The ordered sequences of vertexes, marked as belonging to an hexagonal object, are extracted and analysed separately in order to reconstruct the entire shape of the hexagon, if possible. If the vertex detection and marking procedures were correct one can expect to obtain sequences having 6, 5, 4, 3, 2 or 1 vertexes. When the sequence has only 1 vertex we are not able to reconstruct the shape of corresponding hexagon. In case of 2 vertexes we can reconstruct only the shape of a regular hexagon but without faith in the true shape. Having 3, 4, 5 or 6 vertexes we can reconstruct the shape of regular hexagons and truncated triangular objects.

With 6 vertexes, the shape of the hexagon can be reconstructed simply by sequentially connecting of all of them (see Fig. 4a).

Having 5 vertexes, the shape of a hexagonal microcrystal can be reconstructed by adding the 6th vertex using geometrical properties of the hexagon (see Fig. 4b). Let P_1, P_2, P_3, P_4, P_5 be an ordered sequence of vertexes of a hexagon and P_0 and P_6 vertexes before P_1 and after P_5 respectively not belong to the hexagon (see Fig. 4b). The 6th vertex P'_6 of the hexagon is at the interception of the lines P_1P_0 and P_5P_6. The coordinates of this point can be found as the solution of a system of the equations

$$\begin{cases} \dfrac{y - y_1}{y_0 - y_1} = \dfrac{x - x_1}{x_0 - x_1} \\ \dfrac{y - y_5}{y_6 - y_5} = \dfrac{x - x_5}{x_6 - x_5} \end{cases}$$

representing the lines P_1P_0 and P_5P_6 passing through the points $P_0(x_0, y_0)$, $P_1(x_1, y_1)$ and $P_6(x_6, y_6)$, $P_5(x_5, y_5)$ respectively. Finally, having 6 vertexes the hexagon can be reconstructed as described above.

If only 4 vertexes of a hexagon are available the following procedure can be used for the reconstruction (see Fig. 4c). Let P_1, P_2, P_3, P_4, be an ordered sequence of points representing the vertexes of a hexagon and P_0 and P_5 vertexes before and after the given sequence respectively. The 5th vertex of the hexagon P'_5 to be found belongs to the line P_4P_5 and the length of $P_4P'_5$ is equal to the length of the side P_2P_3. So, its coordinates x'_5 and y'_5 can be calculated using the coordinates of the points P_4 and P_5:

$$x_5^{'} = x_4 + l\frac{x_5 - x_4}{d} \text{ and } y_5^{'} = y_4 + l\frac{y_5 - y_4}{d}$$

where $\boldsymbol{l}$ is the length of $\boldsymbol{P_2P_3}$ and $\boldsymbol{d}$ is the length of $\boldsymbol{P_4P_5}$. The 6th vertex of the hexagon $\boldsymbol{P'_0}$ belongs to the line $\boldsymbol{P_1P_0}$ and the length of $\boldsymbol{P_1P'_0}$ is also equal to the length of $\boldsymbol{P_2P_3}$. Its coordinates can be found in a similar way using coordinates of the points $\boldsymbol{P_1}$ and $\boldsymbol{P_0}$.

Having only 3 vertexes of the hexagon, the remaining 3 can be found in the following way (see Fig. 4d). Let $\boldsymbol{P_1}$, $\boldsymbol{P_2}$, $\boldsymbol{P_3}$ be an ordered sequence of points representing the vertexes of a hexagon and $\boldsymbol{P_0}$ and $\boldsymbol{P_4}$ vertexes before and after this sequence. Vertexes of the hexagon $\boldsymbol{P'_0}$ and $\boldsymbol{P'_4}$ can be found in a similar way as described for 4 vertexes. The 6th vertex $\boldsymbol{P'_5}$ can be found as the interception of two lines parallel to lines $\boldsymbol{P_1P_2}$ and $\boldsymbol{P_2P_3}$ which cross the points $\boldsymbol{P'_4}$ and $\boldsymbol{P'_0}$, respectively. This interception can be found in a similar way as described for the case of 5 vertexes: the line passes the point $\boldsymbol{P'_4}$ and is parallel to the $\boldsymbol{P_1P_2}$ and also passes the point $\boldsymbol{A}$ with coordinates $(\boldsymbol{x_1}+(\boldsymbol{x'_4}-\boldsymbol{x_2}), \boldsymbol{y_1}+(\boldsymbol{y'_4}-\boldsymbol{y_2}))$. Similarly, the line is passing the point $\boldsymbol{P'_0}$ and is parallel to the side $\boldsymbol{P_2P_3}$ also passes the point **B** with coordinates $(\boldsymbol{x_3}+(\boldsymbol{x'_0}-\boldsymbol{x_2}), \boldsymbol{y_3}+(\boldsymbol{y'_0}-\boldsymbol{y_2}))$.

In case only 2 vertexes of a hexagonal microcrystal were found we can only reconstruct a regular hexagonal microcrystal having all sides equal (see Fig. 4e). Let $\boldsymbol{P_1}$ and $\boldsymbol{P_2}$ be an ordered sequence of points representing the vertexes of a hexagon, $\boldsymbol{P_0}$ and $\boldsymbol{P_3}$ be one vertex before given sequence and one vertex after given sequence, as usually. Reconstruction of the regular hexagon is as follows. Two vertexes $\boldsymbol{P'_0}$ and $\boldsymbol{P'_3}$ of the hexagon can be found in the way similar to the case when 4 vertexes are available. The remaining 2 vertexes of the hexagon $\boldsymbol{P'_{-1}}$ and $\boldsymbol{P'_5}$ are defined using the property of central symmetry of a regular hexagon. The centre of symmetry $\boldsymbol{C}$ of the hexagon has coordinates $((\boldsymbol{x'_0}+\boldsymbol{x'_3})/2, (\boldsymbol{y'_0}+\boldsymbol{y'_3})/2)$. The point $\boldsymbol{P'_{-1}}$ belongs to the line $\boldsymbol{P_2C}$ and the distance from the point $\boldsymbol{C}$ to the point $\boldsymbol{P'_{-1}}$ is equal to the distance from the point $\boldsymbol{P_2}$ to the point $\boldsymbol{C}$. Thus coordinates of the point $\boldsymbol{P'_{-1}}$ can be found using equations similar to that used in the case when only 4 vertexes are available. The last vertex $\boldsymbol{P'_5}$ is defined in a similar way. Of course, in the many cases this reconstruction will be wrong and it will not always be possible to check the correctness of the reconstruction even by visual inspection.

Extraction of triangular shaped objects

Partially overlapping triangular microcrystals can also be extracted based on their geometrical properties. This type of silver halide microcrystals are regular triangles with equal sides and vertexes of $\sim 60^{o}$.

After determining the numerical values of each angle of the $\boldsymbol{N}$-sided polygonal, we mark the corresponding vertex as belonging to a triangular object if the angle is between $\boldsymbol{\beta_l}$ and $\boldsymbol{\beta_u}$. Next, all continuous ordered sequences of vertexes previously selected as belonging to triangular objects are extracted and analysed separately in order to reconstruct the shapes. If the vertex detection and marking procedure is done correctly one expects to obtain sequences of vertexes having 3, 2 or 1 points.

When a sequence has only 1 vertex we are obviously not able to reconstruct the corresponding triangular object correctly. If a sequence contains 3 points the shape of the object can be reconstructed simply by sequentially connection its vertexes.

When only two vertexes are available the 3rd vertex of the triangular object can be determined as follows. Let $\boldsymbol{P_1}$ and $\boldsymbol{P_2}$ represent two real vertexes of a triangular object and $\boldsymbol{P_0}$ and $\boldsymbol{P_3}$ two vertexes which were detected in the overlapping ensemble: $\boldsymbol{P_0}$ is located before vertex $\boldsymbol{P_1}$, $\boldsymbol{P_3}$ located after vertex $\boldsymbol{P_2}$ (see Fig. 4f). The Coordinates of the 3rd vertex $\boldsymbol{P'_3}$, belonging to the triangular object, is found as the coordinates of the point of intersection of the lines $\boldsymbol{P_1P_0}$ and $\boldsymbol{P_2P_3}$ in the way similar to the one described above for the case of an hexagonal object having 5 vertexes.

3. RESULTS AND DISCUSSION

Fig. 5 illustrates the main steps of the reconstruction procedure. After the contour of the ensemble of overlapping objects is extracted (Fig. 5b) the tangent direction at every point of the contour is determined (Fig. 5c) and curvature calculated (Fig. 5d). The tangent direction is estimated using M=15 and for the curvature estimation M=2 is used. Large value of **M** in the case of tangent direction determination results in a smoothed estimate whereas small value of **M** in the case of the curvature calculation guarantees than all essential tangent direction changes are detected. There are many local extremes in the curvature plot as one can observe in Fig. 5d. Most of them are caused by the digital nature of the contour and local imperfections of the crystals (noise). Only a few correspond to the real vertexes. Thus the value of $\Delta\Theta$ should be large enough to separate vertexes on the contour from noise. In all our cases $\Delta\Theta$=15 gives good results. In Fig. 5e the vertexes recognised as belonging to hexagonal microcrystals are marked in black. The limiting angles $\alpha_l=105^o$ and $\alpha_u=135^o$ were determined experimentally. With such limits we are able to eliminate vertexes due to noise and vertexes which do not belong to hexagonal objects. Finally, Fig. 5f shows the reconstructed contour of the hexagonal and the truncated triangular microcrystals.

Eighteen ensembles of partially overlapping microcrystals are shown in Fig. 6. They were analysed with the parameters listed above. The limiting angles for the detection of triangular objects were $\beta_l=40^o$, $\beta_u=80^o$. In most cases our procedure is able to reconstruct the shape of partially overlapping microcrystals. For ensemble OC-04 the reconstructed shape of the hexagon is too large and two reconstructed hexagons of OC-14 are too small. In both cases the reconstruction was done having only 2 vertexes of the hexagons. Clearly a reconstruction based on only two vertexes is often subject to large errors.

CONCLUSION

The method described is able to reconstruct the shape of partially overlapping regular objects.. The method is based on the analysis of geometrical information obtained from the position of the vertexes of a ensemble of overlapping objects and is independent of the orientation, location and size. The experimental results on silver halide microcrystals demonstrate that in most cases the shapes of the individual objects can be satisfactory reconstructed. The correctness of the reconstruction depends on the number of available vertexes.

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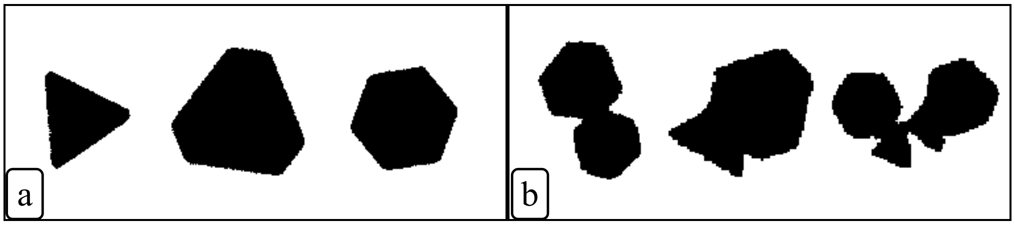

Fig. 1. a) SEM backscattered electron images of individual triangular, truncated triangular and hexagonal silverhalide microcrystals. **b)** The same microcrystals observed as partially overlapping objects in real samples.

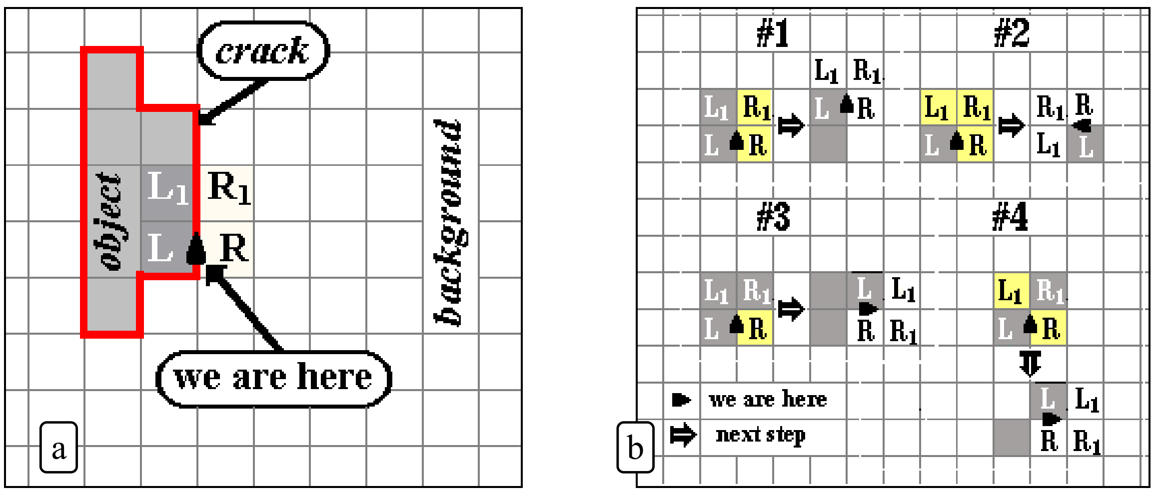

Fig. 2. a) Definition of a *crack* and some important points. **b)** Illustrations of the rules of the border following algorithm.

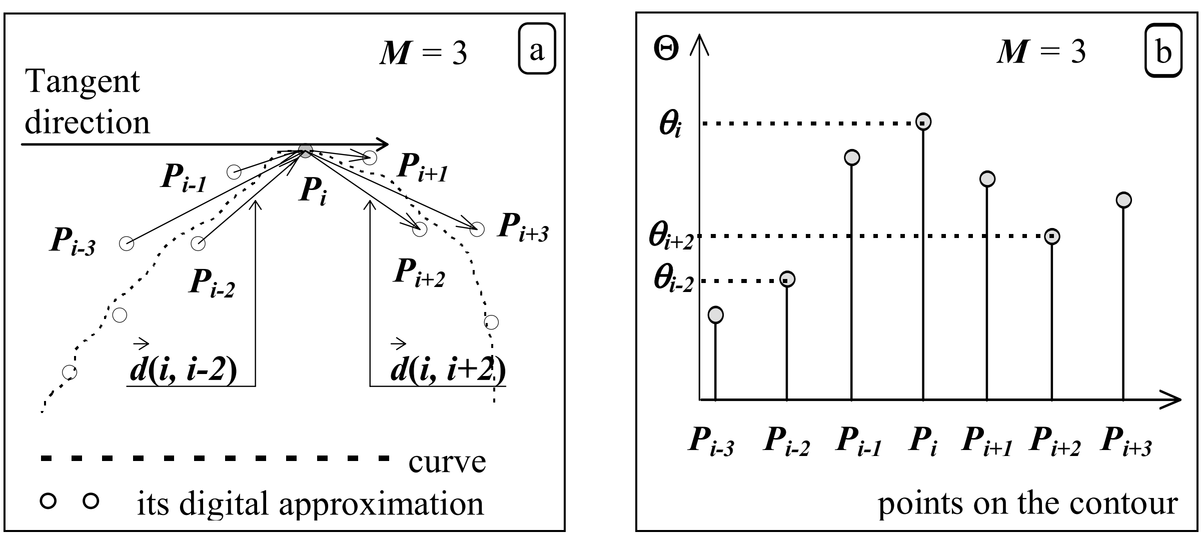

Fig. 3. Median filtered differencing method. **(a)** Sequence of points around $\boldsymbol{P_i}$ and the ***2M*** difference vectors, the tangent direction is defined as the median of corresponding angles of $\vec{d}(i, i+j)$. **(b)** Curvature estimation, the curvature is the median of differences $\boldsymbol{\theta_i}$-$\boldsymbol{\theta_{i+j}}$.

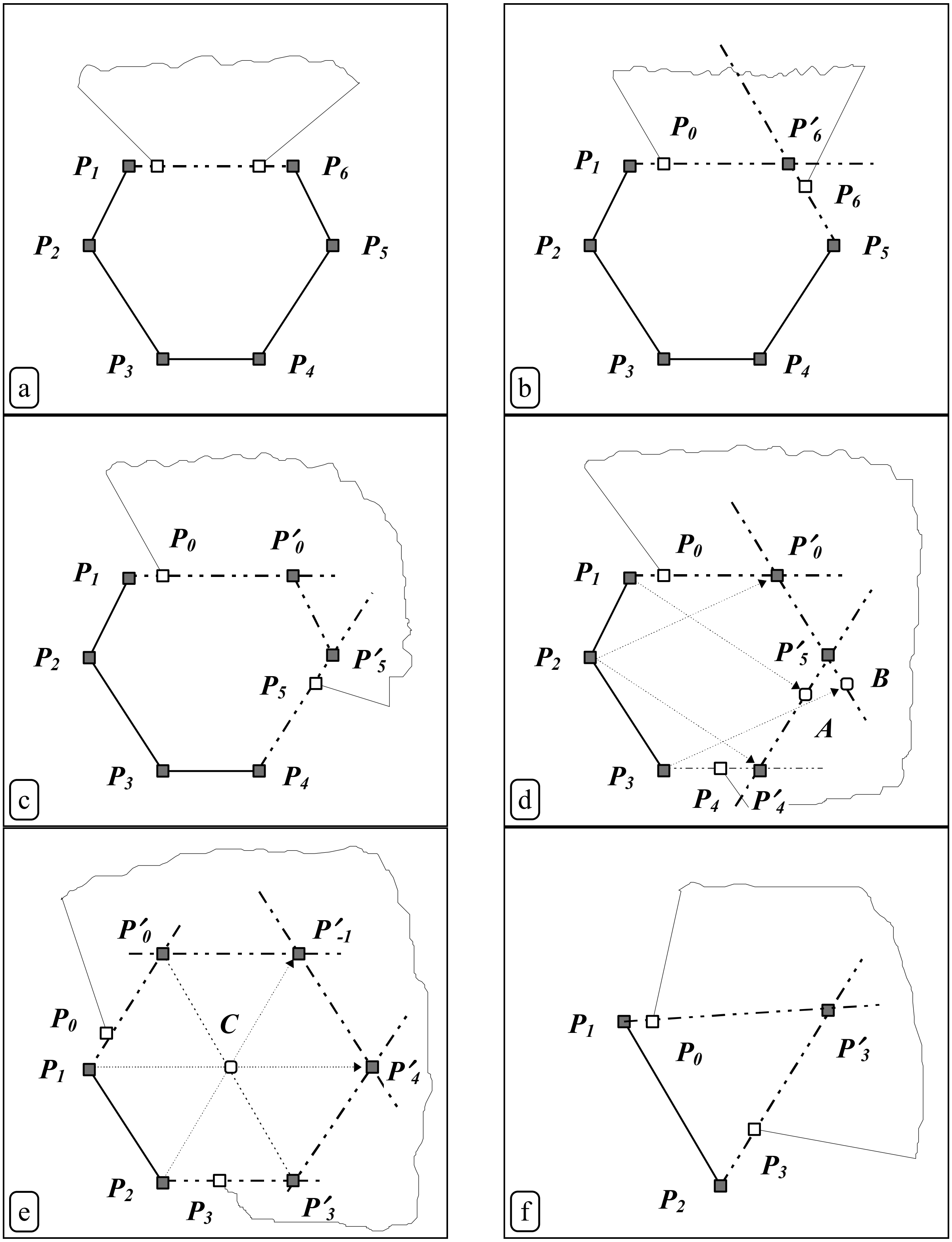

Fig. 4. Illustration of the algorithms used for reconstruction of the shape of partially overlapping hexagonal and triangular objects.

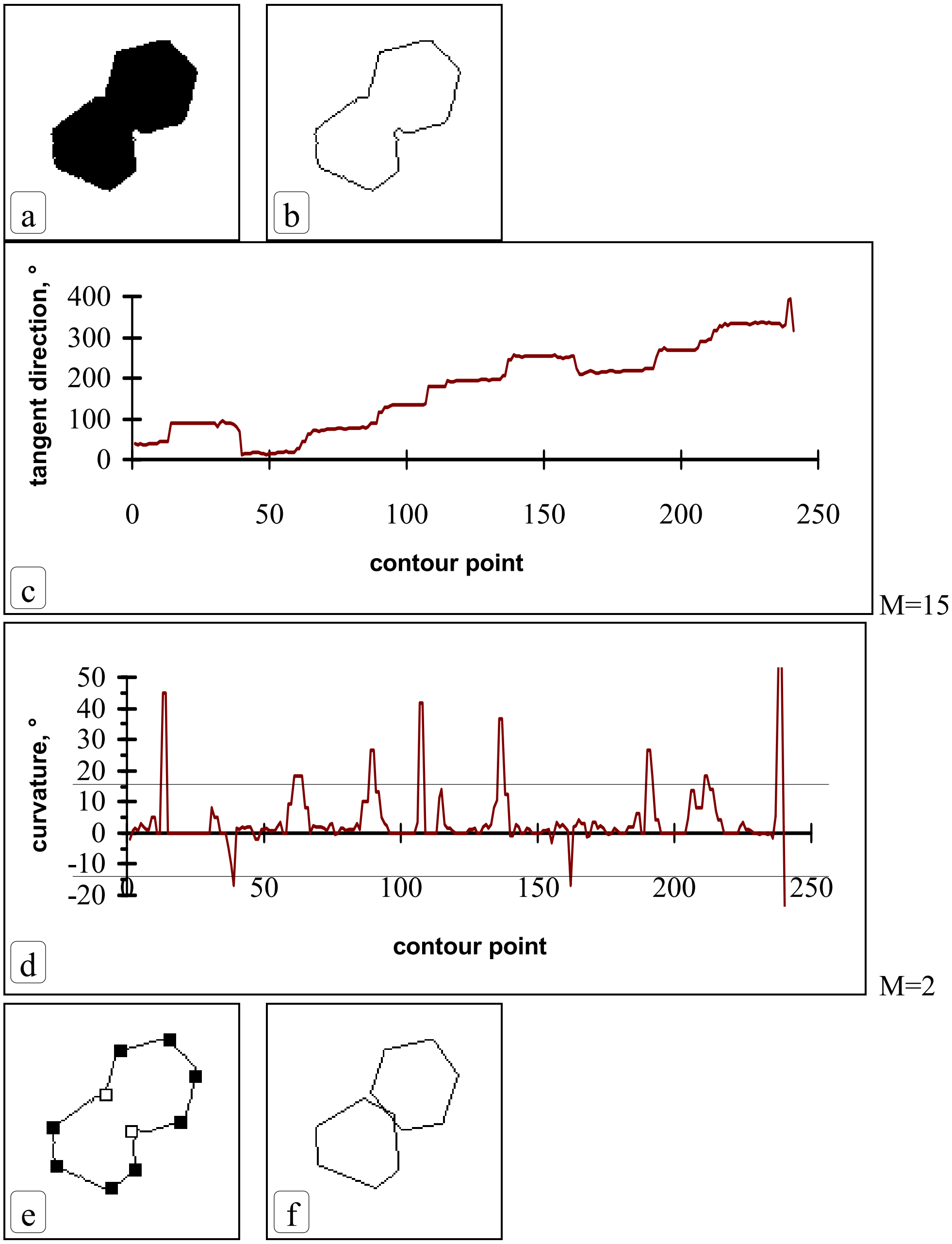

Fig. 5. Illustration of the entire reconstruction procedure. **a)** binary image; **b)** extracted contour; **c)** estimated tangent direction at each point of the contour (***M***=15); **d)** estimated curvature at each point of the contour (***M***=2); **e)** vertexes belonging to hexagonal microcrystals are marked in black ($\Delta\Theta$=15^{o}, α_l=105^{o}, α_u=135^{o}); **f)** contours of reconstructed microcrystals.

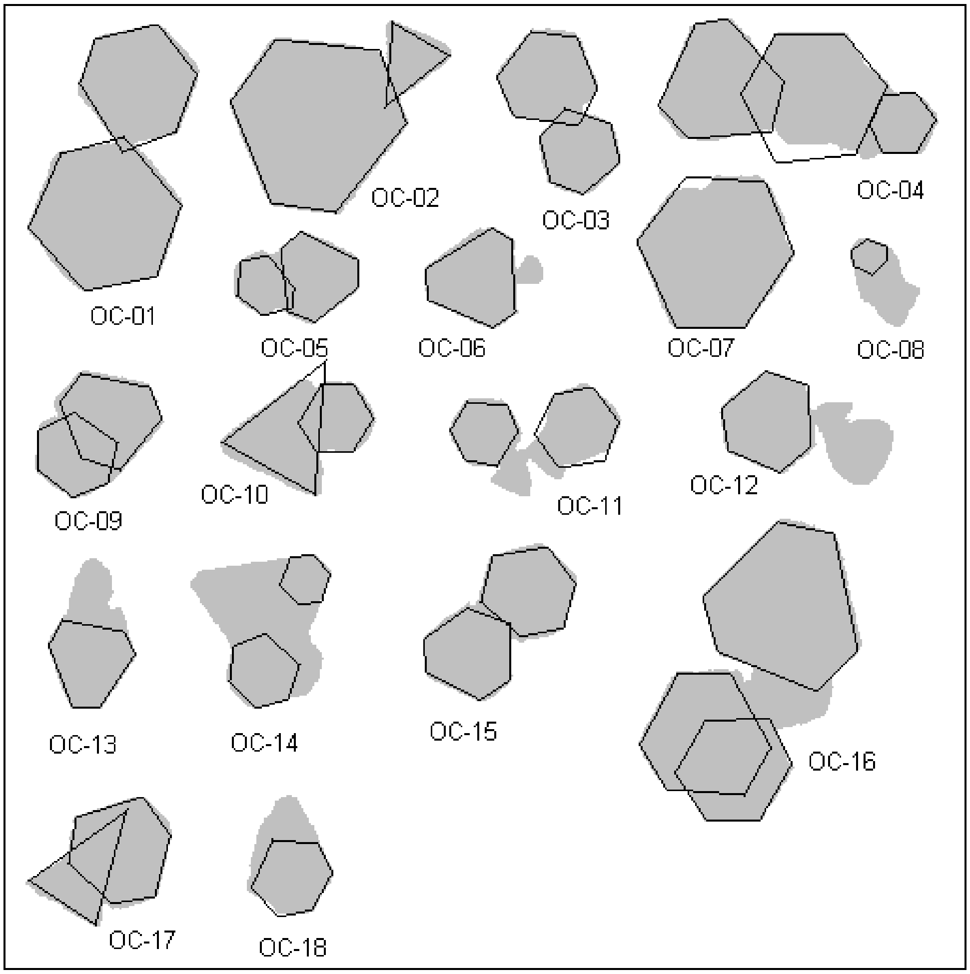

Fig. 6. Results of reconstruction of 18 ensembles of partially overlapping microcrystals.