MECHANISM OF GROWTH OF MONODISPERSED COLLOIDS BY NUCLEATION AND AGGREGATION OF NANOSIZE SUBUNITS

PhD Student in Physics
Igor Sevonkaev

Clarkson University
CAMP

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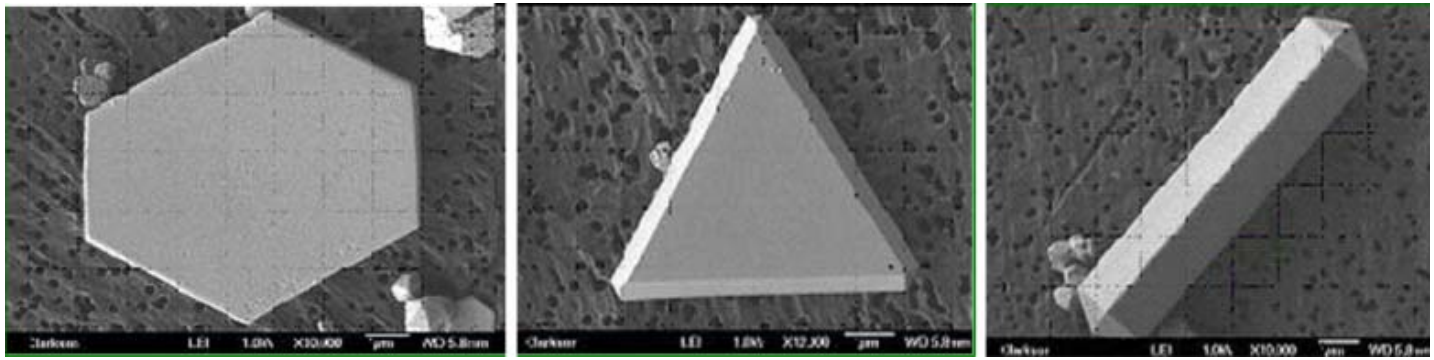
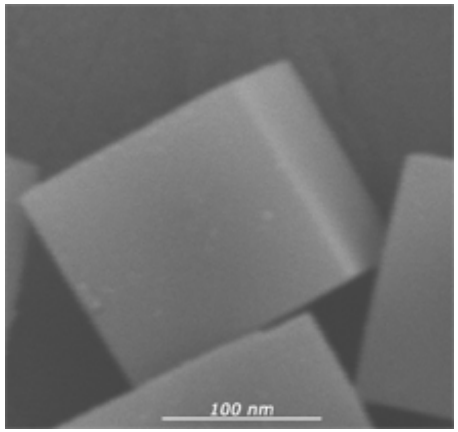
Outline

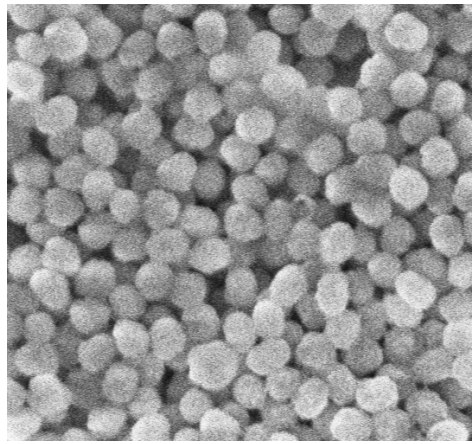
- general description of the problem;
- numerical simulation: 2d and 3d model;
- disadvantages of the numerical model;
- results and discussions of the experimental part;
- XRD results;
- comparison of the numerical model and the experimental observations;
- further directions and goals of the study.

Introduction

Particles of different shapes exist, but nobody knows how and why do these particles choose their shapes.







Nobody can predict a shape of the colloidal particles

Material properties such as:
- **surface reactivity,**
- **magnetism,**
- **ductility,**
- **conductivity;**

are highly important for industry, medicine, and the army.

Understanding coarsening behavior and morphology evolution is critical for efficient material synthesis and quality control.

Theoretical model

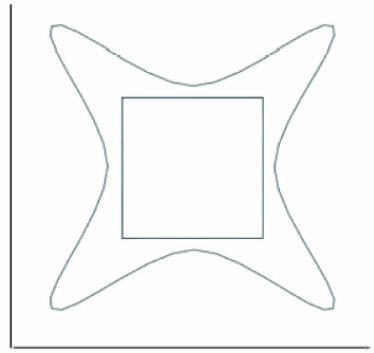
Template: square.

Main deposition rule: Gaussian Distribution Function (GDF) for the arriving building blocks was selected.

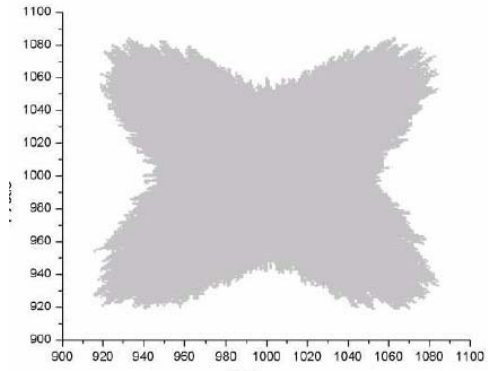
Main mechanism of rearrangement: uniform distribution function (UDF) was suggested.

Two main parameters: the standard deviation σ and the ratio of deposition ρ have been chosen for the shape maintained growth manipulation.

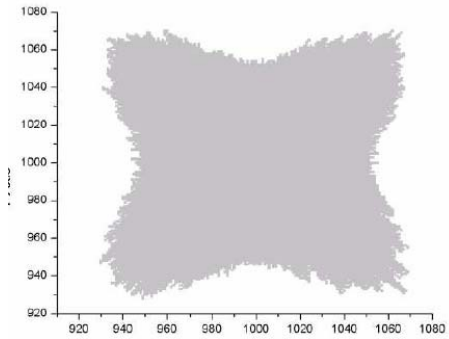
Gaussian distribution function with the peaks corresponded to the edges of the initial particle.



10,000 particles are deposited with the standard deviation $\sigma = 0.3$



10,000 iterations are made with the ratio $\sigma = 0.5$ and $\rho = 0.3$



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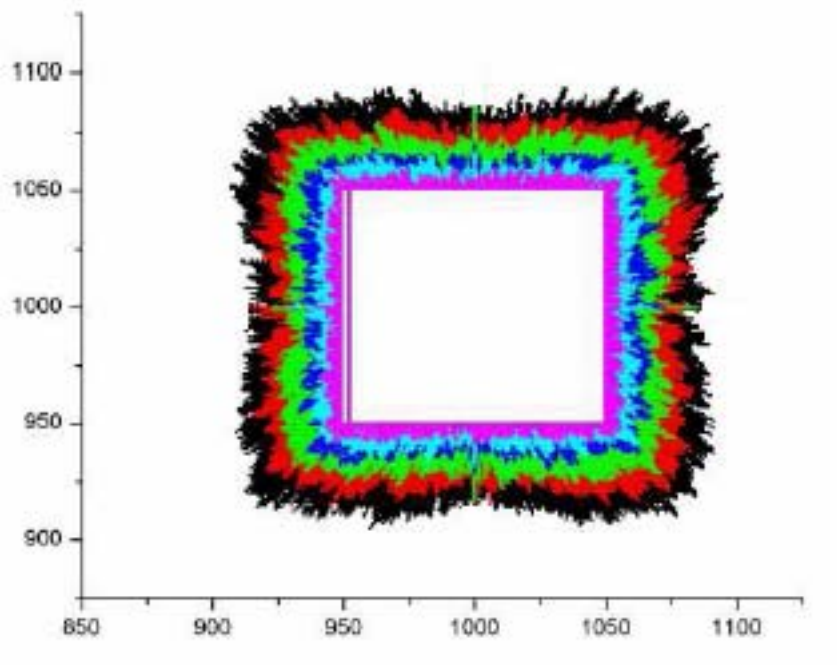
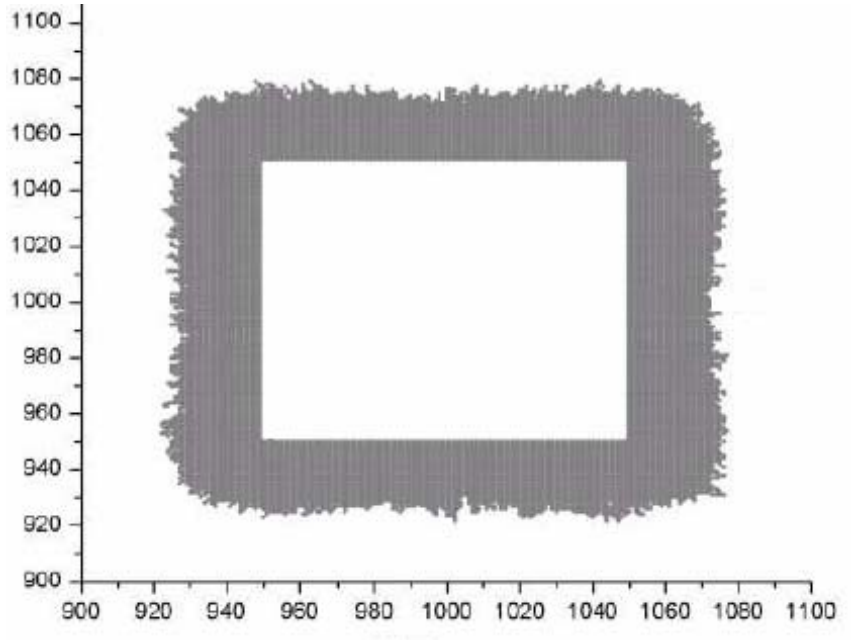


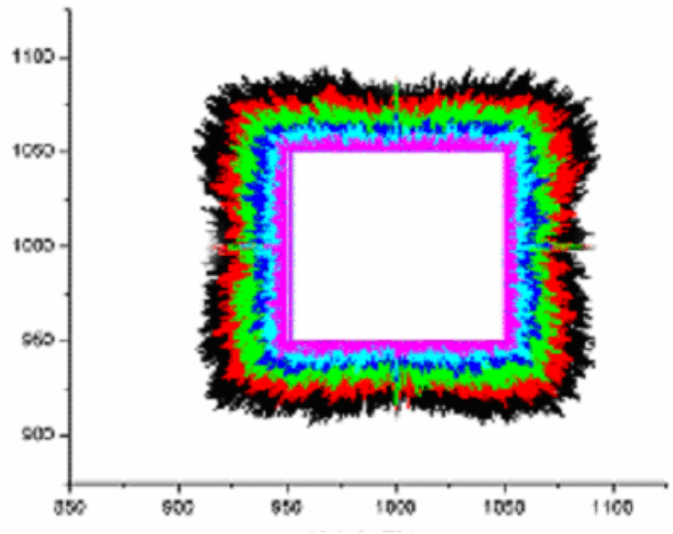


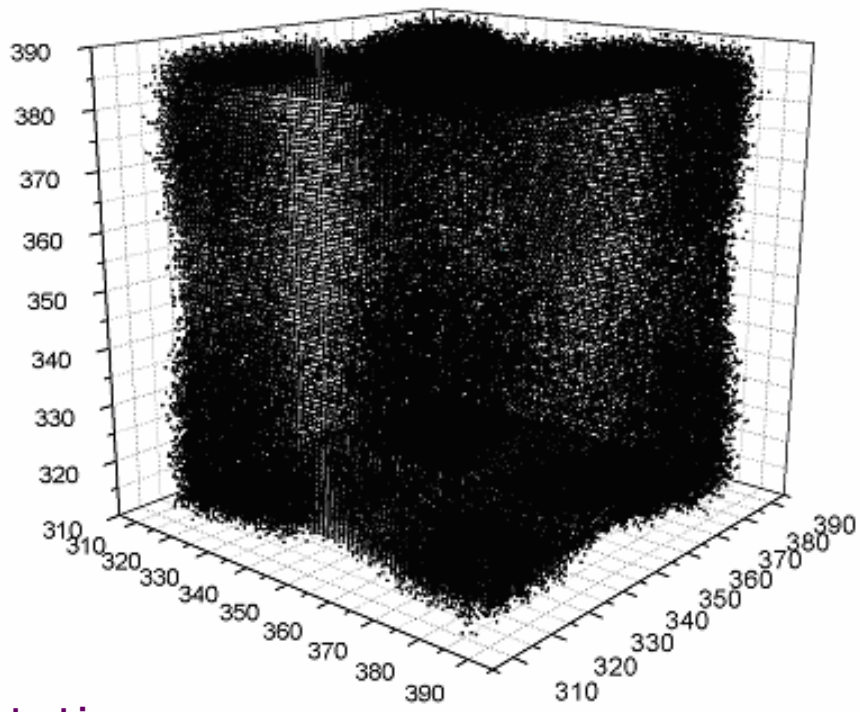
Dynamics of the shape formation of the initial particle.

10^{5i} iterations σ=0.5 and ρ=0.2

Averaged surface after 6 identical simulations for 50,000 iterations each.

Two dimensional model was expanded into 3 dimensions with same conditions.



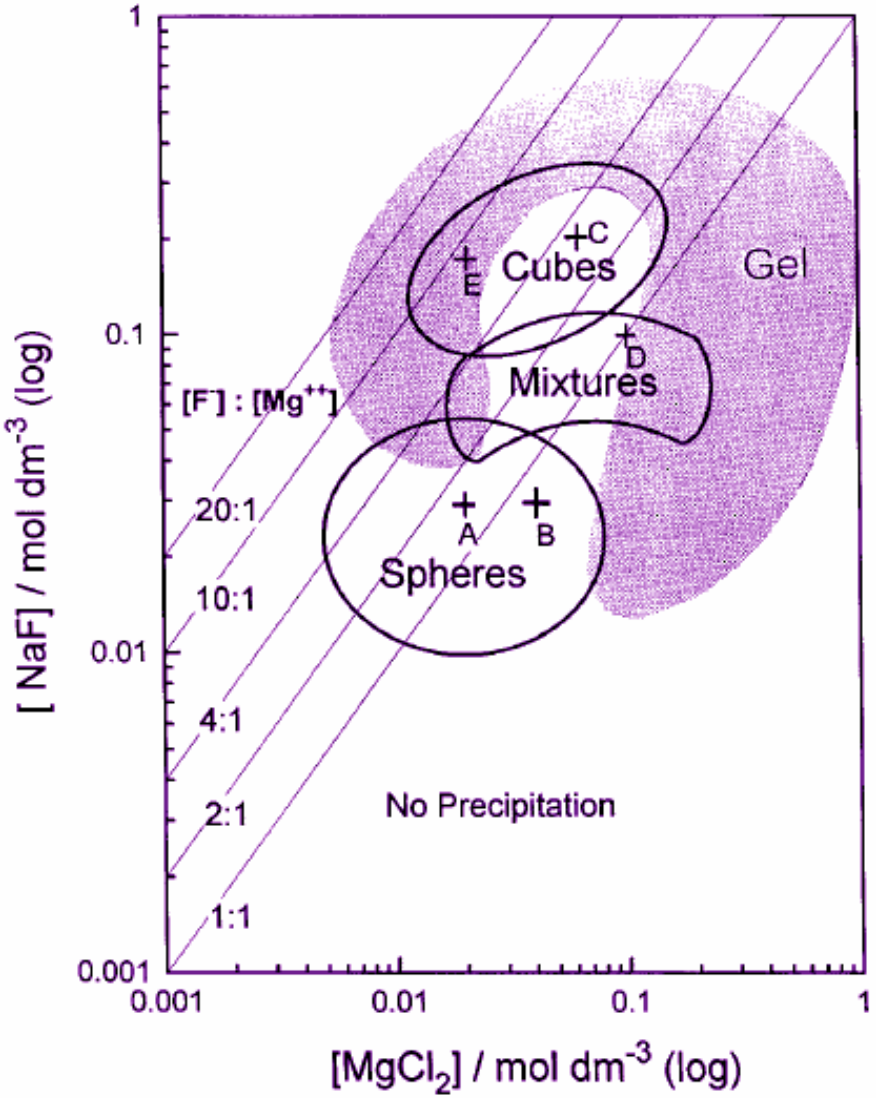


Disadvantages:

- maximum of the GDF is static,
- no real physical background for the parameters σ and ρ.

The Formation of Uniform Colloidal Particles of Magnesium Fluoride and Sodium Magnesium Fluoride,
Wan p. Hsu, Qiping Zhong, and Egon Matijević, Journal of Colloid and Interface Science, **181**, 142–148 (1996).

MgF_2 and $NaMgF_3$ was selected as an experimental model.



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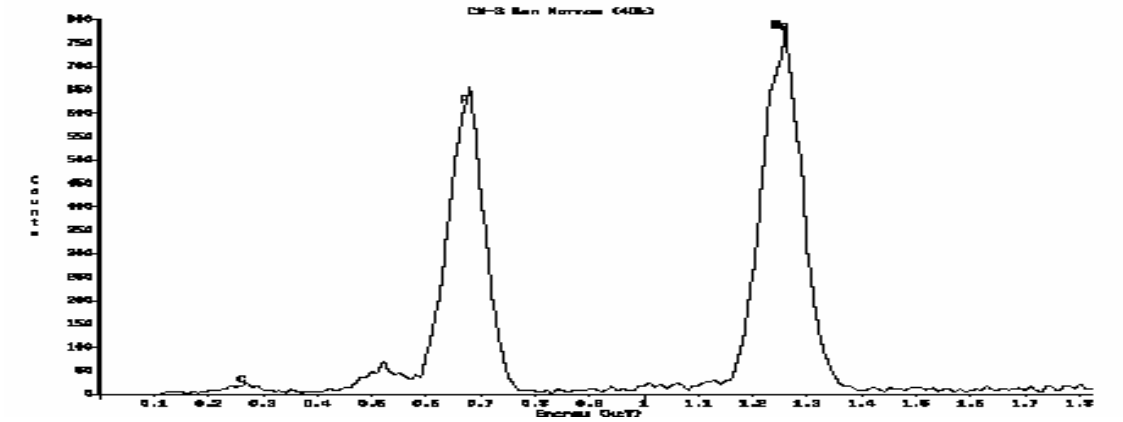
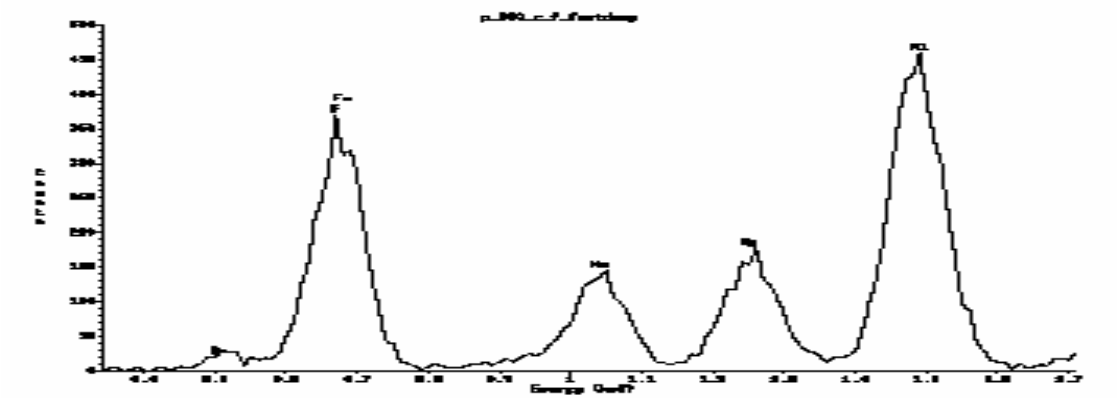
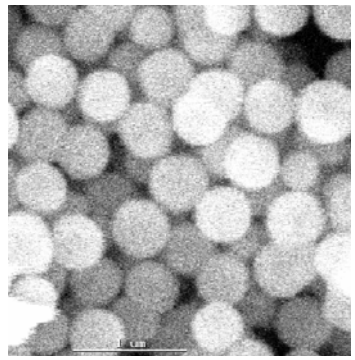
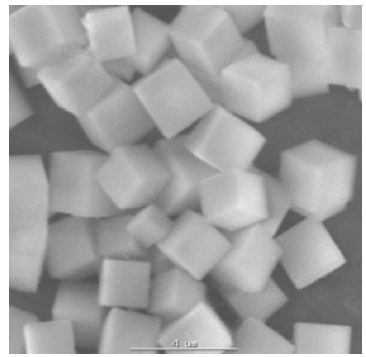
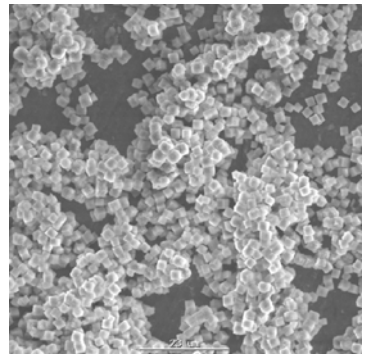
From two simple chemicals we can obtain either spheres or cubes only by changing the relative concentration between them.





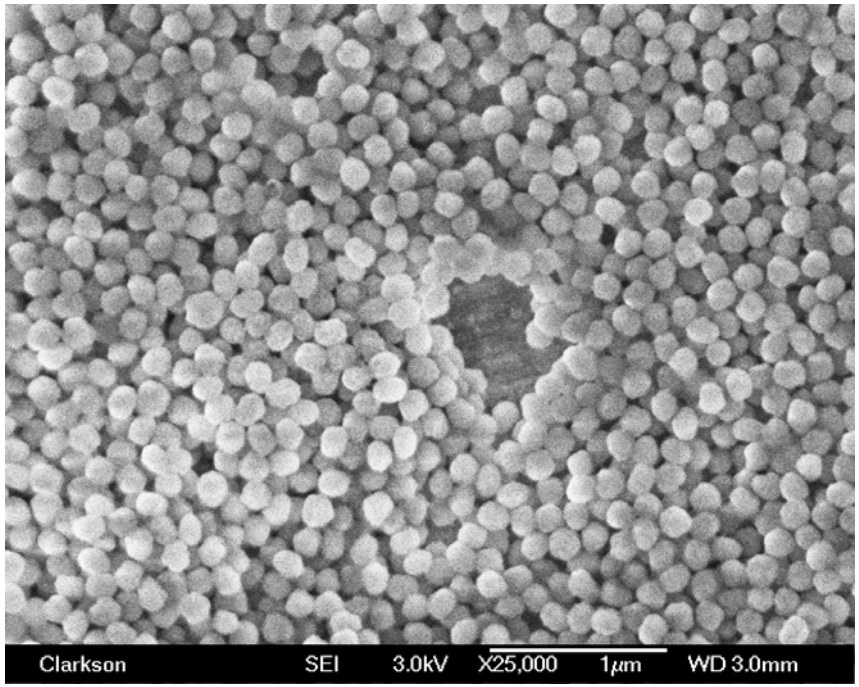


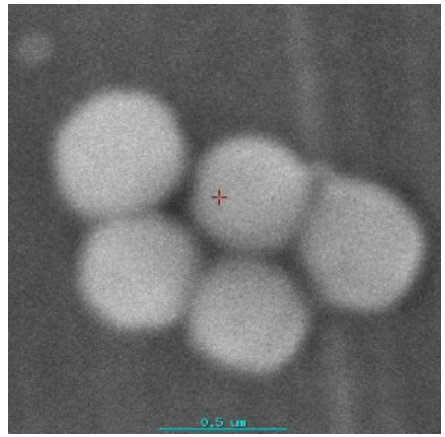


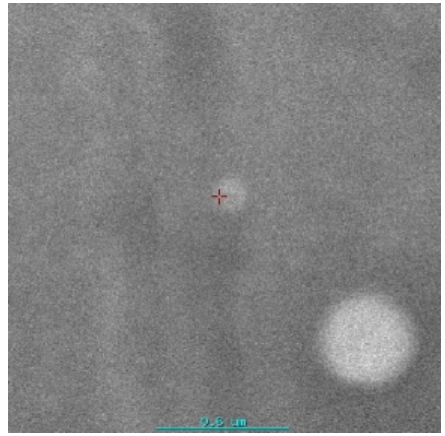


Spherical particles:

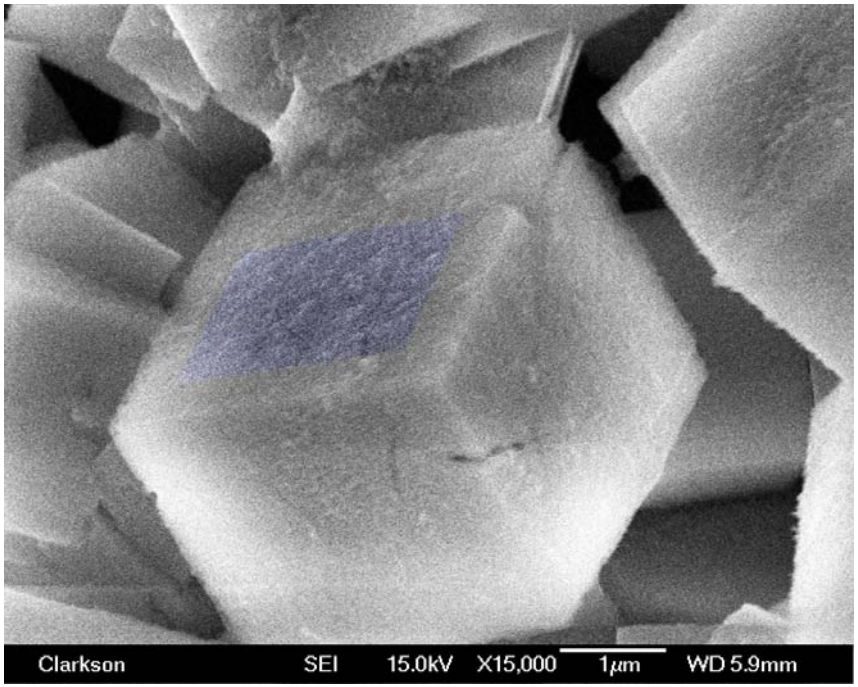
- shape is uniform and smooth;
- size varies with change of concentration.

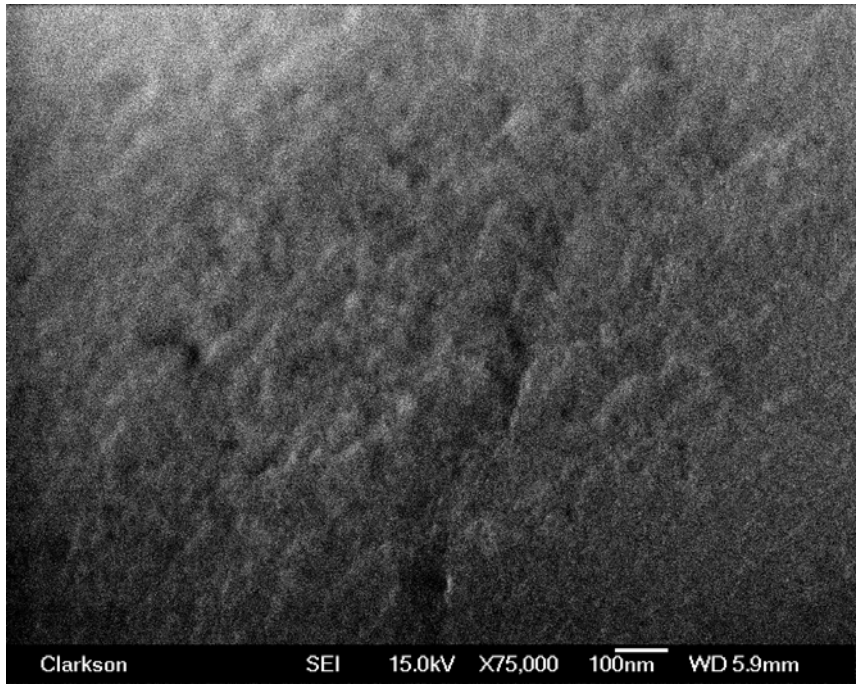




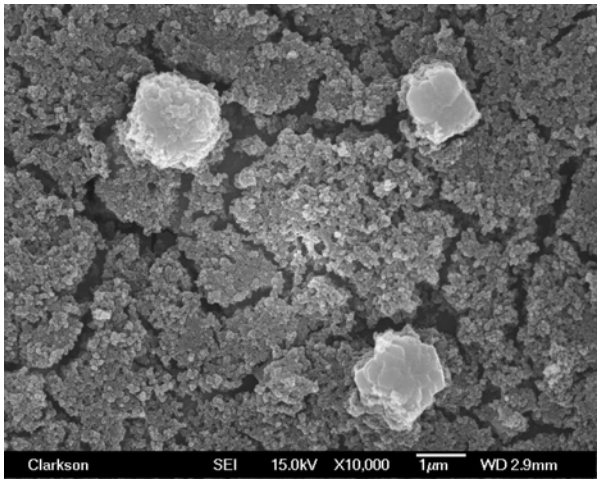


Here more careful work should be done, to explore a surface



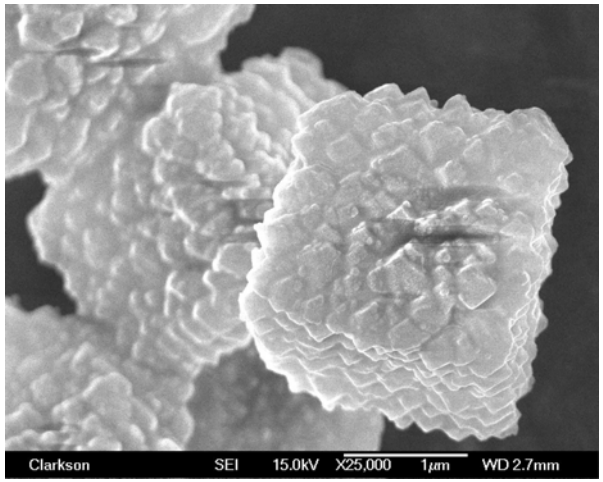


Stages of growth

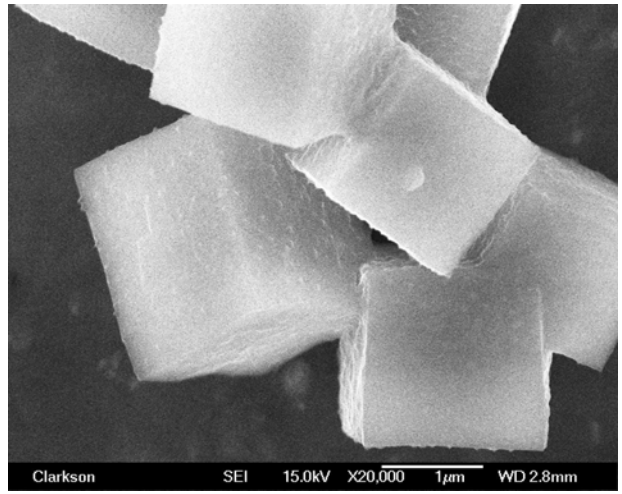


←About 2 minutes after the start

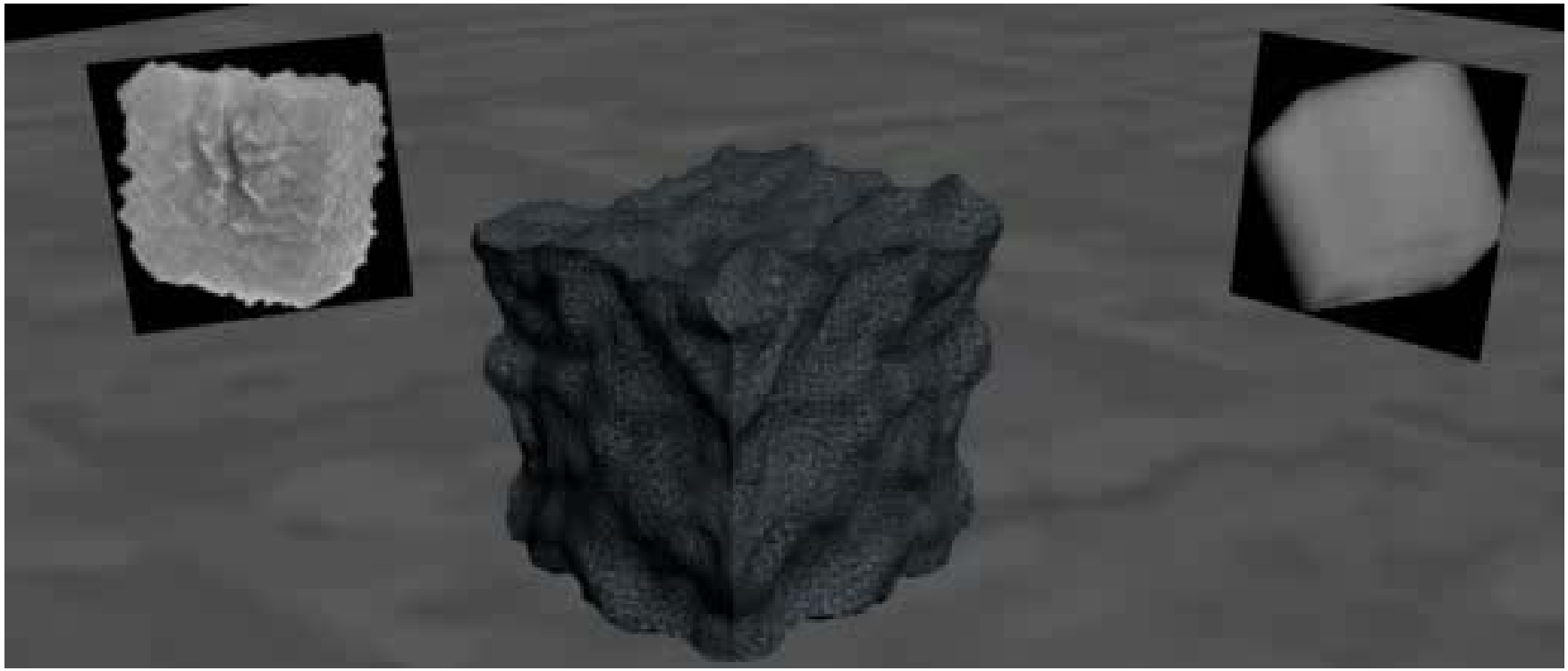
One hour after →



~ Two hours after→

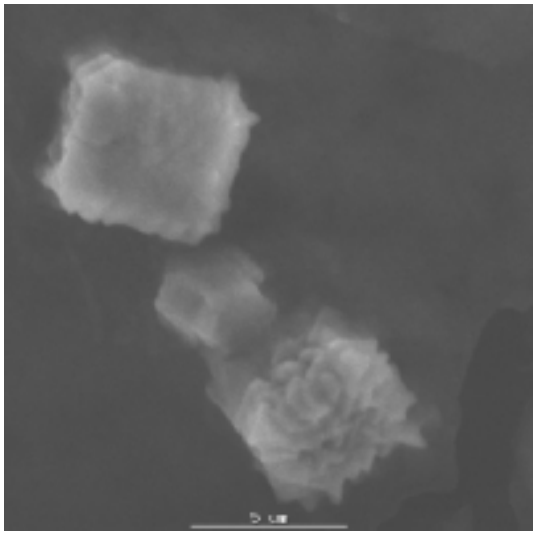


Visualization of the growth process

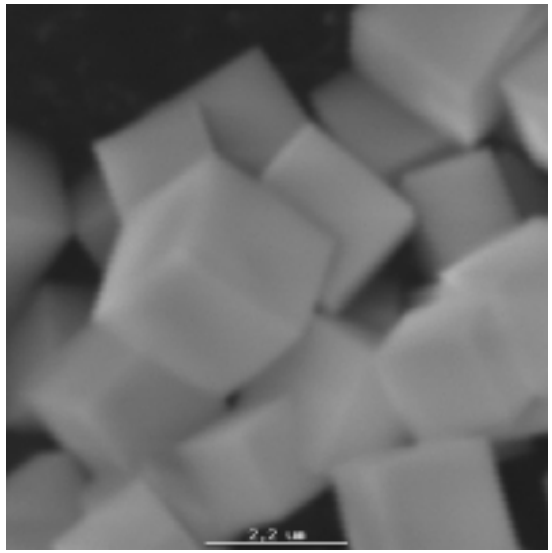


- Size is established and doesn't change,
- Shape formed but become smooth only after some time.

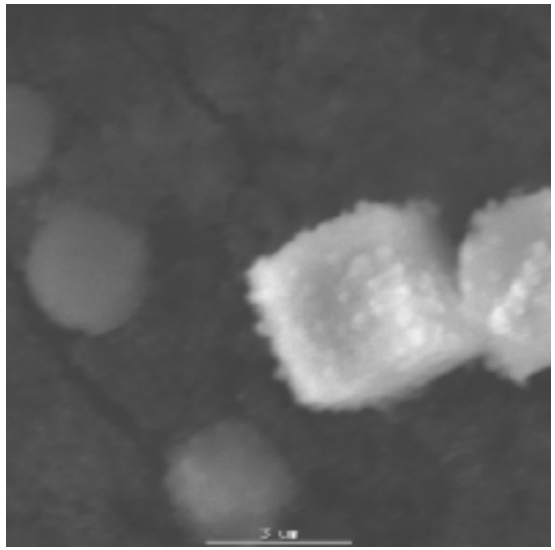
"Acid and water" principle



←$MgCl_2$ + NaF

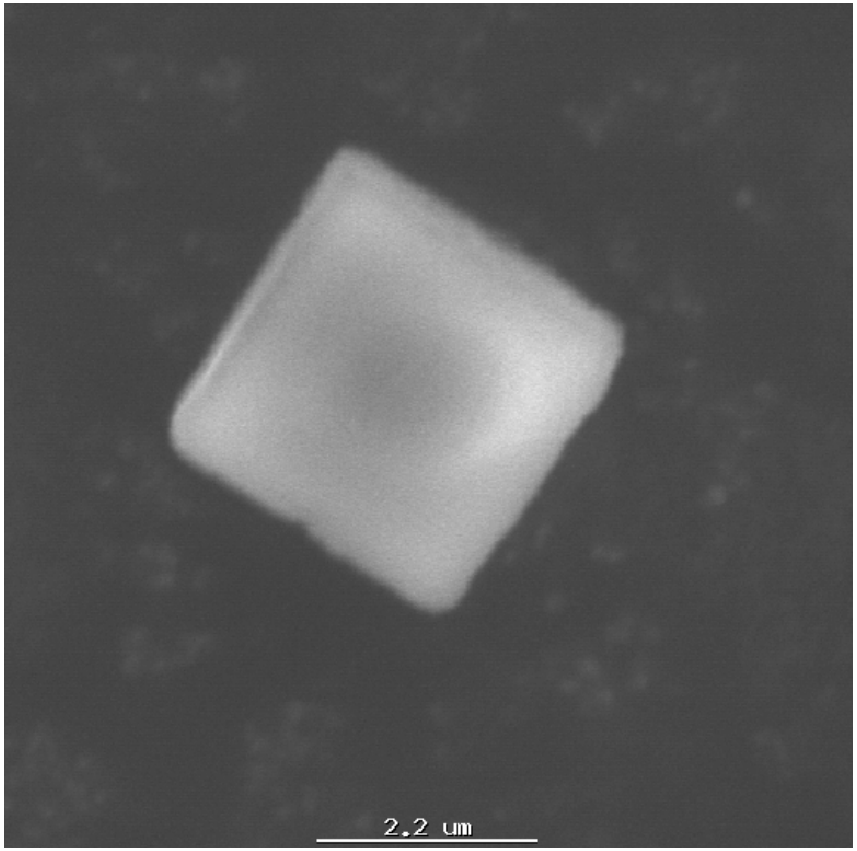


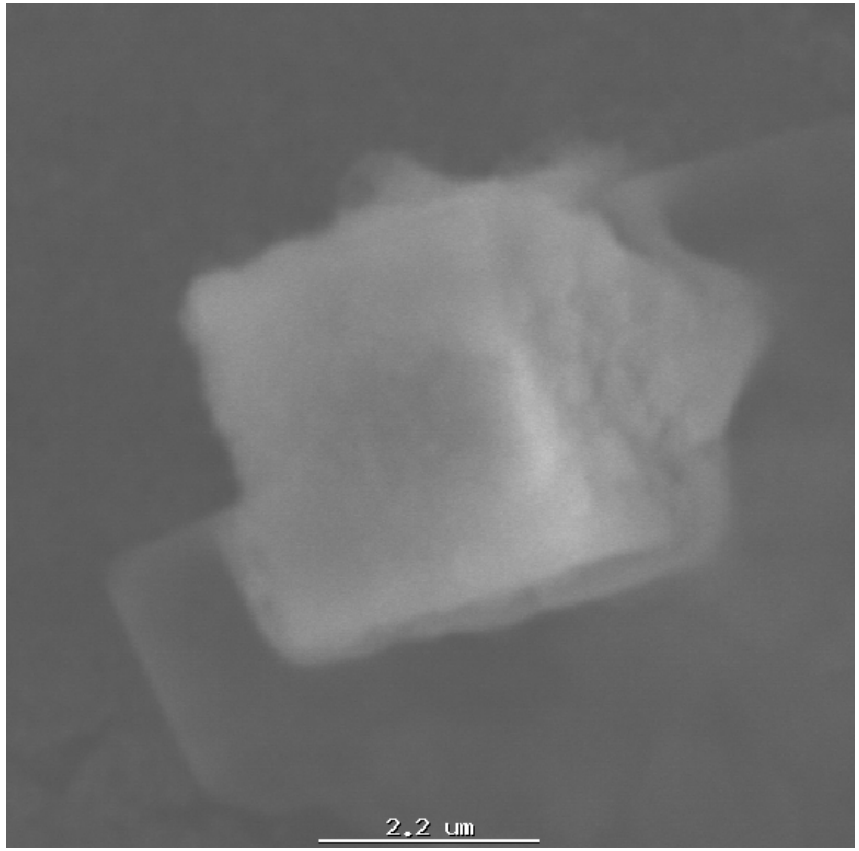
← NaF + $MgCl_2$



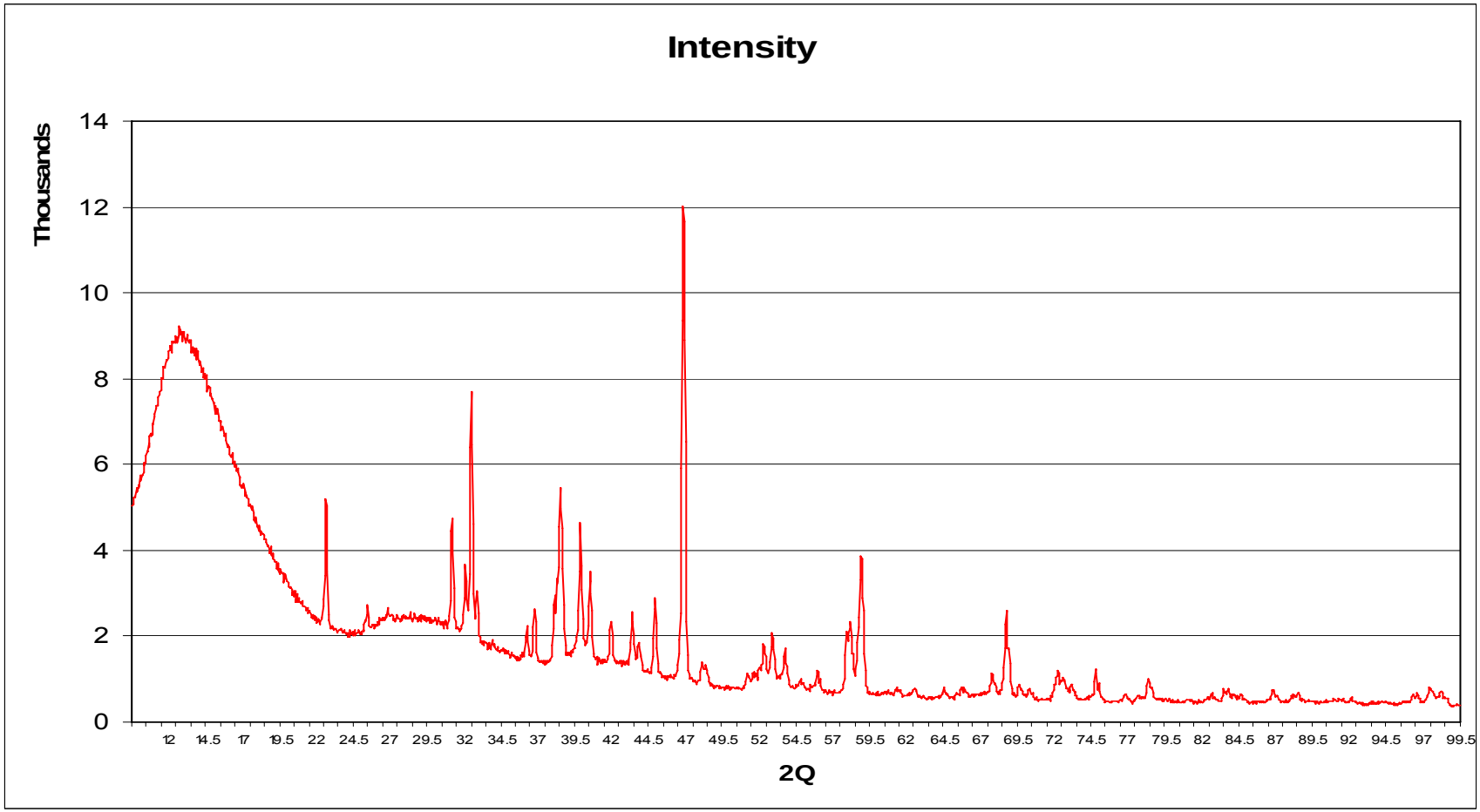
Water + $MgCl_2$ + NaF →

Jet mixing





XRD of the cubic particles
Fits to the template of $MgNaF_3$ from the library PDF-2



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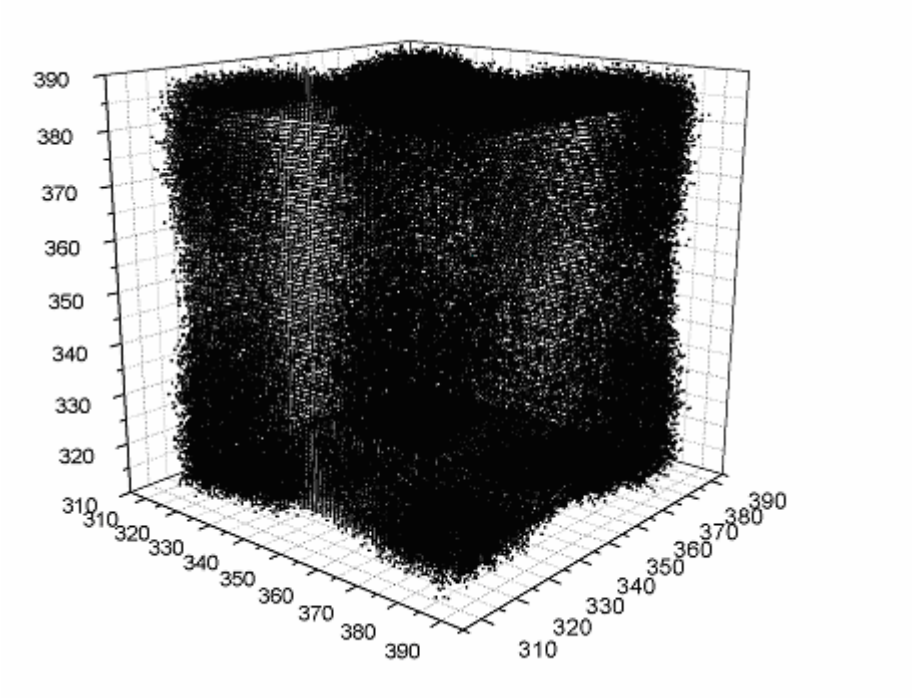
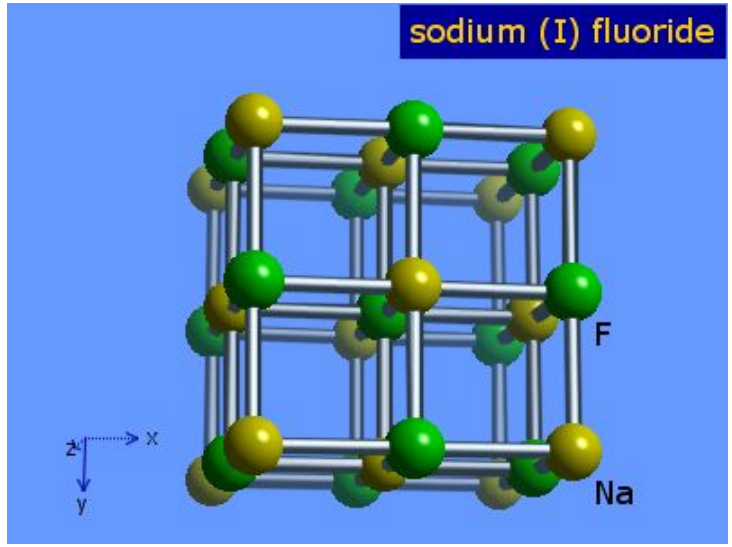
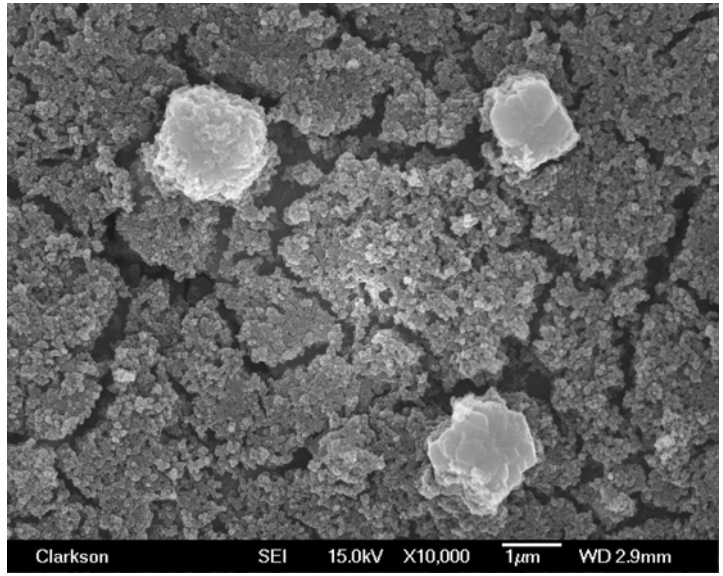
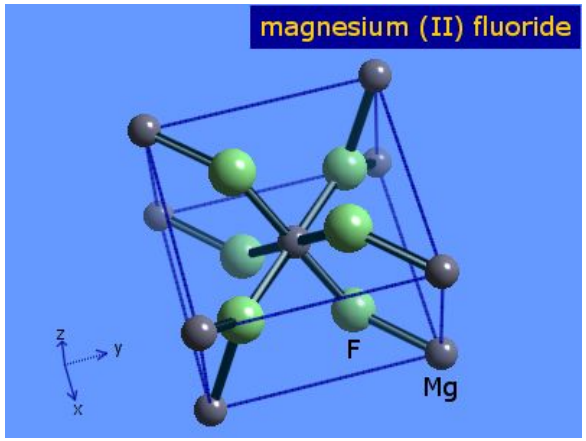
If it can be proved that the particles form cubic structures under the influence of NaF lattice, then the numerical model will be less speculative.

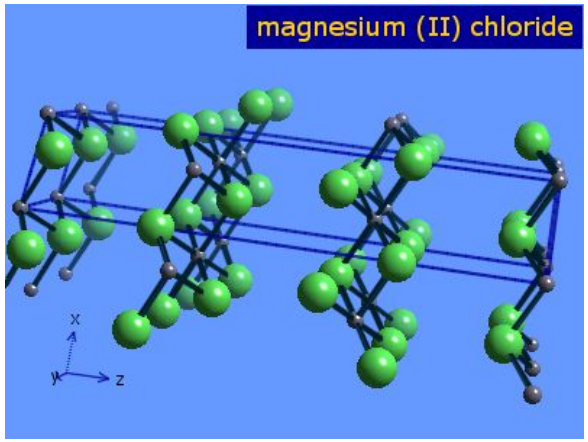


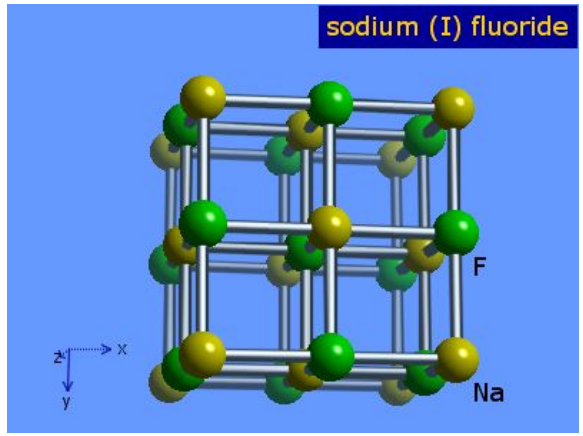




Lattice Comparison of MgF_2, $MgCl_2$ and NaF







Further directions and goals of the study:

- the system should be studied with XRD deeper;
- TEM, SEM, and light scattering should be involved in much more accurate level;
- time of growth of the spherical particles should e increased, to understand if there is a "time-bound" for the aggregation;
- numerical model can be improved:
  - by physical interpretation of the parameters σ and ρ;
  - by involving process-dependent peaks election for DF.

Reference:

1. *The Formation of Uniform Colloidal Particles of Magnesium Fluoride and Sodium Magnesium Fluoride*, Wan p. Hsu, Qiping Zhong, and Egon Matijević, Journal of Colloid and Interface Science, **181**, 142–148 (1996);
2. http://chemistry.about.com

ACKNOWLEDGEMENTS

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SPONSORS:

Questions