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Research Highlights

- A method to define the orientation based on Oriented Bounding Boxes (OBB).
- Compute an OBB using the Extreme Vertices Model (EVM).
- An EVM-based method to compute a true 3D roundness index.
- Study of correlation between the developed methods and those reported in the literature.
- A complete analysis of a real silica nano dataset applying the proposed methods.

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Sphericity and Roundness Computation for Particles using the Extreme Vertices Model

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Abstract

Shape is a property studied for many kinds of particles. Among shape parameters, sphericity and roundness indices had been largely studied to understand several processes. Some of these indices are based on length measurements of the particle obtained from its oriented bounding box (OBB). In this paper we follow a discrete approach based on Extreme Vertices Model and devise new methods to compute the OBB and the mentioned indices. We apply these methods to synthetic sedimentary rocks and to a real dataset

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of silicon nanocrystals (Si NC) to analyze the obtained results and compare them with those obtained with a classical voxel model.

Keywords: Binary volumes, Shape description, Length measurements, Oriented Bounding Box, Sphericity, Roundness.

1. Introduction

Computed-based experimentation is getting a growing interest in many fields where scientific data coming from real samples are used to compute structural parameters as porosity, connectivity, sphericity and roundness among others. In the bioengineering field, these parameters allow to evaluate physical properties such as the osteoporosis degree of bones [30] and the suitability of biomaterials to be used as implants [42]. In geology, they allow to analyze the transport and distribution of fluids into sedimentary rocks for petrographic purposes [33] and the grain shape and sphericity index in silica sand for industrial and manufacturing applications [40]. In the nanoscopy field, the size and sphericity of silicon nanocrystals are useful parameters to determine their applicability as optoelectronic materials [15, 48] in Si based light emitters, as sensor material with optical readout, or as label material in bio-imaging.

In this work we focus on sphericity and roundness parameters. Sphericity is a measure of the degree to which a particle approximates the shape of a sphere, and is independent of its size. Roundness is the measure of the sharpness of a particle's edges and corners. They measure two different morphological properties: sphericity is most dependent on elongation, whereas roundness is largely dependent on the sharpness of angular protrusions (convexities) and indentations (concavities) from the object. Sphericity and roundness are ratios and, therefore, dimensionless numbers. Some of these indices are based on length measurements of the three representative axes of a reference ellipsoid of the particle that can be computed from its oriented bounding box.

The contribution of this paper is focused on rock-like objects as those shown in Figures 1 and 5 (sand particles, pebbles or gravel) as well as on Si nanocrystals (NCs). The presented methodology performs well with these two types of objects although they have very different sizes which is a guaranty of its validity. They are 0-genus objects that may show protrusions and concavities and we are not restricted to star-shaped objects as in [9].

In most of the reported literature, the operations to study the structural parameters are performed directly on the classical voxel model. In this paper, we propose new geometric methods to compute sphericity and roundness based on the Extreme Vertices Model (EVM). EVM is a concise representation model for binary volumes and we have developed an EVM-based platform which offers a series of operations for binary volumes that have been used in the methods and results presented in this paper, as erosion, dilation and connected component labelling. The conversion cost from the initial voxel model (VXM) to EVM is shared by all of these operations. See Section 3. The main contributions of this paper are:

- Two EVM-based methods to compute the oriented bounding box (see Section 4.1) and a 3D roundness index (see Section 4.3).
- Results showing the efficiency and accuracy of the presented methods applied to two sets of data: a set of 30 synthetic rocks (Section 5) and a real Si NC dataset (Section 6).

This paper is based in part on the doctoral thesis by the corresponding author [10]. Here we improve and extend the obtained results. Concerning the rock dataset (Section 5), we present a discussion on the OBB volume obtained with VXM and EVM, a comparative between VXM and EVM model to compute the sphericity and roundness based on length measurements, and an analysis of how the resolution affects the computation of the OBB, sphericity and roundness indexes.

Concerning the results with a Si NC datasets, in a recent publication [23] an accurate description of the acquisition method and samples is presented and the obtained results concerning the computation of shape and true sphericity with VXM are validated by the NC experts. These results have encouraged us to further extend and improve this study by including an analysis of values of sphericity based on length measurements, true sphericity and roundness computed with VXM and EVM for this Si NC dataset (Section 6).

2. Related Work

2.1. Sphericity

Sphericity is one of the most used compactness measure of a shape [49]. There are basically two formulation theories for the sphericity index. One of

them is based on length measurements and the other one on the volume and surface area (true sphericity).

Length measurements are the lengths of the three representative axes of an object, $a = d_L$ (longest), $b = d_I$ (intermediate) and $c = d_S$ (shortest) and correspond to its OBB or reference ellipsoid. They can be computed by principal component analysis (PCA) on the corresponding voxel model [3, 24].

There are several formulations of this type. A simplified sphericity index is defined as $\Psi = d_n/a$ [45], where d_n is the nominal diameter (diameter of the sphere having the same volume as the object).

Krumbein defined the intercept sphericity as $\Psi = \sqrt[3]{bc/a^2}$ which is a function of the volume ratio of the reference ellipsoid to the circumscribing sphere. A more widely accepted sphericity index is [41]:

$$\Psi = \sqrt[3]{c^2/ab} \quad (1)$$

From these length measurements the three elongation parameters can be computed: $e_{yx} = b/a$, $e_{zx} = c/a$ and $e_{zy} = c/b$.

The so-called true sphericity index was defined by Wadell [44] as the ratio of the nominal surface area, S_n (surface area of a sphere having the same volume as the object), to the actual surface area of the object, S :

$$\Psi = \frac{S_n}{S} = \frac{\sqrt[3]{36\pi V^2}}{S} \quad (2)$$

where V is the volume of the object. The circularity index, $c = 4\pi S/\text{perimeter}^2$ is the 2D equivalent of the true sphericity index. Both indices range from 1 (perfect sphere or circle) to 0 (elongated shape).

Volume and surface are computed directly from the voxel model [4, 24] by summing voxels and external surfels respectively. A better estimation of the surface area can be obtained by a weighted average of the boundary voxels [46] or extracting a triangulated mesh with MC (Marching Cubes) [29].

Other sphericity indices can be defined as $\Psi = V_p/V_s$ [3] where V_p is the actual volume of the particle, computed summing voxels, and V_s is the volume of a sphere with diameter c .

Approaches based on the continuum representation use spherical harmonic expansions to compute S and V [9, 51].

Sphericity related indices have also been computed at nanoscopic scale. An equivalent spherical diameter is used to obtain a pore size distribution in nanoporous materials [18].

Si NCs are analyzed with 2D software, ImageJ, to obtain the equivalent diameter [19] and circularity index [28], and a 3D software, Amira, is used to compute size and Lent measurements [25] of quantum dot particles.

A different approach uses cross-correlation to adjust the three elongation parameters of the ellipsoid best fitting the particle [34].

Finally, another measure in use to compute the compactness is the convexity (C_x), which describes how closely a particle represents a convex hull and can be defined as $C_x = V/V_{CH}$, where V is the volume of the particle and V_{CH} the volume of the convex hull enclosing the particle [49].

2.2. Roundness

Although roundness is a 3D property, some methods work with the maximum 2D projection plane (silhouette) of the object looking for a trade-off between accuracy and time.

Roundness (\mathcal{R}) was defined by Wadell [44] as the ratio of the average radius of curvature of the corners of the object's silhouette to the radius of the maximum inscribed circle: $\mathcal{R} = (\frac{1}{n} \sum_{i=1}^n r_i) / r_{max}$, where n is the number of corners, r_i the radius of the i -th corner curvature, and r_{max} the radius of the maximum inscribed circle. \mathcal{R} is 1 for a perfectly round object and less than 1 for any other object.

The Krumbein chart (KC) [26] shows examples of pebbles for which the roundness has been calculated using this equation and grouped into nine classes (see Figure 1).

2D methods can be based on granulometry (morphological opening) [14] or on discrete geometry (distance transform of the silhouette) [39]. They exhibit a correlation with KC of 0.96 and 0.92 respectively. A recent approach computes roundness [50] by fitting circles at the corners. There is also a ray-casting based approach [35]. In it, equally spaced rays are traced from the centre of a least-squares circle and the roundness is obtained as the average of distances $d_i - r$, where d_i is the distance from the circle center to the intersection point between the i -th ray and the object and r is the radius of the circle.

There are 3D approaches following Wadell definition. From the voxel model, a MC triangulated mesh is computed and from them principal, mean and Gaussian curvatures can be estimated [49]. Another approach uses only the maximum principal curvature and computes it with spherical harmonic expansions [9]. Both approaches are very time consuming and the first one simplifies the initial mesh in order to reduce the computation cost.

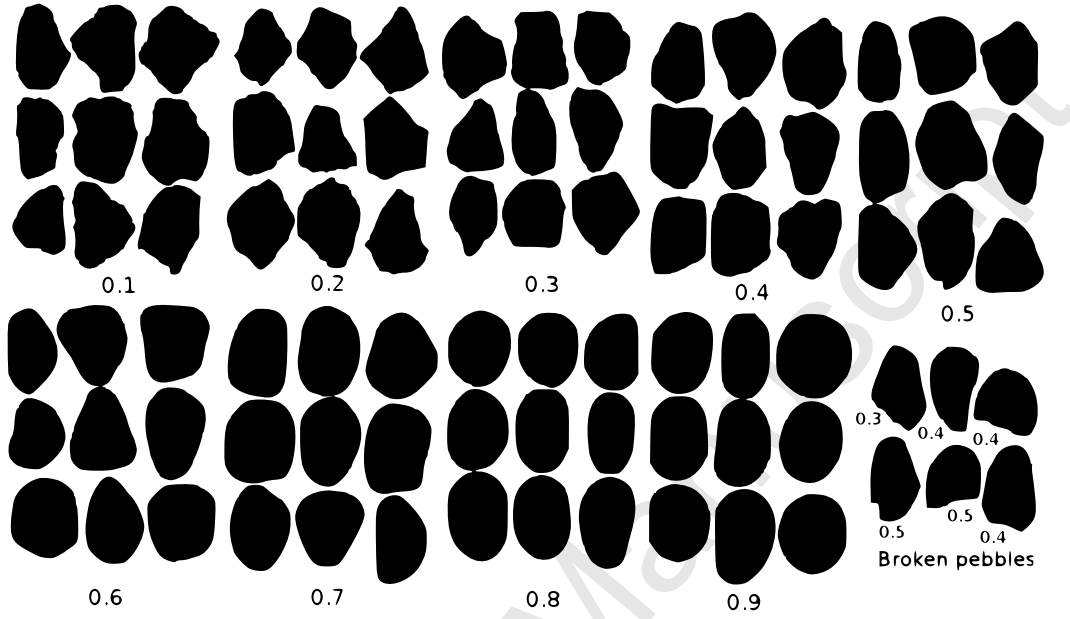


Figure 1: Krumbein's chart for visual determination of roundness [26].

Other authors [20] propose new formulations for the roundness index based on length measurements, surface area and volume. Based on the idea that the ratio between the volume and surface area reflects the roundness, this index is defined as:

$$\mathcal{R} = \frac{V}{S\sqrt[3]{abc}} \quad (3)$$

In this work, a specific software Pixform is used to compute it.

In another work [3], the roundness index is defined as:

$$\mathcal{R} = \frac{S}{4\pi\left(\frac{a+b+c}{6}\right)^2} \quad (4)$$

i.e., as the ratio between the surface area of the particle and a sphere with a diameter equal to the arithmetic mean of the three length measurements, and it is computed from the voxel model.

There is a 3D approach based on ray-casting. Using spherical harmonics expansion, the roundness index is computed as a surface integral of the dot product between the surface position vector \mathbf{r} and the unit normal vector to the surface \mathbf{n} , $\mathbf{r} \cdot \mathbf{n}$, [9]. However, the computation of this index is restricted to star-shaped particles.

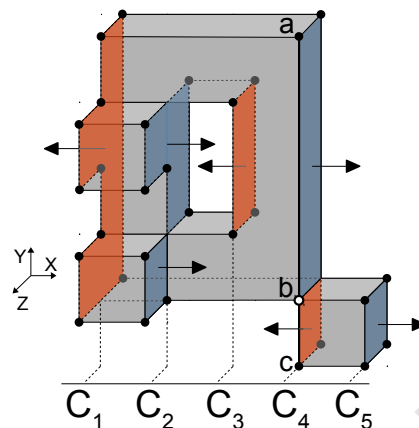


Figure 2: An OPP with its *extreme vertices* marked with dots; a vertical *brink* from vertex **a** to vertex **c** is marked where these vertices are both *extreme vertices* while vertex **b** is not; cuts perpendicular to X-axis are shown with its corresponding faces in red and blue according to their orientation

In this paper, we present an efficient method to compute a 3D roundness index. It is based on a discretized model, the Extreme Vertices Model, follows a ray-casting approach based on distances and is not restricted to star-shaped particles.

3. Extreme Vertices Model

The most common model to represent 3D binary digital images is the voxel model. The continuous analog of a 3D binary voxel model is an orthogonal pseudo-polyhedron (OPP) [27], i. e., an orthogonal polyhedron with a possible non-manifold boundary.

The Extreme Vertices Model is an alternative representation model for 3D binary digital images in which the object is represented by a subset of the corresponding OPP vertices, called extreme vertices.

Let P be an OPP, a *brink* of P is the maximal uninterrupted segment built out of a sequence of collinear and contiguous two-manifold edges of P . The brink ending vertices are called extreme vertices (EV). An OPP, and hence a 3D digital image, can be unambiguously represented by this EV set. A *cut* is the set of vertices lying on a plane perpendicular to a main axis of P . The Extreme Vertices Model (EVM) represents objects by the EV set, sorted lexicographically. Figure 2 shows an example of an OPP. Extreme

vertices are marked with a dot. There are only 4 vertices of the OPP that are not extreme vertices. Segment from vertex **a** to vertex **c** is a brink and therefore vertices **a** and **c** are extreme vertices while vertex **b** is not. Cuts perpendicular to the X-axis (from C_1 to C_5) are coloured. The different colors and corresponding arrows show faces perpendicular to the X-axis with its orientation.

EVM is a complete B-Rep model as all the geometry and neighboring information of faces, edges and vertices of the corresponding OPP can be obtained [43]. The storage requirements for an OPP P in its EVM representation is $O(n)$, n being the cardinality of the EV set which is $O(nv)$, nv being the total number of vertices of the OPP. EVM is a more concise scheme than the voxel model and even than models that store only boundary voxels as the semiboundary and shell models [37]. For more details concerning EVM see [2] and [37].

OPP have been used in several 3D applications as Boolean operations [8, 17], direct skeleton computation (instead of iterative peeling techniques) [16, 31], orthogonal hull computation [6, 7] and in theory of hybrid systems to model the solutions of reachable states [8, 13].

Concerning the EVM model the following operations have been developed: object volume and surface, and Boolean operations [1]; lossless model simplification [12]; morphological erosion and dilation operations and connected component labeling [36, 38], and structural parameters computation as connectivity (genus) [11] and porosity with a virtual porosimetry method that doesn't need previous skeleton computation [38].

4. Indices Computation

In this section, we present methods to compute the OBB and the corresponding length measurements as well as the sphericity and roundness indices of particles represented with EVM.

4.1. OBB Computation

The method presented in this paper applies PCA to the set of extreme vertices, EV , of the EVM-represented object. Although the number of vertices of the EV set is significantly smaller than the number of voxels, the OBB produced from the EVM is very similar to the OBB produced from the voxel model and the computation time is greatly reduced in the EVM-based

method. In Section 5 and Section 6 we discuss the results for both approaches applied to synthetic rock objects and real silica dataset, respectively.

4.2. Sphericity Computation

The sphericity indices based on length measurements are obtained straightforward from the OBB.

To estimate the true sphericity index (Equation 2), the volume is computed from the EVM [1] giving the same result than computed from the voxel model. However, the surface area is computed from the voxel model with a method [46] that minimizes the mean square error. It performs a traversal of the boundary voxels assigning weights to them depending on its typology.

4.3. Roundness computation

Roundness can be estimated with a ray-casting-based approach. Uniformly distributed rays are traced from the center of the object to some sample points on its surface. For each ray, the difference between the distance from the center to the corresponding sample point and the radius of a reference shape at this point is computed. Then, roundness is estimated as an average of these distances.

Based on this idea, in this paper we propose a new 3D roundness index computation method. It uses the ellipsoid inscribed in the OBB of the object under consideration as a reference shape. The presented approach traces rays from the center of this ellipsoid to each vertex of the EV set in the EVM-represented object. For any vertex $\mathbf{v} \in EV$, the difference between the distance from the center to \mathbf{v} and the radius of the ellipsoid passing through \mathbf{v} are computed and the roundness index is obtained as the average of these distances. The EVM-based roundness index is computed in four steps:

1. Compute the principal axes of the reference ellipsoid inscribed in the OBB of the object with the method presented in Section 4.1. See Figure 3(a).
2. Compute a geometric transformation matrix, M , that aligns the OBB with the frame of reference and centers it at the origin O . Apply M to each $\mathbf{v} \in EV$. See Figure 3(b).
3. For each $\mathbf{v}^k \in EV$, trace a ray from the origin to \mathbf{v}^k , and compute the intersection point between this ray and the reference ellipsoid, \mathbf{q}^k , and the distance between \mathbf{v}^k and \mathbf{q}^k , Δ_k . The intersection point \mathbf{q}^k can be obtained solving the quadratic equation $t^2|\mathbf{p}^k|^2 - 1 = 0$ for t , with $\mathbf{p}^k = (2v_1^k/a, 2v_2^k/b, 2v_3^k/c)$. See Figure 3(c).

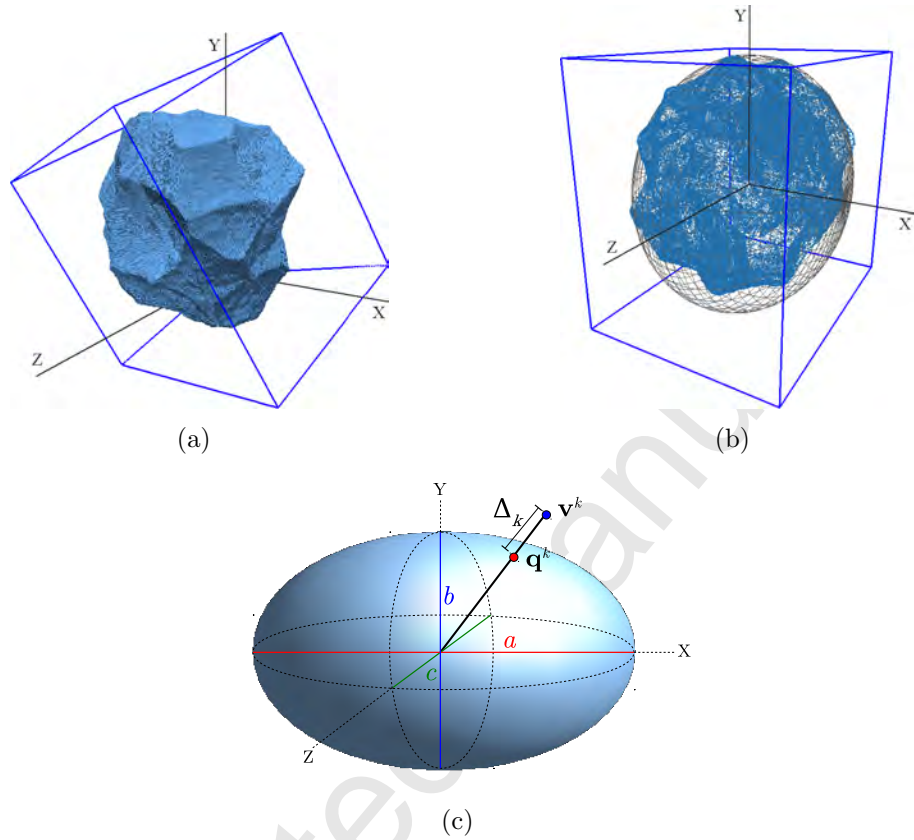


Figure 3: (a) An object and its OBB. (b) Object and reference ellipsoid after applying the geometric transformation matrix that aligns and centers them with the frame of reference. (c) A ray through a point $v \in EV$, the intersection point between the ray and the ellipsoid q and the difference Δ .

4. Compute the roundness \mathcal{R} as the average of the previous computed distances. To remove the size effect, the average is divided by a normalization factor. We use the geometric mean of the principal axes lengths of the reference ellipsoid (a , b , c). This is the same normalization factor applied in the method that will be used to compare the present EVM-based method [20], which have proven to have a strong correlation with Krumbein's roundness. The average is also multiplied by a factor of 10 to enhance the readability of the results. Finally, we subtract the result to 1 in order to keep the roundness definition, where 1 correspond to a perfectly round object and less than 1 for any other

object. Finally, roundness \mathcal{R} is expressed as:

$$\mathcal{R} = 1 - \frac{10}{n(abc)^{\frac{1}{3}}} \sum_{k=1}^n \Delta_k \quad (5)$$

where n is the cardinality of EV .

Note that Equation 5 can give negative values for non rock-like objects, which are not studied in this paper. On the other hand, the factor of 10 we apply does not affect the correlation formula, since it depends on the mean and the covariance of the data.

5. Results with synthetic data

This section and the following show a comparative between VXM-based methods and EVM-based methods in three experiments. The corresponding programs have been written in C++ and tested on a PC Intel®Core i7-4600M CPU@2.90GHz with 7.6 GB RAM and running Linux.

5.1. EVM-roundness Correlation using Krumbein's chart

In order to show the correlation of the EVM-roundness index (Equation 5) with the roundness index defined by Wadell, the silhouettes of the Krumbein's chart (see Figure 1) have been tested in a 2D version of the proposed method. Each tested image was created with a resolution of $\approx 320 \times 320$ pixels. Figure 4 shows the relationship between Krumbein's roundness and EVM-roundness. These results have a linear correlation of 0.898. The EVM-roundness index has also been computed applying the OBB computed from the voxel model. It results in a slightly better (almost the same) correlation of 0.902.

5.2. Indices computation for synthetic rocks

We have used a GPL Blender extension, *rock Generator* (wiki.blender.org/index.php/Extensions:2.6), to create a set of thirty 3D models of rocks with different expected sphericity and roundness (see Figure 5). These models simulate sedimentary rocks whose sizes can range from mm to hundredths of mm. Each model was converted to a voxel model with a resolution of $\approx 512 \times 512 \times 512$ voxels. Distribution of the set of rocks according to their computed sphericity and roundness is shown in Figure 6.

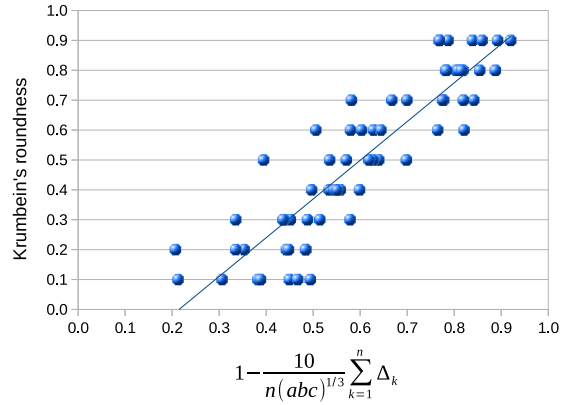


Figure 4: Relationship between Krumbain's chart roundness and EVM-roundness (Equation 5).

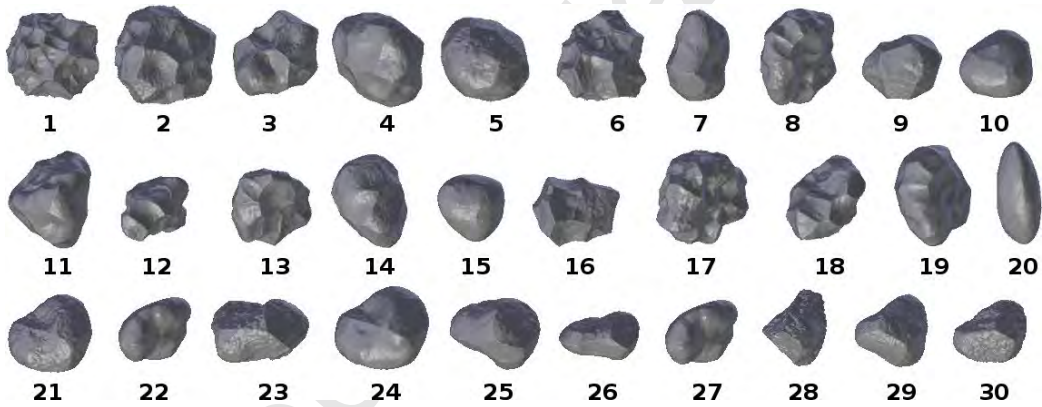


Figure 5: Thirty 3D rock samples created with rockGenerator.

Statistics for the 30 rock datasets are listed in Table 1. For each dataset it shows the size in voxels, the number of used points to compute the VXM-based OBB and its volume. Next, it shows the same parameters for the EVM-based OBB. The last column shows the volume difference between both approaches.

From the results obtained in the 30 rock datasets we have observed that in 14 rocks (marked in bold in Table 1) the EVM-based OBB is tighter than the VXM-based OBB. Moreover, the volume difference between both approaches ranges from 0.10%(R6) to 2.63%(R2); in both cases the VXM-based OBB is tighter than EVM-based OBB. The minimum and maximum

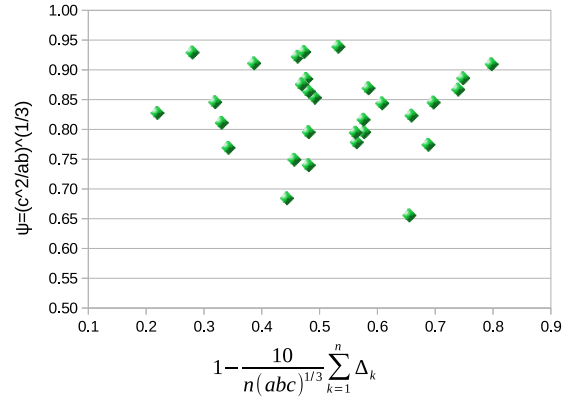


Figure 6: Distribution of the rock samples according to their sphericity (Equation 1 and roundness (Equation 5).

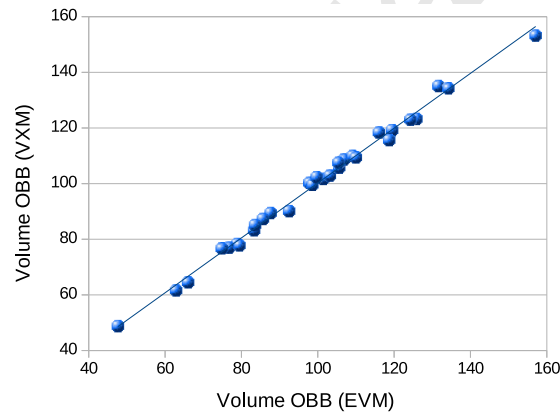


Figure 7: Relationship between the OBB volume computed with VXM and EVM.

differences considering the datasets in which the EVM-based OBB is tighter are 0.12%(R9) and 2.60%(R25) respectively. In the sphere dataset the VXM-based OBB is tighter than EVM-based OBB and the difference is just 0.04%.

Moreover, Figure 7 shows the relationship between the OBB volume computed with VXM and EVM. These results have a strong correlation of 0.997. Therefore we conclude that the EVM-based OBB is, at least, as accurate as the VXM-based OBB.

Table 2 shows the sphericity and roundness indices computed from Equation 1 and 5 respectively. Next the times to compute: the EVM-based OBB,

Table 1: Statistics of datasets for resolution $512 \times 512 \times 512$.

D.	Size	VXM		EVM		%v.d.
		pts., 10^5	OBBVol, 10^6	pts., 10^3	OBBVol, 10^6	
R1	485x512x508	483	157	592	153	2.47
R2	495x512x506	554	132	652	135	2.63
R3	511x465x510	502	107	577	109	1.73
R4	511x510x495	560	126	561	123	2.05
R5	485x485x512	596	123	535	123	1.02
R6	512x396x491	349	106	461	106	0.10
R7	511x370x357	302	63	346	62	2.02
R8	511x409x402	349	79	434	78	0.80
R9	414x391x512	369	83	440	83	0.12
R10	473x419x512	489	101	492	102	0.26
R11	511x507x422	424	103	502	103	0.27
R12	420x512x441	342	105	419	108	2.01
R13	495x466x512	404	98	525	100	2.57
R14	511x504x417	478	99	492	100	1.02
R15	511x440x509	564	119	505	119	0.25
R16	405x437x512	321	77	444	77	0.32
R17	484x512x475	440	119	533	116	2.59
R18	511x475x482	460	116	510	118	2.04
R19	512x410x389	340	75	386	77	2.54
R20	511x360x224	185	38	256	38	0.17
R21	471x419x512	404	88	475	89	2.00
R22	453x471x512	461	109	459	110	0.77
R23	334x385x512	278	66	360	65	2.28
R24	451x426x512	385	86	470	87	1.93
R25	404x443x512	370	93	425	90	2.60
R26	310x356x512	230	48	328	49	2.34
R27	429x456x512	374	100	493	102	2.57
R28	511x466x432	301	79	451	78	2.13
R29	463x512x464	436	110	529	109	0.48
R30	430x393x512	329	84	435	85	1.81
Sph.	512x512x512	698	134	575	134	0.04

the EVM-roundness, the VXM-based OBB and the VXM-based surface area. In this case, the average time to compute the EVM-roundness and the VXM-roundness indices for the rock samples is 115 and 9592 milliseconds respectively, i.e., our approach is more than an order of magnitude faster. This is mainly because we do not need to compute the surface area.

Our method has the disadvantage of the cost of conversion, the average time to convert VXM to EVM for the rocks samples is 13611 milliseconds.

Table 2: Results of datasets for resolution $512 \times 512 \times 512$.

D.	Ψ (Eq. 1)	\mathcal{R} (Eq. 5)	Time in milliseconds			
			OBB-EVM	\mathcal{R} -EVM	OBB-VXM	SA-VXM
R1	0.93	0.28	65	79	5088	8686
R2	0.94	0.53	74	74	4646	8970
R3	0.84	0.61	63	91	4641	7777
R4	0.85	0.70	63	81	4951	8684
R5	0.91	0.80	59	72	4289	8591
R6	0.85	0.32	51	64	3046	5607
R7	0.77	0.69	43	50	2460	4628
R8	0.74	0.48	48	59	3465	5413
R9	0.87	0.58	49	60	3434	5755
R10	0.89	0.75	54	66	4036	6993
R11	0.88	0.48	54	69	3480	6387
R12	0.83	0.22	46	59	3030	5528
R13	0.68	0.44	63	69	3583	6630
R14	0.82	0.66	57	65	3294	6701
R15	0.87	0.74	56	66	3651	7749
R16	0.92	0.46	48	61	2647	4935
R17	0.81	0.33	59	71	4047	6697
R18	0.80	0.48	55	67	4410	7200
R19	0.78	0.56	44	53	2927	5097
R20	0.66	0.66	28	35	1494	2711
R21	0.80	0.58	52	64	3447	6101
R22	0.75	0.46	49	62	3690	7031
R23	0.85	0.49	39	47	2155	3876
R24	0.82	0.58	51	62	3242	5662
R25	0.86	0.48	46	51	3063	5324
R26	0.79	0.56	35	43	1802	3356
R27	0.77	0.34	55	65	3375	6141
R28	0.91	0.39	49	59	3091	5189
R29	0.93	0.47	58	69	3790	6363
R30	0.88	0.47	47	60	2727	4964
Sph.	1.00	0.99	63	76	4708	9649

However, we have developed an EVM-based platform which offers a series of operations for binary volumes. The cost of converting VXM a EVM is shared by all these processes. Besides the length measures, sphericity and roundness presented in this paper, other structural parameters can be computed faster than in their VXM-representation, such as the genus [5, 11], the skeleton [31, 32] and the pore-size distribution for porous materials [38].

The values of sphericity (Equation 1) and roundness (Equation 3 and 4),

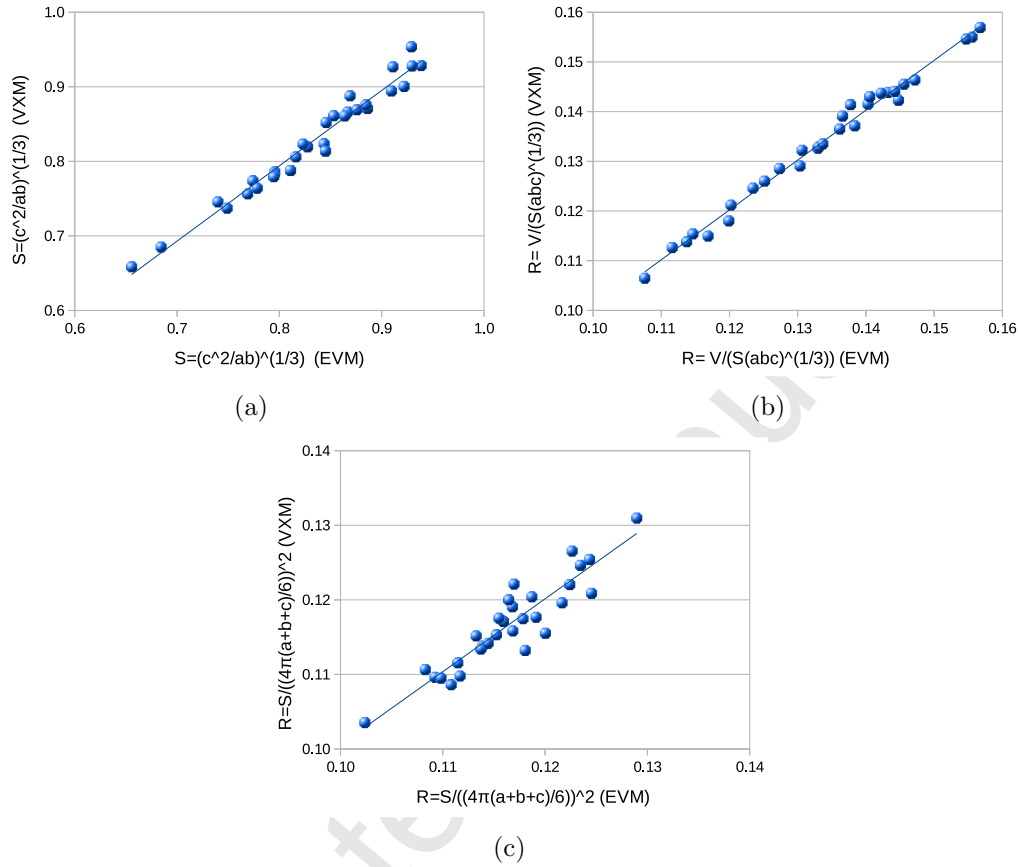


Figure 8: Relationship between VXM and EVM in the computation of (a) sphericity Equation 1, (b) roundness indices Equation 3 and (c) Equation 4.

based on length measurements will also be as accurate computed with VXM than computed with EVM and the resulting correlations are 0.985, 0.995, and 0.922 respectively. Figure 8 shows the graphs with these correlations.

Finally the VXM-roundness index (Equation 3) has been compared with the roundness index proposed (Equation 5). The correlation is 0.933 and the corresponding graph is shown in Figure 9.

5.2.1. Resolution study

We also show that, the model resolution has little effect on the computation of the OBB, sphericity and roundness indices. For this study, we have selected six rocks and the sphere, which cover a wide range of sphericity and

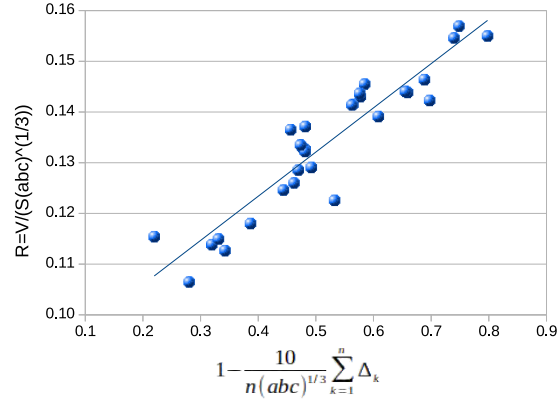


Figure 9: Relationship between VXM-roundness (Equation 3) and EVM-roundness (Equation 5).

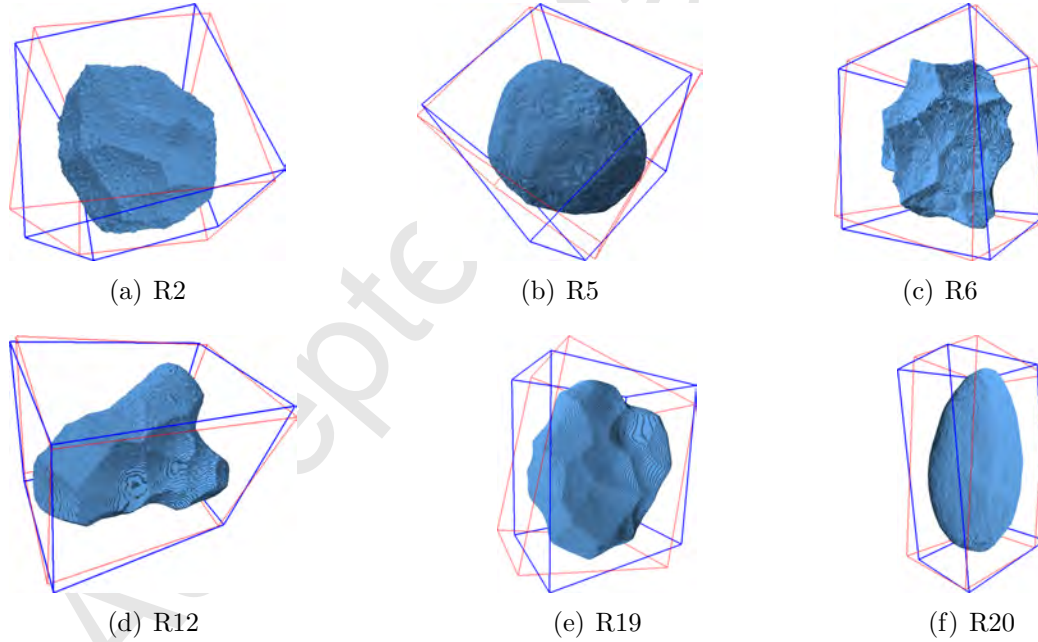
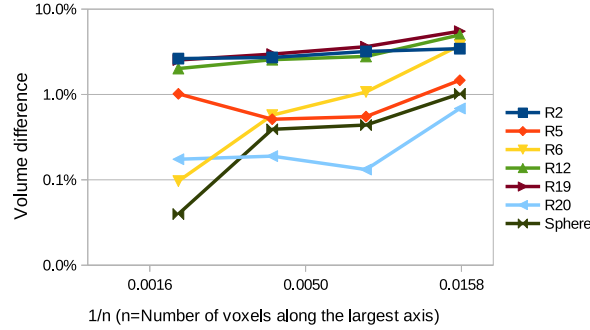
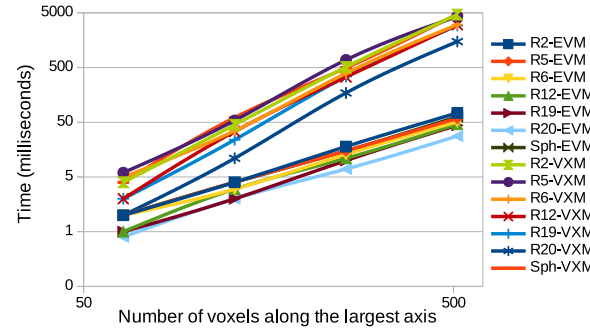


Figure 10: Datasets of the 6 selected rocks and their OBB. The EVM-based and VXM-based OBB in continuous (blue) and stippled (red) line respectively.

roundness indices (see Figure 10). We have tested the selected models with space resolutions of $64 \times 64 \times 64$, $128 \times 128 \times 128$, $256 \times 256 \times 256$ and $512 \times 512 \times 512$. Figure 11(a) shows, in a log-log scale, the volume difference



(a) Volume difference in a log-log scale.



(b) Computation time in a log-log scale.

Figure 11: Resolution test for OBB computation: volume difference and computation time.

computed between a VXM-based and an EVM-based OBB. Note that the volume difference decreases while resolution increases and that, even with a low resolution of $64 \times 64 \times 64$, the difference is less than 6%. Moreover, for some samples (R2, R12, and R19) the dependence is almost linear.

Figure 11(b) shows, in a log-log scale, how resolution affects the computation time in both methods. From the analysis of these data it can be deduced that the VXM-based method is of cubic order (cn^3) whereas the EVM-based method is of quadratic order (cn^2) as they depend directly on the number of points in the respective representation.

Figures 12(a) and 12(b) show how resolution affects the computation of sphericity and roundness respectively using the proposed methods. We have computed the relative difference respect the model in the $512 \times 512 \times 512$ space resolution. Note that the sphericity index is almost invariant, in the worst

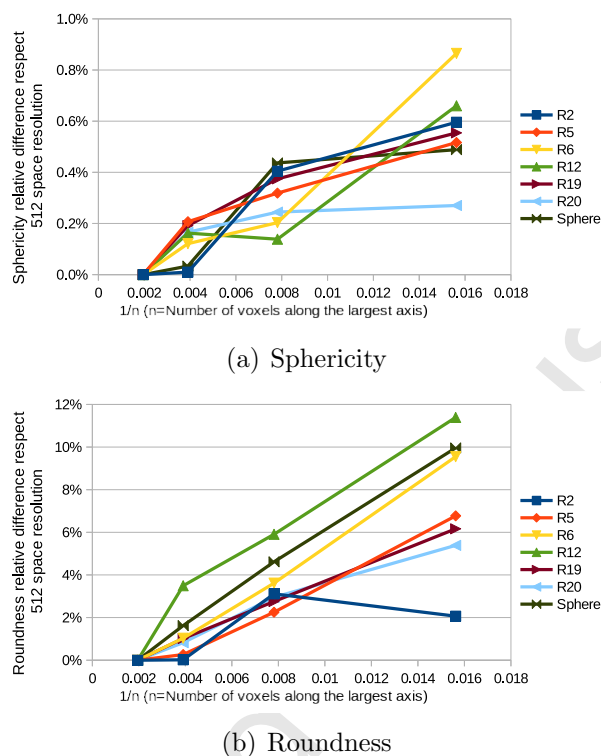


Figure 12: Resolution test for OBB computation: sphericity and roundness variation.

tested case, the relative difference is less than 1%. Regarding the roundness index, in the worst tested case, the relative difference is less than 12%, this difference is bigger than that of the sphericity index due to EVM-roundness is highly dependent on the number of points. For instance, the R12 sample in the $64 \times 64 \times 64$ space resolution has just 1.5% of points that are in the $512 \times 512 \times 512$ space resolution. Therefore, this is a good result as the resolution in which real models are acquired is increasing constantly.

6. Analysis of a Real Silicon Nanocrystals dataset

A real silicon nanocrystals (Si NCs) dataset has been obtained. In this section we use this dataset to compare values obtained with EVM-based and with VXM-based approaches.

A more detailed discussion on the NCs sample growth, the acquisition EFTEM method and the results obtained using the VXM-based approach

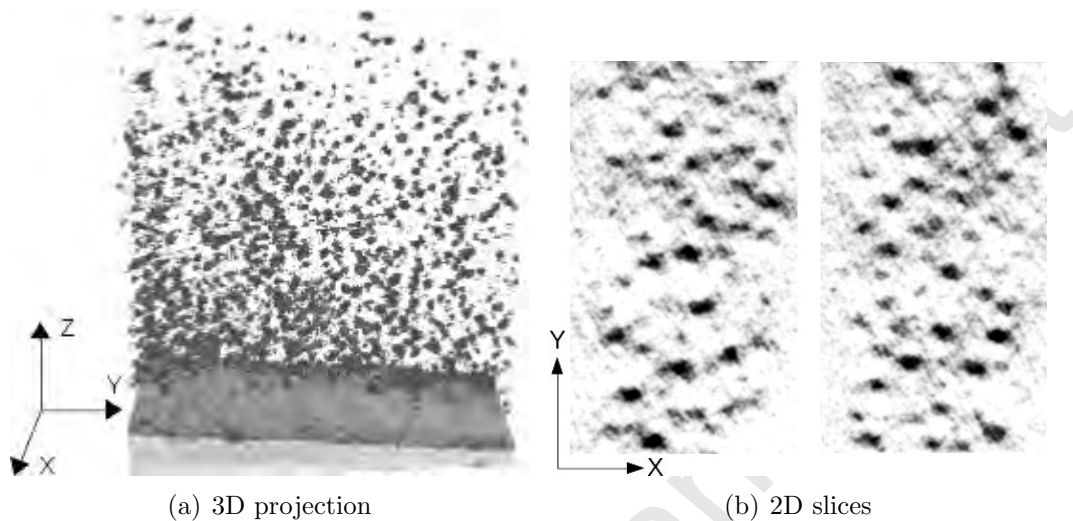


Figure 13: Some views of the silicon nanocrystals dataset tomography.

can be found in [23] which are also briefly included in this section.

Concerning this application, the contribution of this paper is the comparison of values obtained with EVM-based and with VXM-based approaches. Moreover we also describe in detail the required preprocessing to convert the raw format tomography into a suitable VXM model.

6.1. Sample acquisition and preprocessing

Size controlled Si NCs embedded in a SiO_2 matrix were grown on Si substrates by thermal evaporation of a superlattice comprised of 20 $\text{SiO}_2/\text{SiO}_{x=1.2}$ bilayer stacks and a 10 nm thick capping oxide [22]. The sample has 3 nm thick SiO_x layers and 5 nm thick SiO_2 spacing layers.

EFTEM (energy filtered transmission electron microscopy) was performed and tilt series from -68° to $+76^\circ$ at an increment of 4° were acquired [21, 47]. Due to the limited tilt range, objects appear elongated along the Y-direction in the tomographic reconstruction. The elongation factor can be estimated from the tilt range and is ≈ 1.3 for the conditions specified above. From the complete image we have considered the undisturbed 10 first layers as the few NCs in the topmost layers maybe some specimen preparation artefact. Therefore the final considered sample size is $49 \times 106 \times 157$ nm.

The complete tomography is a 32-bit gray scale dataset in RAW format and size $131 \times 281 \times 332$. The 3D projection and some 2D slices of this dataset are depicted in Figure 13.

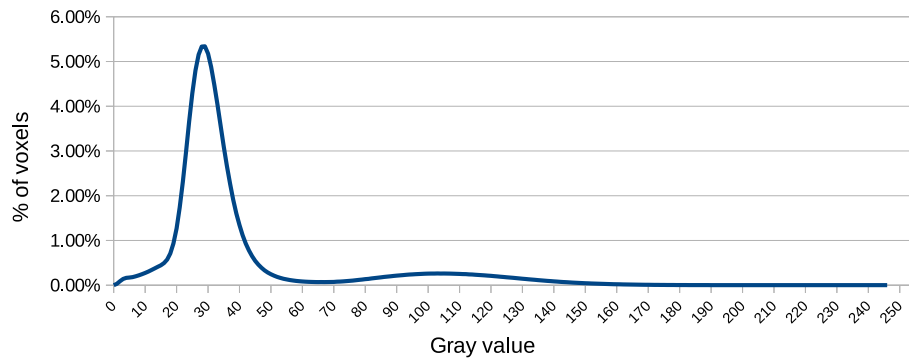


Figure 14: Gray value histogram of the sample.

The following preprocessing steps have been applied:

1. Convert the original dataset to a 8-bit voxel model.
2. Scale the voxel model via trilinear interpolation, to twice its size in order to better define the grain shapes.
3. Apply an elongation factor of 1.3 to the Y axis: $262 \times 730 \times 664$ voxel model.
4. Crop the model in order to remove the base plate and consider only the 10 first layers: $262 \times 730 \times 286$ voxel model
5. Apply a binary threshold filter.
6. Remove noise applying morphological opening and closing operations

Step 5 requires a threshold that allows yielding a good segmentation of the particles. The gray value histogram is shown in Figure 14, in this case, high values of gray represent the foreground and the curve helps to determine where the background ends and the foreground begins. Note that the curve falls off around the value of 50. Therefore, thresholds of 45, 50 and 55 have been used to binarize the dataset.

Figure 15 shows the sample after the corresponding threshold and noise removal, where for each threshold, the number of connected components (CC), considering 6-connectivity, is indicated. Observe that the result of applying a threshold of 45 looks like a model having several agglomerated particles. The result of applying a threshold of 55 seems to lose information. Therefore, we consider that the particle shapes are better defined applying a threshold of 50.

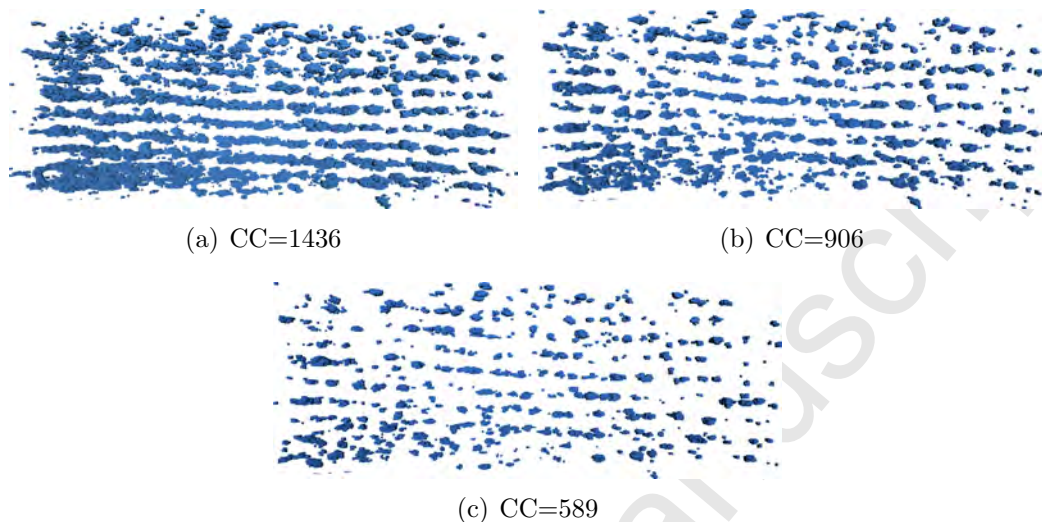


Figure 15: Dataset after segmentation and noise removal with thresholds (a) 45, (b) 50 and (c) 55.

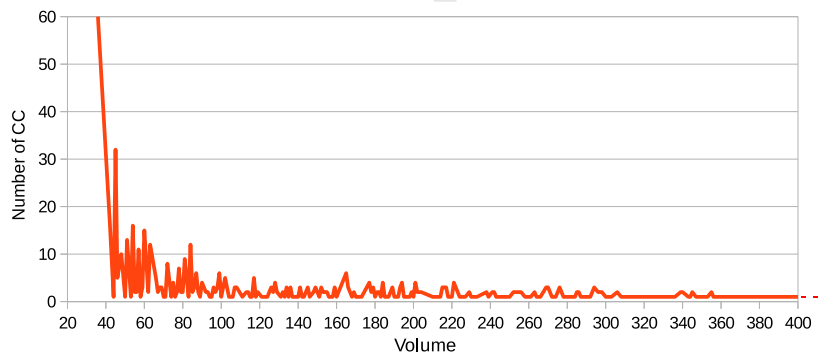


Figure 16: Number of connected components according to their volumes.

After the preprocessing, we compute the connected components, which represent the quantum dot particles. Figure 16 shows a graph of the number of CC according to their volumes.

From the previous data, a voxel size of 0.19 nm approx results. The average size of a particle (diameter) is expected to be around 2 nm or 3 nm. Considering spherical particles this size would correspond to 1190 voxels approx. However, for the size distribution computation, only particles with a volume of 200 or more voxels will be considered. Therefore, the resulting

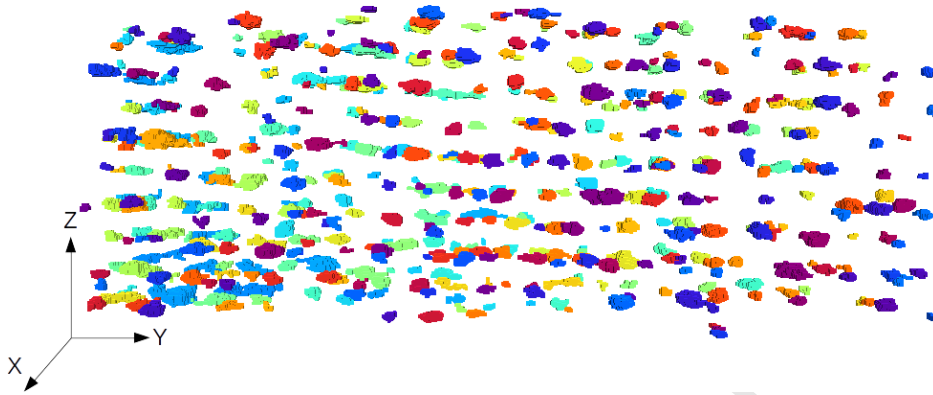


Figure 17: Resulting particles with volume larger than 200 voxels.

dataset consists of 496 CC. See Figure 17 where the resulting particles are depicted.

6.2. Particles Properties Computation

Results obtained using the VXM-based approach [23] showed that NCs in superlattices are non-agglomerated, individual clusters with slightly oblate spheroidal shape. Length measurements and sphericity computation were used for these conclusions which were validated by the NCs experts. Now we show the obtained values using the VXM and EVM approaches.

One of the studied shape parameters was the mean diameter computed as $(a + b + c)/3$. The value obtained with EVM and VXM were 2.72 nm and 2.67 nm respectively. Both values fit very well to the photoluminescence results [22] and the fact that the original SiO_x -layer from which the Si NCs formed was 3 nm thick.

Ratios c/a , c/b and a/b have also been computed. From our understanding the NCs are not perfectly spherical but a bit like a rotational ellipsoid with the lateral shape quite circular since the nanocrystals have no restrictions in X-Y direction and these lateral dimensions are larger than the vertical dimension (Z) due to the self-organized growth with the limiting upper and lower SiO_2 barrier. The obtained average ratios with VXM were $c/a = 0.41$, $c/b = 0.61$ and $a/b = 1.48$, and with EVM were $c/a = 0.42$, $c/b = 0.61$ and $a/b = 1.45$. These values corroborate the previous assumption. Moreover a mean c/b of 0.61 corresponds to an oblate spheroid with just 12% more surface-to-volume ratio than a real sphere.

The true sphericity (Equation 2) has only been computed with VXM and the obtained value of 0.80 as average with a peak value of 0.86 in the normal distribution is a good result, as there are almost no perfectly spherical NCs with $\Psi = 1.0$, but only few have significantly small Ψ -values.

The average sphericity based on length measurements a, b, c (Equation 1) gives a different value than the true sphericity but the values obtained with the two compared approaches are very similar: 0.64 (VXM) and 0.65 (EVM).

Roundness is not a really useful parameter for this NC application, since the scale in which these sharp or round edges are, is at sub-nanometer level, i.e. close to or even beyond the resolution limit of EFTEM tomography. However, in order to further test the EVM-based presented approach we have computed the roundness using VXM (Equation 3) and EVM (Equation 5) and the obtained values are also very similar: 0.15 and 0.16 respectively.

7. Conclusions

We have presented new methods based on EVM to compute length measurements, sphericity and roundness of 3D objects represented as binary volume datasets.

Length measurements have been computed from the OBB of the object obtained by PCA applied to the restricted set of vertices of the EVM representation. Experimental results have shown that this method is as accurate as the same method with VXM and is more than an order of magnitude faster.

We have proposed a new EVM-based roundness index. The method to compute it is based on the ray-tracing paradigm and uses the vertices of the EVM representation. Besides, the time to compute the proposed index is also more than an order of magnitude faster compared with previous VXM-based methods, which depend on the surface area computation.

We have computed the correlation between our approach and the approach based on the voxel model for two sphericity indices and for the roundness index obtaining good results.

One of the advantages of EVM is that the cost of most of the involved processes are less affected by the increasing resolution than in VXM. We have corroborated this fact for the computation of the sphericity and roundness indices: the EVM approach is of quadratic order while the VXM is of cubic order with increasing resolution.

A complete study of a Si NCs dataset has been presented and the computed parameters are equally accurate using VXM or EVM while the computation time is reduced by an order of magnitude.

As a future work, we are devising an alternative method to estimate the real surface area directly of an EVM-represented object so that we could compute the true sphericity without using a VXM-based scheme. We are also studying a method to partition the pore space (for porous materials) without having to compute the skeleton.

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