# **Zeolite Synthesis and the Crystallization Process**

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Zeolites, as a class of crystalline minerals, find a wide range of applications in various fields, such as catalysis, separation, and adsorption. These materials have also been developed for advanced applications, such as gas storage, medical applications, magnetic adsorption, and zeolitic-polymeric membranes. To effectively design zeolites for such intriguing applications, it is crucial to intelligently adjust their crystal size, morphology, and defect population in relation to crystal perfection. Optimizing these fundamental parameters necessitates a deep understanding of zeolite formation mechanisms, encompassing the thermodynamics and kinetics of nucleation steps as well as crystallite growth.

Keywords: zeolites crystallization ; nucleation mechanism ; growth mechanism

# 1. Introduction

The factors governing the crystallization process are important tools to understand the physicochemical properties of a wide range of crystalline materials. Such elements also help us to predict how the crystallization is propagating through the lattice and how to tune the functionality of these materials by controlling the crystallization mechanism [1]. In this context, zeolites, as a class of crystalline materials with a variety of applications (catalysis, sorption, separation, etc.), demonstrate excellent versatility with chemical modifications <sup>[2]</sup>. However, they are sometimes very sensitive to adding new particularities to their existing specifications, meaning that their formation chemistry has some boundaries; outside of those areas, pure phase cannot exist [3]. For example, high degrees of delicacy should be considered for the synthesis of zeolite using some metals such as Ti (Titanium), Sn (Tin), Zr (Zirconium), or Hf (Hafnium), in the presence or in the absence of Al. The insertion of these atoms inside the framework of zeolites is tough work unless some additional components are added to the primary suspension to assist the crystallization step [4][5]. Namely, we can use special and sometimes expensive structure-directing agents (SDAs) or -environmentally noxious mineralizers, such as HF, to incorporate such metals in the framework <sup>[G][Z]</sup>. The conventional synthesis of zeolitic materials containing the abovestated elements is troublesome since their atomic radius and chemical reactivity are remarkably different and slower compared to Si and Al atoms; therefore, they can form amorphous metal oxide phases instead of being grafted into the zeolitic framework. The formation of amorphous phases, which has been observed by the introduction of such metals into the synthesis mixture, can also decrease the surface area of the final material due to the blockage of the porous network [4]

In addition to the compositional adjustment, crystal morphology and dimensions of zeolitic particles are important parameters influencing the functionality of zeolites for novel applications <sup>[8]</sup>. The so-called "crystal habit" generates a wide range of geometric appearances for crystallites, such as acicular, tabular, or striated, as specified by crystal aspect ratios (e.g., length, width, and thickness) plus numbers of crystal planar surfaces <sup>[9]</sup>. The crystal habit of formed zeolite is influenced by synthesis parameters, such as the type of inorganic species (e.g., heteroatoms as stated above), type and amount of organic SDAs, synthesis temperature, and presence of impurities. So, the final morphology is the outcome of the interplay between these different parameters; and thus, based on the various and empirical combinations of these factors, a wide range of zeolites, from nano-crystalline to gigantic crystals (centimeter range or higher) as well as equi- or multidimensional crystalline zeolites, can be crafted by the engineering of crystal habits <sup>[9][10]</sup>.

# 2. Nucleation Mechanism

Nucleation is the first step of crystal formation that is initiated by atoms accumulating in a small cluster inside the primary suspension. Dissolved species tend to form a quasi-solid phase, which is called nuclei, and likely contribute to the irreversible formation of the ultimate crystalline product through smart selections of conditions <sup>[11][12][13][14][15]</sup>. It also indicates that inappropriate conditions can make this process reversible and the formed clusters can be redissolved in the mixture of precursors. The motive force, which is exerted on the suspended particles to begin the nucleation, is called supersaturation and acts as chemical potential between the dissolved species and forms a quasi-solid phase. In fact, the

discrepancy between the actual concentration of zeolite precursors and the concentration at a solubility equilibrium at a certain temperature is known as supersaturation. As a possible effect, elevating the temperature can increase the entropy and chemical potential for a given synthetic system and, thus, facilitate the supersaturation condition in favor of the primary nucleation step <sup>[16]</sup>. However, it should be noted that increasing the temperature does not always positively affect the nucleation step and may suppress the nucleation by assisting the formation of different phases that are not thermodynamically desired for the nucleation step. In contrast, if the system shifts under supersaturation condition, clusters are dissolved in the primary solution [17]. Thermodynamically, two parameters govern how and at what speed the nucleation step is proceeding: (i) the difference in the total free energy of the system between the two final states (i.e., dissolved particles as State 1 and formed cluster as State 2, which is known as a bulk term; and (ii) the interaction between the solid centers and suspension phase at the interfaces, which is known as a surface term [17]. By realizing this, the nucleation rate can be altered by setting the supersaturation condition, indicating the higher the supersaturation, the faster the rate of nucleation, and the smaller the crystal size distribution. There is a threshold amount for supersaturation (i.e., so-called critical supersaturation zone, also characterized as the meta-stable zone); This is a region which above it, the nucleation occurs exponentially [18], yet, very close to this region, the crystal growth dominates the negligible nucleation and only a few large crystals are formed. In other words, when the system shifts to a critical supersaturation condition, nucleation occurs in a short time and stops quickly because the process reaches a phase that is incapable of forming crystals [19][20]. Furthermore, in the critical supersaturation region, the formed nuclei possess a critical radius which below this radius nuclei dissolve; in contrast, above it, nuclei can reduce the formation of Gibbs energy and further grow <sup>[21]</sup>. The primary nucleation classically occurs via two different pathways: (i) homogeneous nucleation in a pure phase, which uniformly grows from the parent phase via local fluctuations; or (ii) heterogeneous nucleation at low supersaturation, which occurs by adding seeds or in general in the presence of impurities [12][13][14][15]. However, both types of nucleation assists lowering the surface energy to the maximum possible negative value <sup>[22]</sup>. Despite these routes and regardless of which one is the cause of primary nucleation, secondary nucleation is the result of several dynamic interplays in the nucleating medium as well as surface interactions eventuating in polycrystalline breeding.

### 3. Growth Mechanism

Crystal growth initiates via atom migration from the suspension of precursors toward the forming crystalline surface and continues with atom attachment and rearrangement in the crystalline lattice. It is worth mentioning that when the growth step reaches a steady state condition, the supersaturation levels off and decreases because nutrients are gradually consumed during crystal growth. Cluster growth can be assumed to happen initially through Ostwald ripening and further proceeds with the gradual aggregation of small species <sup>[23]</sup>. From the classical point of view, zeolite crystal growth is a surface phenomenon including several sub-steps, the slowest of which is kinetically controlling the growth process. In this respect, the growth occurs on the surface and subsequently spreads toward the edges and kinks of the crystal unit <sup>[24][25]</sup>. However, it should be noticed that due to the presence of an organic structure directing agent (SDA) in the synthesis of zeolites and presence of some other elements (e.g., Na, K, etc.), the growth step is a complex process and its reaction mechanism is not yet fully clear. For instance, the interaction between inorganic precursors and the organic phase (SDA) impacts both the crystallization process and crystal size <sup>[1][26]</sup>.

Developing knowledge about zeolite growth mechanisms has shown to be very fruitful for the construction of new and innovative structures, such as chiral pores, extra-large pores, and extremely complex framework topologies <sup>[27][28]</sup>. On this subject, several surface growth models have been theorized in past decades, such as monoatomic layer growth as a model in which terraces and vacancies on the layer formation step demonstrate a less ideal and more practical mechanism of growth <sup>[24]</sup>.

The growth step is highly promoted at high supersaturations, which are thermodynamically regions with high levels of potency required to overcome energy barriers for 2D nuclei formation. However, low supersaturations are also capable of generating nuclei and fostering crystals. The ability of crystallization in these domains originated from the presence of dislocations, which can cut off the crystalline surfaces and gradually construct more steps on the crystal surfaces. This growth behavior of crystalline surfaces removes the necessity for 2D nucleation <sup>[29]</sup>. Nonetheless, the second and next steps should dimensionally grow beyond the critical diameter (i.e.,  $2r_{critical}$ ) to make the stepping process thermodynamically feasible <sup>[29][30]</sup>. In practice, lower supersaturations alter the growing behavior of the crystalline surface, which digresses from birth/spread growth type and shifts to spiral growth format with self-stepping patterns around dislocation centers <sup>[29][30]</sup>. This type of crystal growth also produces smooth crystalline surfaces <sup>[29]</sup>.

Supersaturation can directly affect the crystal growth patterns <sup>[29][31][32][33]</sup>. At lower supersaturations, smooth surfaces are developed by a spiral type of growth while increasing supersaturation replaces the spiral pattern with birth/spread growth, which still develops smoothly. Indeed, birth and spread growth is achievable after passing the critical supersaturation

region for 2D nucleation in the phase diagram. In both domains, crystals grow with polyhedral morphologies and flat faces. In contrast, highly concentrated supersaturations produce rough surfaces with the adhesive type of growth. Generally, increasing supersaturation increases the possibility of adhesive growth with higher degrees of irregular interfaces, such as fractal, spherical, and other complex morphologies <sup>[29][31][32][33]</sup>.

Apart from the study of growth phenomenon on microscopic scale, zeolitic-phase formation can be systematically controlled during the synthesis and by means of setting precisely experimental parameters. In this context, the crystalline particles in the nanometer range are obtained by restricting the growth step of conventional micron-size crystals <sup>[33]</sup>. For instance, the type and amount of SDAs <sup>[1]</sup>, aging time <sup>[5]</sup>, crystallization time, and temperature <sup>[5]</sup> can be regulated to produce fine crystalline particles <sup>[33]</sup>. Increasing the amount of SDA and lowering the temperature of synthesis in the absence or deficit of Na<sup>+</sup> <sup>[1]</sup> or the application of hard templates, such as porous carbons or polymers, can prevent crystal growth through suppressing nanoparticle aggregation. In addition, 2D zeolites are an interesting family of zeolites which are specified by their lamellar crystalline and porous structure <sup>[34][35]</sup>. These zeolites are obtained by the growth and following assembly of nano-layers in one particular dimension and due to the weak or absence of covalent bonds between their layers. In this class of zeolites, the stacking sequence can be modified, which enables scientists to synthesize diverse structures <sup>[34][35]</sup>. 2D zeolites are interesting materials because they produce better accessibility with enhanced mass transfer to active sites, which are desired properties for catalysis and adsorption processes.

# 4. Types of Structural Defects in Zeolites

Crystal defects are built by different structural and lattice imperfections in zeolite domains. Stacking faults and complex intergrown subunits are the two most common defects in zeolitic frameworks <sup>[36][37][38]</sup>. In the context of stacking faults, zeolite Beta (BEA framework) is an interesting example because of the presence of three polymorphs with different stacking faults (i.e., chiral polymorph A, achiral polymorph B, and polymorph C) as well as having a lot of hydroxyl groups in its structure. The high population of silanol groups in the framework of zeolite Beta has been explained by the occurrence of two different stacking faults at the same layer, which cannot be connected at edges or boundaries; therefore, they create too many abnormal pores with open bonds which end with terminal silanol groups <sup>[36]</sup>.

From a synthetic point of view, thermal treatment (calcination at elevated temperatures), elemental extraction using acid or base solutions, and steaming can also introduce defects in zeolite network; they are considered defects that are structurally generated in as-synthesized zeolites but are not considered inherent defects, those which are generated simultaneously with zeolitic crystals building <sup>[39]</sup>.

From a structural point of view, defects are divided into four types: volume defects, surface defects, line defects, and point defects. In general terms, volume defects, as stated above, are created due to the lack of chemical bonds, resulting in the formation of T-OH bonds. Volume defects are also known as bulk defects and can also be produced by missing tetrahedrally coordinated T atoms, and leads in the formation of voids in the structure [39][40]. Some factors can enhance the generation of these defects during the zeolite synthesis, such as contact with water molecules, the presence of heteroatoms (e.g., Ti), the presence and type of organic template, or dual templating [40][41][42][43]. Bulk defects also depend on the synthesis parameters and by their well-adjusting for each zeolite sample, the density of defects can be reduced or the grain boundaries can be healed. In line with these facts, some frameworks are more prone to bulk defects than others [10][40][41][42]. The surface type of defects can be generated during the steps of growth at twin boundaries and are assumed to be the major mechanism of growth resulting in the densification of polycrystalline zeolites, such as faujasite (FAU framework) [44]. In this type of defect, the growth takes place at the boundary of two crystals, which could connect the crystals together and produce disorders that are known as surface defects [44]. Surface defects are mainly observed in the absence of seeding techniques and owing to the linkage between the crystals, the original morphology of crystals are changed. In the case of the faujasite framework, the hexagonal geometries of the crystallites are altered and more irregular shapes are constructed [44]. The line defects in zeolites are formed due to the dislocated fringes and, thus, can change the stacking orders [45]. They can also be formed by the dissemination of point defects with a 2D pattern in the framework system. Point defects are created due to a missing atom in the connecting regions [45][46][47].

The structural defects alter the physicochemical properties of crystals in comparison with the case of ideal crystal perfection. However, such defects are caused by the intrinsic behavior of forming crystals and due to the crystal habits, they are inevitable. Furthermore, despite their presence, they are controllable and can be adjusted to be reduced, healed, or optimized for a given demand <sup>[48]</sup>. For instance, organic SDA-free synthesis, which is limited to a narrower range of Si/Al for each framework, can change the crystal structure as well as the crystal habits because these properties are functions of the molar composition (e.g., Si, Al, OH), temperature of synthesis, and time of crystallization. Using a specific experimental setting for these parameters, the crystal habit, morphology, as well as type, and population of defects can be

modified. To exemplify these alterations, one protocol is the use of acid treatment, by which higher degrees of volume and surface defects are inserted into the framework. These centers can accept open metals or hydroxyl sites as active sites for catalysis.

# 5. Modeling of Zeolite Crystallization Using Machine Learning

More recently, machine learning and computational statistics have been applied to zeolite science <sup>[49]</sup>. The target is to use machines for predicting the quantitative output of synthesis pathways, providing a greater ability to predict zeolite yield and performance <sup>[49][50]</sup>. In this regard, different mathematical models, such as linear regression, ridge regression, regression tree, random forest, XGBoost, and artificial neural network models, can be employed <sup>[49]</sup>. Using these models by means of synthesis variables as input, the model versatility and machine ability have been assessed. The promising results of such modeling for zeolite LTA indicated that machine learning in combination with experimental techniques can be used as a tool in zeolite science <sup>[49]</sup>. In addition, computational statistics were used for extracting data, including synthesis information and trends from zeolite journal articles, to predict different features of Germanium-containing zeolites, such as framework density <sup>[50]</sup>. Machine learning has also been employed for the prediction of the zeolitic framework <sup>[51]</sup>. By developing a nine-dimensional feature vector consisting of novel topological descriptors designed by computational geometry methods, a tool for the accurate prediction of a new framework has been modeled by the integration of the above-stated mathematical model with a series of physicochemical properties of zeolite crystals <sup>[51]</sup>.

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