International Advance Journal of Engineering, Science and Management (IAJESM)
Multidisciplinary, Indexed, Double Blind, Open Access, Peer-Reviewed, Refereed-International Journal.
SJIF Impact Factor =7.938, January-June 2024, Submitted in March 2024, ISSN -2393-8048

Solid State Chemistry

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ABSTRACT

This course provides a solid foundation in a dynamic field while simultaneously examining possible new areas of innovation. Through the use of interesting applications, the topics are presented in context. utilizes a pattern of two colors with a section of four colors in order to make crystal forms more accessible to the user. It has a lengthy bibliography as well as reading suggestions, which will assist you in finding further works that are relevant to it more quickly. Contains not just a list of questions and answers but also a handbook that explains how to respond to those questions. The students who are in their first and second years of college are the target audience for this introductory course on solid state chemistry. It provides students with real-world examples of how their knowledge may be used, as well as an overview of recent breakthroughs in the field.

Keywords: - solid state, state chemistry, crystal, Material Properties

INTRODUCTION

As a result of the fact that genuine crystals have a multitude of defects and imperfections that have an effect on their electrical, mechanical, chemical, and physical characteristics, it is impossible to construct a crystal that is absolutely faultless. A wide variety of technical phenomena and processes, including as annealing, precipitation, diffusion, sintering, oxidation, and many others, are dependent on the existence of flaws. It is essential to keep in mind that problems with materials do not always have a negative impact on the quality of the materials. It is possible that the desired attributes may be achieved by carefully managing the different types and amounts of flaws that are present in a system. This is a possibility if the appropriate processing techniques are used. To provide a more concrete example, "defect engineering" is rapidly becoming into a significant area of research.

There are four basic forms of faults and imperfections: point defects, line defects (also known as dislocations), planar defects (also known as interfacial or grain boundary defects), and volume defects. Point defects are the most prevalent type of problem. Macroscopic or bulk faults, such as holes, fractures, and foreign particles, may also be included in this category. These flaws are introduced during the manufacture and processing of the solid state. In a system, the existence or absence of point defects is determined by the composition, temperature, and pressure of the system. This is due to the fact that point defects are inherent to the equilibrium state. On the other hand, the original production of the solid and the subsequent processing of the solid are the factors that define the presence of new faults and the concentration of those faults.

Think about a few important characteristics of solids and how faults or crystal imperfections might impact those characteristics. As an example, crystal defects play a crucial part in the process of controlling the electrical characteristics of semiconductors. Conductivity of silicon may be altered in type (n or p) and by more than eight orders of magnitude with the introduction of trace amounts of electrically active dopant elements with the purpose of modifying the conductivity. Because of substitutional incorporation, each dopant atom in this structure represents a point defect in the silicon lattice when it is present. Because of the finding that even minute concentrations of impurity atoms may radically modify the electrical properties of semiconductors, a whole new field of solid state device technology has opened up, and the transistor was developed as a result of this discovery. Even in a perfect crystal, nearly none of the semiconducting properties that may have made these technological advancements possible would be present. It is only the shattered solid state that has these particular features.

It is possible for crystals to undergo mechanical deformation or a permanent change in shape due to the presence of dislocations, which are line defects. Because of its crystalline form, an engineering material that does not include any dislocations is brittle and has very limited practical use. Although the existence of dislocations ensures the ductility of crystals, which is defined as the ability to undergo deformation, the potential strength of crystalline solids is greatly reduced as a result of their presence. For the purpose of identifying essential characteristics such as ductility and strength, it is of the utmost importance to understand that dislocations are significant elements. In point of fact, the behavior of line faults is ultimately responsible for controlling practically all of the mechanical properties of crystalline materials. The magnetization and demagnetization capabilities of ferromagnetic materials are significantly impacted by the presence of Bloch walls, which are flaws that are two-dimensional in nature. The elements iron, nickel, and iron oxide are included in these materials. At these interfaces, two crystal regions that have magnetic states that are opposing to one another meet. Whenever magnetization takes place, these imperfections move about, and the movement of these faults provides the material with a net magnetic moment. If Bloch barriers did not exist, then it would be reasonable to assert that all ferromagnetic materials operate as permanent magnets. The presence of surface imperfections such as cracks makes it feasible for delicate materials such as glass to break with relatively little weights; in fact, electromagnets would not be conceivable if these flaws did not exist. This fact is one that will be familiar to anybody who has ever split open a glass tube by drilling a small notch into the surface of the tube. When surface fractures in glass are eliminated by etching with hydrofluoric acid or flame polishing, the fracture strength is nearly always enhanced. This is because the surface fractures are removed. As an example, the fracture strength of glass is around 1010 Newton/m2 when it is devoid of surface cracks. This is in contrast to the actual fracture strength of glass, which is approximately 107 Newton/m2.

OBJECTIVE

1. Determine atom, ion, or molecule organization in solids.
2. Examine how crystal structure affects material physical and chemical characteristics.

Point defects

Formation of point defects

There is a proverb that states, "Nothing is perfect." The natural world is a reality that cannot be refuted. In addition to being relevant to living things, this rule, which may be represented as the second law of thermodynamics, is also applicable to inanimate stuff, such as crystalline solids:

$$F = H - TS$$

Free energy, which is indicated by the letter F, is connected to the heat content of a system, which is marked by the letter enthalpy, as well as the disorder term, which is denoted by the letter TS. In the event that a reaction takes place at a temperature T, the change in F (ΔF) is linked to a change in H (ΔH), which is the amount of heat present, and maybe also a change in TS ($T\Delta S$) if the reaction takes place. The following is what takes place when defects appear in a solid that is otherwise of perfect quality: In accordance with the Maxwell-Boltzmann theory of the distribution of solid energy, it is possible for some atoms to acquire sufficient heat to migrate out from the equilibrium lattice site and into the interstitial space. As was indicated earlier, the formation of point defects leads to an increase in the heat content of the system (ΔH is positive and rises linearly with the number of defects formed). This comes about as a consequence of the energy that is needed and the lattice strain that resulted from the production of point defects. Disorganization arises when there is a deviation from perfection, which leads to the creation of flaws (ΔS is positive). A significant amount of disorder is created (ΔS) during the first stage, which is characterized by a transition from perfection to a modest disarray. On the other hand, as the overall disorder progresses, the rise in disorder (with a specific number of defects generated) decreases from time to time. Similarly, $T\Delta S$ experiences a dramatic decline at the beginning of the process, before reaching a level. It can be seen in figure 1 that the outcome of the free energy reaches its lowest point when a certain quantity of solid faults are present. Due to the fact that the equation for equilibrium defect density is f(temperature), this demonstrates that the transition from a faultless structure to an equilibrium one occurs in a natural way.

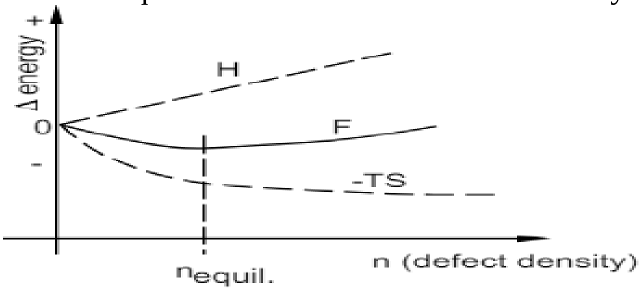

Figure 1 Thermodynamics of point defect formation

In the scientific world, the particular mechanisms that lead to atomic vacancies in solids are still a matter of intense controversy; nevertheless, the equilibrium energies that follow these events are clearly clear: Upon doing an analysis of the thermal energies of the lattice atoms, it has been shown that the average vibrational energy of the lattice atoms is much lower than 1 eV when the temperature is at room temperature. This is the estimated energy change that is connected with the production of a vacancy, as well as the minimal amount of energy that is required to produce a vacancy. Therefore, in order to acquire the energy ΔHd, which is essential for defect creation, a lattice atom must endure a significant energy fluctuation since it is the only way to do this. Given that the relative probability of an atom having an energy that is either greater than the ground state energy or different from the ground state energy is denoted by the symbol e, the probability of an atomic site being vacant likewise varies in the same way. With the assumption that a (molar) crystal has N atomic sites, the number of vacant sites may be calculated as follows:

$$n_d = ANe^{-\Delta H_d/kT}$$

Number of flaws in equilibrium at T: nd
Total atomic sites per mole = N.
ΔHd = energy required for defect formation.
T = absolute temperature (K).
Boltzmann constant: k
A = proportionality constant

Point Defects in "Pure" Metallic Systems

Impurity atoms, missing matrix atoms, and misplaced matrix atoms are examples of point defects that may be found in "pure" crystalline metals. Point defects are faults that are atomically sized. A selection of these point faults are shown in Figure 2. A substitutional impurity atom is one that is positioned in a normal lattice site, while an interstitial impurity atom is one that is situated between atoms that are part of the matrix. The size of the foreign atom in relation to the site is the determining factor in determining whether it will position itself in an interstitial or substitutional location. For the most part, tiny atoms are considered to be interstitial impurities, while large atoms are often substitutional impurities.

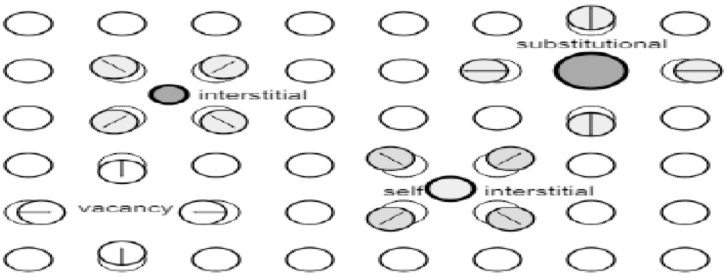

Figure 2 Point defects in crystalline solids

The term "vacancy" refers to the vacant space that an atom would normally occupy in a crystal that is perfect in every way. When an atom or ion transfers from a normal lattice site to another one on the surface of the crystal, this phenomenon is referred to as a Schottky defect. The term "vacancy" is often used to characterize this defect. Atomic mobility is high at high temperatures because of the heightened thermal vibrations, which may encourage atomic rearrangement in an existing crystal. Atomic mobility is high because of the higher thermal vibrations. There is also the possibility that a vacancy will arise during the process of crystallization as a result of localized disturbances that take place when new atomic planes appear on the surface of the crystal. Most of the time, point defects that are referred to as vacancies have an energy of creation that is less than one electron volt and are almost as big as the site that was first occupied.

Using Equation (2), one can determine the number of vacancies present in a crystal at any temperature. The energy needed to transport an atom from an atomically regular point inside the crystal to its surface for a Schottky-type defect is denoted by the symbol ΔHd. An enhanced equilibrium concentration of vacancies is formed in a heated solid, often near the crystal surface and then around dislocations and grain boundaries. This is because these are the places where atoms that have moved away from their typical lattice position have the potential to find a new home. As time passed, vacancies traveled from the surfaces of the crystal into the mass of the crystal. As a result of the "diffusion of vacancies" to grain boundaries or dislocations, which act as sinks, the concentration of vacancies decreases as the material is cooled. The new equilibrium vacancy concentration can only be formed after a short period of time has passed in each of these situations. In proportion to the decrease in temperature, the pace at which vacancies move across the lattice slows down at an exponentially decreased rate. As a consequence of this, the bulk of the voids are said to be "frozen in" when the material is quickly cooled (quenched) from a high temperature that is quite near to the melting point. As a consequence of this, the concentration of vacancies in quenched specimens is much larger (also known as "non-equilibrium") than what is implied by the value of that which represents thermal equilibrium.

In the lattice of a pure material, there is only one vacancy for every 108 atom sites while the material is at ambient temperature. However, when the material melts, this number increases to around one vacancy for every 103 sites. The presence of vacancies plays a significant role in the movement of atoms inside a crystalline solid. Void spaces have an effect on the rate at which matrix (or substitutional) atoms diffuse. It is consequently essential to have vacancies. (The process by which they move is the same as thatassociated with transferring a car in a full parking lot to the exit). A graphical illustration of this may be seen in Figure 3. Extremely few instances of self-interstitials may be seen in densely packed systems that make use of metals, regardless of the fact that radiation may introduce them. The high-energy neutrons that are produced by atomic fission, for example, have the potential to generate vacancy-interstitial couples by displacing metal atoms from their typical positions and causing them to move into the interstitial gaps.

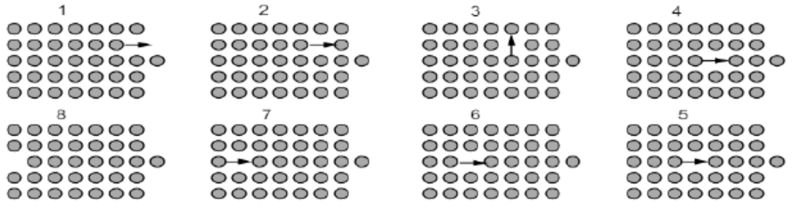

Figure 3 Dynamics of vacancy movements in a close packed solid

CONCLUSION

Solid state chemistry is a dynamic and crucial discipline of chemistry that focuses on the study of solid materials, including their synthesis, structures, and features. Solid state chemistry is dedicated to the study of solid materials. In the field of solid-state chemistry, the objective is to gain an understanding of crystal structures, investigate the characteristics of solids, develop novel materials, describe them via the use of sophisticated techniques, examine faults and defects, design materials for technological applications, and employ theoretical and computational modeling. Furthermore, they investigate phase transitions as well as reactions.

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