



## **A STUDY ON PROGRESS OF CRYSTALLINE MATERIALS IN GROWTH AND ITS CHARACTERIZATION**

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### **Abstract :**

*The crystalline introduces considerable simplifications into the description of structure and the formulation of theories for the physical properties. Two main strategies currently in use for crystal engineering are based on bonding and coordination complex. The Crystalline Sstructure Design today contains atomic positional parameters for nearly 300 000 crystal structures, and this forms the basis for heuristic or synthon-based or "experimental" crystal engineering. A primary goal of this paper is to understand the structure of materials with the resulting reviews by making this theoretical connection, and able to create predictive models which will help materials , further analyze the nanocomposite structures and anticipate the effects those microstructures .*

*Key words: crystalline materials, solid state physics, molecular, nano, composite*

### **1. INTRODUCTION**

The study of crystalline materials has played a prominent role in the traditional approach to solid state physics. The crystalline introduces considerable simplifications into the description of structure and the formulation of theories for the physical properties. Therefore it is natural that the study of solid state physics emerged from crystallography and that the basic theories were formulated for the case of crystalline matter. Crystal engineering is the design and synthesis of molecular solid-state structures with desired properties, based on an

understanding and exploitation of intermolecular interactions. The two main strategies currently in use for crystal engineering are based on bonding and coordination complexation. These may be understood with key concepts such as the supra molecular synthon and the secondary building unit. A useful modern definition is that provided by Gautam Radhakrishna Desiraju, who in 1988 defined crystal engineering as "the understanding of intermolecular interactions in the context of crystal packing and the utilization of such understanding in the design of new solids with desired physical and chemical properties."<sup>[2]</sup> Since many of the bulk properties of molecular materials are dictated by the manner in which the molecules are ordered in the solid state, it is clear that an ability to control this ordering would afford control over these properties. Crystal engineering relies on no covalent bonding to achieve the organization of molecules and ions in the solid state. Much of the initial work on purely organic systems focused on the use of hydrogen bonds, though with the more recent extension to inorganic systems, the coordination bond has also emerged as a powerful tool. Other intermolecular forces such as  $\pi \dots \pi$ ,



halogen...halogen, and Au...Au interactions have all been exploited in crystal engineering studies, and ionic interactions can also be important. However, the two most commonly used strategies in crystal engineering exploit hydrogen bonds and coordination bonds. Molecular self-assembly is at the heart of crystal engineering, and it typically involves an interaction between complementary hydrogen-bonding faces or a metal and a ligand. By analogy with the retrosynthetic approach to organic synthesis, Desiraju coined the term "supramolecular synthon"<sup>[3]</sup> to describe building blocks that are common to many structures and hence can be used to order specific groups in the solid state. The carboxylic acid dimer represents a simple supramolecular synthon, though in practice this is only observed in approximately 30% of crystal structures in which it is theoretically possible. The Cambridge Structural Database (CSD) provides an excellent tool for assessing the efficiency of particular synthons. The supramolecular synthon approach has been successfully applied in the synthesis of one-dimensional tapes, two-dimensional sheets and three-dimensional structures. The CSD today contains atomic positional parameters for nearly 300 000 crystal structures, and this forms the basis for heuristic or synthon-based or "experimental" crystal engineering. High temperature materials are divided into two main categories—semi-crystalline and amorphous—based on their difference in molecular structure. Semi-

crystalline materials have a highly ordered molecular structure with sharp melt points. They do not gradually soften with a temperature increase, instead, semi-crystalline materials remain solid until a given quantity of heat is absorbed and then rapidly change into a low viscosity liquid. These materials are anisotropic in flow, shrinking less in the direction of flow vs. transverse to flow. They have excellent chemical resistance.

## 2. MATERIALS - CRYSTALLINE STRUCTURE

A primary goal of this work is to connect the microscopic structure of materials with the resulting mechanical properties including their elastic and plastic responses. By making this theoretical connection, we will create predictive models which will help materials scientists and mechanical engineers analyze nanocomposite structures and anticipate the effects those microstructures have on the onset of failure mechanisms in such materials.

1. Crystalline solid can be either Single Crystal Solid (crystal lattice of entire sample is continuous and unbroken to edges of sample with no grain boundary) or Poly Crystal Solid (aggregate of many crystals separated by well-defined boundaries)
2. Cluster of crystals with identical structure (same crystallographic planes & directions) are known as Grains separated by Grain Boundaries



3. X-ray diffraction analysis shows that atoms in metal crystal are arranged in a regular, repeated 3-D Pattern known as Crystalline Structure

Materials have a fundamental understanding of what occurs on the atomic scale in a crystal under high stresses during elastic or plastic deformation, but in materials that do not have an underlying crystalline structure we've only just begun to understand how deformation affects the atomic scale structure. Most materials can be created in an amorphous state in which the atoms have no long-range structural order. One common example is silica, which can be made into common glass or can crystallize into one of several phases of quartz. Metallic alloys, which are commonly found only as crystalline phases in nature but can also be forced into an amorphous state if they are deposited energetically, can be composed of carefully chosen elemental constituents or cooled very quickly from the liquid state. This research focuses on situations in which a material is composed of both amorphous and nanometer scale crystallites. Our goal is to help guide the development of new, emerging nanocomposite materials with high strength and hardness.

### **3. PROSPECTS FOR CRYSTAL ENGINEERING**

From recent literature it appears that knowledge gained over the past century and increasingly sophisticated screening techniques developed within the last decade are paving the way towards design of co-crystals with potentially improved properties in the field of crystal engineering and developing the retro-synthetic understanding

of crystal structure using reasoning that is analogous to that applied by organic chemists. The assemblies that define the crystalline arrangement of the molecules as they self-organize into the solid-state. The parallels between the development of crystal engineering and synthetic organic chemistry run still deeper. Methodologies for carrying out these crystallizations are being developed alongside the development of new robust motifs. The importance of the solubility and dissolution relationships of the components of a putative co-crystal is becoming a matter of significant investigation. The same can be said for the roles of additives in templating novel forms. Mechanical milling of materials has also been documented as a means to make co-crystals, and a recent example of polymorphic forms of caffeine:glutaric acid illustrates the opportunities of this type of processing to influence crystal form. With an increase in the understanding of the modes of self-assembly, one can start to address the design aspect towards making co-crystals. The field of crystal engineering has experienced significant development. Importantly, crystal engineering principles are now being actively considered for application to pharmaceuticals to modulate the properties of these valuable materials. Because the physical properties that influence the performance of pharmaceutical solids are reasonably well appreciated, there is a unique opportunity to apply crystal engineering techniques and the appropriate follow-up studies to solve real world problems. As structures and series of co-crystals have begun to appear, we again find that properties cannot be predicted from the structures. The co-crystal options presented retain the stability inherent in a crystalline state, while allowing for solubilization that significantly exceeds that of crystalline



itraconazole base and rivals the performance of the engineered amorphous bead formulation. There remain several limitations to the application of what is currently known to the design of useful materials. As mentioned earlier, it remains intractable to reliably predict crystal structure. Multi-component crystals are well out of reach for prediction due in part to complex energetic landscapes, lack of appropriate charge density models and a large number of degrees of freedom, making computation unfeasible. Moreover, there is only a qualitative understanding of the interplay between intermolecular interactions and materials performance, especially for properties such as solubility, dissolution profile, hygroscopicity and melting point. But the saving grace of the co-crystal approach comes in two guises: Complementarity and diversity. On the topic of complementarity, it is possible, by way of CSD database mining for instance, to identify trends of hetero-synthion occurrence in model systems. As for the diversity aspect, the space of possible co-crystal formers is large, limited only by pharmaceutical acceptability. Coupled with parameters such as stoichiometry variation and increase in the number of components, the opportunities appear vast.

**4. THE SCOPE OF CRYSTALLINE MATERIALS:** Materials especially crystalline materials provide the foundation of our modern technologically driven world. The domination of materials is achieved through detailed scientific research. Advances in the techniques of growing and assessing ever more perfect crystals of a wide range of materials lie at the roots of much of today's advanced technology. Crucially important applications in information technology, photonics, energy

storage and harvesting, environmental protection, medicine and food production require a deep understanding of and control of crystal growth. This can involve suitable growth methods and material characterization from the bulk down to the nano-scale.

Crystal growth is an important field of materials science which has got scientific as well as technological importance. Scientific importance of the subject is mainly related to the growth of single crystals and its characterization while the technological importance is dealing with the growth of large single crystals and its application on device fabrication. The present research work (reported in this thesis) is scientific in nature and not technological. It is possible to grow large size crystals of (BTCC - BTCl) mixed crystals with improved quality by carefully adopting either the SR method or some innovative techniques with modified apparatus. The effect of pH value on the growth conditions and morphology of the grown crystals can be investigated. Since the nucleation studies for these samples are not carried out, attempts can be made in future to investigate the nucleation parameters such as metastable zone width, induction period, interfacial tension, etc to improve and investigate the optimized growth parameters for industrial crystallization. Attempts can be made to identify suitable dopants, which could provide better optical properties and thereby enhance the NLO property of these crystals. It will be interesting to study the micro hardness studies for different orientations of the grown crystals. The grown crystals can be subjected to Z-scan studies to estimate the absorption coefficient. Grown crystals could also be subjected to Nuclear Magnetic Resonance (NMR), Scanning Electron Microscopy



(SEM) and Atomic Force Microscopy (AFM) studies to visualize the structure and defect mechanisms. Etching studies can be made on different crystallographic faces of the crystals with suitable etchants in order to identify the dislocations. Several studies are to be carried out on the fabrication of devices with the grown crystals.

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