



STUDIES ON MIXED CRYSTALS: AN OVERVIEW

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ABSTRACT:

There are many returns to controlling structures and properties in crystalline materials which explain the increasing efforts in this direction. Crystal implementation has historically focused on the rational nature of single-component molecular crystals or supramolecular compounds. Recently, studies on crystalline solid solutions have become popular in research involving crystal implementation..

KEYWORDS: Crystals, Mixed Crystals, Solid Solutions, Crystal structures, Crystal Properties.

INTRODUCTION:

A "solid solution" ("ss") refers to a crystal or crystallite consisting of at least two different chemical elements, with the foreign atoms being distributed statistically within the host lattice.

However, what is characteristic about a solid solution is that the lattice structure of the initial crystal remains unchanged by the integration of a second particle type, which must have a similar crystal lattice. Therefore, an element's original atomic lattice is conserved, whether the foreign atoms are interstitially or substitutionally inserted into the host lattice.

Many metals may integrate certain species of atoms into their (matrix) atomic lattice structures. Such foreign atoms can be either inserted at the lattice's interstitial sites or occupy a site within the matrix's atomic lattice.(FIG.1)

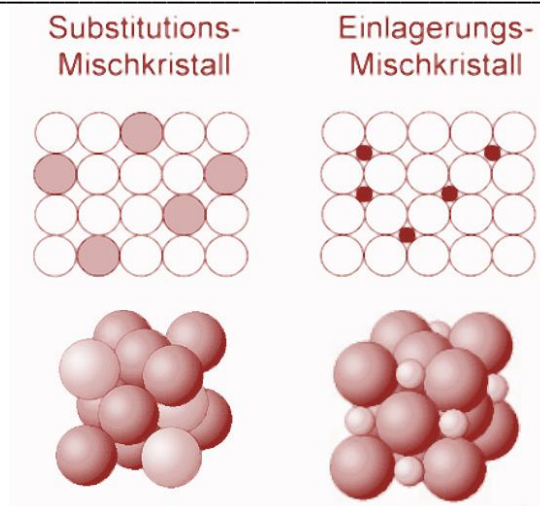


Figure 1: atoms in a solid solution

The lattice is always more or less stretched due to the different lattice parameters, resulting in an increase in strength (so-called solid solution hardening or reinforcing solid solution, see also Reinforcing mechanisms). On this basis, solid solutions have a higher level of hardness and tensile strength and a lower temperature of melting than the substance. In addition, there is decreased electrical conductivity in the metallic solid solutions.

The Fe-C system includes examples of the solid solutions produced by interstitial atoms.

- Zn in Cu or Cu in Al are examples of strengthening through substitutional foreign atoms.

Crystalline solid solutions are long known solid phases that allow to fine-tune the structure and properties of a material. Some of them, such as metal alloys, have been used for thousands of years in everyday life. These phases thus constitute an important part of the science of materials. On the contrary, solid solutions containing organic molecules and their compounds have had a slower rate of development. However, the number of publications on molecular solid solutions (i.e. mixed crystals) has increased considerably in recent decades, and studies on molecular solid solutions have become popular in crystal implementing. The studies have provided new information that can help to explain these phases and show how to obtain materials with improved and tunable properties. Practical concepts for designing, synthesizing and characterizing molecular solid solutions are outlined (Figure 2) and discussed from a crystal implementing perspective.[1]

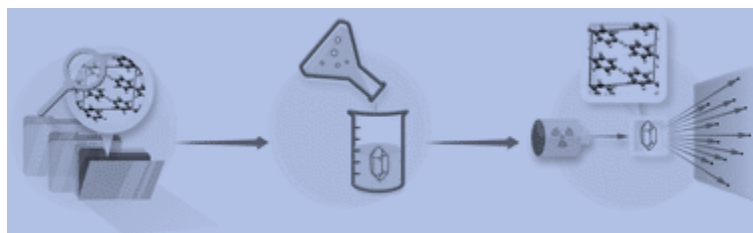


Figure 2

Single Component Crystals

Crystals are solid structures with a homogeneous makeup which due to their homogeneity exhibit specific properties. Crystalline structures' mechanical properties play a critical role in dictating the dissolution rate, solubility, and other characteristics of the crystal, as well as the variety of their applications. Now the elasticity of the first known single-component, bendable pharmaceutical crystal has been elucidated by researchers. A pharmaceutical crystal's homogeneity helps ensure product purity as well as predictability of certain properties that contribute to the formulation of pharmaceutical products such as elasticity (Figure 3).

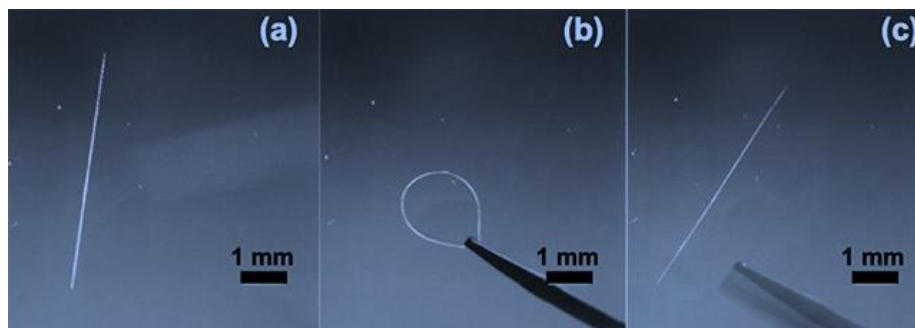


Figure 3: (a-c) Looping of the elastic celecoxib

The degree and ease with which an active pharmaceutical ingredient like celecoxib can be milled or compressed into tablet form depends largely on the mechanical properties of the crystal. Crystals must meet certain criteria to be classified as "bendable-faced elastic":

- interlocking isotropic packing devoid of slip planes that ensure the structure remains intact by retaining its original physical features; and
- reversible bending elasticity as a result of multiple dispersive interactions in orthogonal directions, which help ensure the crystal regains its shape after manipulation by a metallic needle.

The researchers conducted a series of experiments to elucidate the mechanical properties of celecoxib. When a metallic needle depressed the crystal containing the celecoxib molecules, the crystal immediately rebounded, fully intact, and regained its original shape upon removal of the needle. Such results demonstrate how elastic this single-component crystal is.[2]

Multi Component Crystals:

Supramolecular self-assembly permits the molecules and ions to be used as constructing blocks or tectons. The supramolecular interactions (synthons) and their motifs and patterns are so sturdy in lots of cases that the equal supramolecular structures are continuously generated by means of constructing blocks which pose the proper practical companies. This technique permits a honest change of the crystal structure wherein the degree of nice tuning is decided by means of the difference between

comparable building blocks in size and shape. [3-4] when carried out to multicomponent crystals, one of these supramolecular technique is in particular convenient. In truth the mixture of a couple of substance increases the potential for structural variability, which in unmarried component crystals is restrained to the phenomenon of polymorphism (determine four)[5]. Self-assembly turned into efficiently exploited to create neutral and charged species multicomponent crystals, in addition to composite solids with multiple levels. In those merchandise, comprising metallic complexes, salts, cocrystals and, extra currently, ionic cocrystals, cocrystallize more than one components in a stoichiometric ratio and act as a supramolecular compound. Those compounds obey dalton's more than one-proportion regulation, and every issue typically occupies nicely-defined crystallographic positions in their crystals.[6]

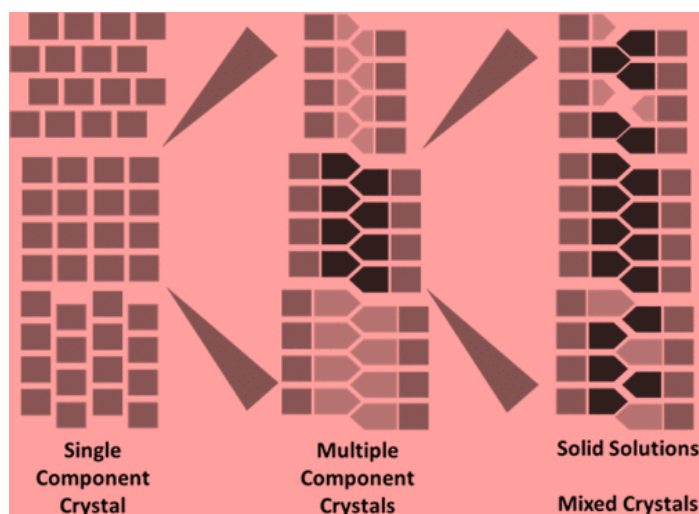


Figure 4 Multi Component Crystals

Strong answers constitute a distinct kind of multicomponent fabric.[7] those levels are characterised with the aid of a structural disorder, which is accountable for the homes common of liquid answers. The stoichiometry of solid answers, as with their liquid equal, isn't constrained to a single indispensable value but may be numerous in spectrum. Certainly, as for liquid answer, solubility inside the stable country does now not want to be entire however can be discovered in a constrained composition variety. Greater considerably, the variation in stoichiometry creates a non-stop version of (colligative) structural, thermal and chemical houses, making these materials particularly appropriate for best tuning (determine four). Sturdy answers regularly have properties that are between those of the pure components, however new homes arise in a few conditions. Either way, crystalline robust solutions provide an possibility to apprehend the connection of structure homes, as outlined beneath.[8]

Mixed Crystals:

The term "solid solution" has been used in a variety of contexts since its invention in the 19th century, to refer to both crystalline and amorphous solids. Historically, perhaps

because of the technical limitations that hindered accurate structural characterisation, their chemical composition (stoichiometry) was the main criterion for the identification of these phases. In this sense the word has implied any solid which has not obeyed multiple proportions of Dalton's law. This included substitutional crystals and host / guest structures partly occupied, as well as interstitial and intercalated compounds [9].

The time period mixed crystal has been used with more than one meaning which imply both crystalline stable answers and bodily combinations. Kitaigorodskii in his seminal e book used "mixed crystals" in the broadest sense to consult molecular crystals. If so, the expression turned into also used for single element systems with $z' > 1$ or bodily combos of polymorphs. Even currently, the time period turned into used for not unusual cocrystals, aggregate of levels, and easy salts. Frequently combined crystal is likewise used for natural and structured polymers, that are single macromolecules or mixtures rather than molecular crystals. Despite the fact that, using combined crystal is most usually restrained to crystalline solid answers of discrete molecules. Extra lately the terms blended cocrystal or solid cocrystal answer were defined as nicely. Those materials are cocrystals wherein the structural characteristic of a single conformer is ensured by means of two or more molecules that may be present in a variable ratio. The word alloy, originally used exclusively for metallic substances along with strong solutions, combinations and intermetallic and non-stoichiometric compounds, additionally cautioned molecular crystals as well as polymers for coordination. In this example the organic clause is inserted to underline the gap from the initial approval. The term multivariate mofs has also been used in the area of metallogranic frameworks to indicate solid solutions of porous polymers in coordination[10].

CONCLUSION:

Ideally, the crystal designer has assembled all molecules in the desired form and will be able to control unit size and symmetry and any physicochemical properties as well.

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