

## **Density, Hardness, and Melting Points: Key Physical Properties of Binary Crystals**

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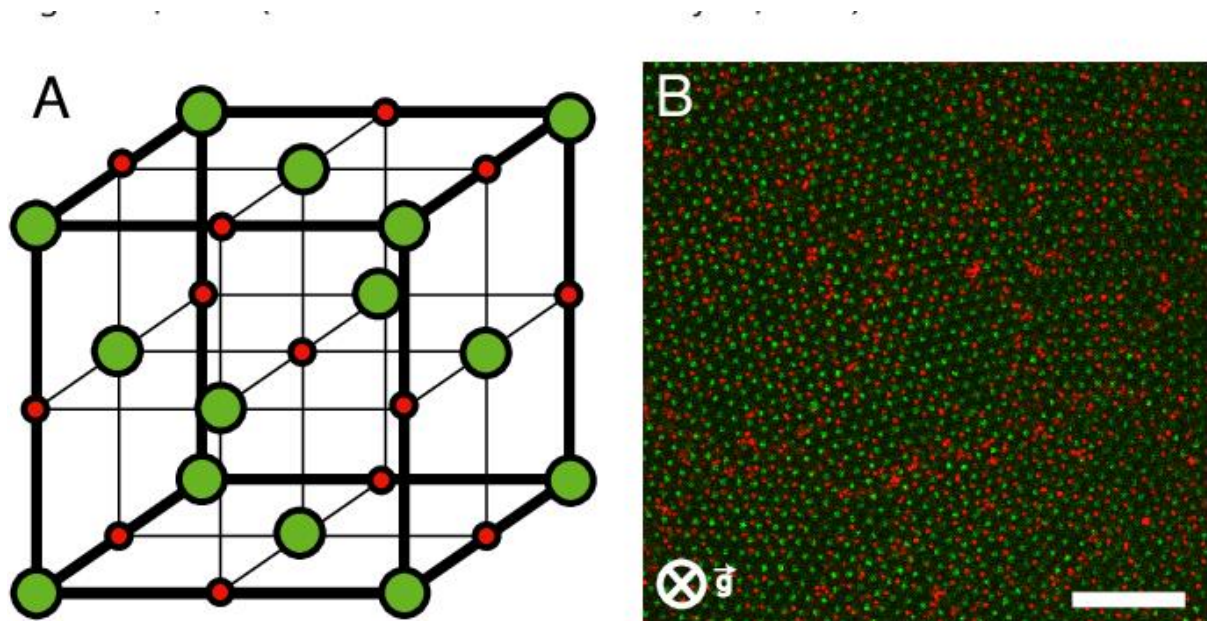
### **Abstract**

Binary crystals, composed of two distinct atomic or ionic species, exhibit unique physical properties such as density, hardness, and melting points, which are critical for their application in materials science and technology. The mechanical and structural stability of these crystals depends on the density, i.e. mass and spatial arrangement of the constituent atoms. It is an important parameter for industrial facilities due to hardness, a measure of resistance to deformation or scratching, that is under the control of interatomic bonding strength, crystal lattice structure and defect density. Bond energy and crystal cohesion of alloys define the range of temperatures in which they can be practical and melting points, indicative of thermal stability, depend on these characteristics. The interdependence of these properties with the atomic size difference, electronegativity difference and coordination number of the binary components is demonstrated. Recent advances in computational modeling and experimental techniques now allow the precise determination and prediction of these properties and the design of binary crystals with tailored properties for applications such as semiconductors, optical devices, or high strength materials. The relationship between composition, structure and physical properties of materials is serving as a cornerstone for understanding and driving innovation in many technological domains. In this article, we examine how density, hardness and melting points are linked in binary crystals to deepen our understanding of how material science functions.

### **Introduction**

Binary crystals consisting of two distinct atomic or ionic species are a fundamental class of materials with a wide range of application in science and industry. The crystals we have characterized possess special physical properties (density, hardness, and melting point) that are pertinent to their performance and effectiveness in different technological domains. Density is a key physical property and can only be explained by the combination and packing efficiency of its constituent atoms in the crystal lattice. Whether through cooperative or competition, it has a great bearing on the mechanical strength and stability and suitability for structural applications of these materials. In the same way, hardness, used to denote resistance to deformation or scratching, is equally directly proportional to the kinds of

bonding, lattice structure, and atomic interactions in binary crystals. Hardness is an extremely important condition for a material to be chosen for cutting, wear resistant applications or in other areas that involve high stress. Another important property is the melting point that indicates thermal stability of the material, its ability to withstand high temperatures with no change in structural breakdown which is important for thermal and refractory applications.



The atomic characteristics, bonding nature and crystal structures of the binary components are found to affect the interplay between these physical properties. Binary Crystals density, hardness, and melting points depend on atomic size, electronegativity difference, coordination number and lattice energy. Recent technological advances in material synthesis and characterization have allowed us to alter these properties for the desired applications; from semiconductors and optical devices to the shearing materials used in cutting edge aerospace applications. Knowledge of how these physical properties interact and are controlled by intrinsic and extrinsic factors of binary crystals allows scientists and engineers to design materials with optimized performance characteristics. In this paper, the relation between melting points, hardness and density in binary crystals is discussed along with their importance, and different related applications are explored in scientific and industrial fields.

### **Definition and significance of binary crystals**

Crystalline materials comprised of two distinct atomic, ionic, or molecular species arranged in a well defined periodic lattice are called binary crystals. These species are stable against breakup into monomeric species or chemical decomposition and combine in fixed stoichiometric ratios to form a structure whose stability is governed by the nature of the

bonding, that is, ionic, covalent, or metallic. Arranging these components in binary crystals creates unique structural, electronic, and thermal properties and makes them essential to a wide spectrum of scientific and industrial applications.

Binary crystals are important due to their tunable diverse physical properties, for instance density, hardness, melting points, electrical conductivity, etc. The atomic or ionic arrangement, bonding strength and crystal lattice symmetry are the properties from the arrangement of atoms or ions which from these properties are a direct consequence. For instance, ionic binary crystals (such as sodium chloride (NaCl)) have high melting points and high stability because of strong electrostatic forces and covalent binary crystals (such as silicon carbide (SiC)) are extremely hard with a remarkable thermal conductivity. Binary crystals are critically important for modern technology. As foundational in the semiconductors used as the basis of electronic devices, and in terms of the high performance materials used for aerospace, optical systems and energy storage, they are central. In addition, because of their crystallographic predictability and property versatility, they can provide a means to investigate fundamental principles in crystallography and materials science. In this regard, knowledge of binary crystals opens new doors into materials behavior and will enable design of advanced materials for future applications.

### **Importance of density, hardness, and melting points as key physical properties**

In binary crystals, the density, hardness and melting points of the materials are vital fundamental physical properties that determine performance and the applicability of materials. Density, expressed as mass per unit volume, is dependent of how compactly the atomic or ionic structure of a material is arranged, and influences its mechanical stability and strength. With higher structural integrity and resistance to deformation, high density materials are very much desired for applications where durability is essential e.g. construction and heavy machinery. The strength of atomic bonds and the crystal lattice arrangement cause a material to have hardness, the measure applied to the resistance a material has to scratching, indentation or plastic deformation. High hardness materials, such as diamond, or silicon carbide, are indispensable in wear resistant materials, cutting tools and industrial abrasives. Melting point, the temperature at which a material moves from solid to liquid, is a very important indicator of thermal stability and strength of a bond as well. Materials in environments of high temperatures, including turbines, refractory, and materials used in space, need to have high melting points because of strong ionic or covalent bonds. These properties are interrelated and dependent on factors such as type of bonding, atomic arrangement and external conditions; therefore, they are critical selection and engineering

criteria. A substantial amount of research has been devoted to rationalizing the structure and unique properties that arise at interfaces, and to understanding the relationship between these properties, which can be leveraged to guide the design and optimization of materials for particular functionalities, including semiconductors and optoelectronics, as well as high performance structural materials. Because of it, density, hardness and melting points are not just material properties that define the material, but they are also the determining factors for the future of material science and industrial applications.

## **Density**

### **Factors affecting density in binary crystals**

#### **Atomic Mass and Volume**

The density of binary crystals is given fundamentally by the atomic masses and volumes of the constituent elements. (A measure of density) is mass per unit volume, and density depends on not only the combined mass of atoms in a unit cell (the molar mass,  $M$ ) but also the volume occupied by those atoms. The reason for this is that, of course, heavier atoms have a greater contribution to the crystal lattice so they lead to higher density overall. For example, binary crystals comprising elements with high atomic mass, for example, lead or gold, usually possess higher density than crystals containing elements of low atomic mass, for example, lithium or aluminum.

Volume, however, is dependent on the size of the atoms and the geometry and electron cloud arrangement in the crystal lattice. Due to having a larger atomic radii, interatomic distances are greater, and therefore the unit cell volume can be increased which will decrease the overall density. Additionally, atomic volume is dependent on the type of bonding between atoms, ionic, covalent, or metallic. For instance, the ionic radii of its elements, or the resulting lattice structure, may cause the density of ionic crystals to vary. Density is affected by the atomic volume, which in turn is changed by temperature and pressure. Thermal expansion increases crystal volume, which lowers density, as temperature is raised. On the other hand, when under high pressure, atoms are forced closer together, reducing the volume and elevating density. To tailor materials for aerospace applications including lightweight but strong materials, concomitantly, radiation shielding requiring higher densities, it is critical to understand the balance between atomic mass and volume.

#### **Crystal Packing Efficiency**

The term crystal packing efficiency represents how efficiently the atoms or ions are arranged in a volume of a crystal lattice. The density of binary crystals is an important factor which

depends on the anisotropy. Packing efficiency refers to the proportion of the unit cell volume which is comprising of atoms; higher packing efficiency means denser materials, and vice versa. The type of crystal structure has a huge contribution as to how well they pack together. Simple cubic, body centered cubic (BCC) or face centered cubic (FCC) binary crystals have different efficiencies. For example, FCC structures, which exist in many metals and some binary crystals, have a packing efficiency around 74% that is denser than that of the BCC structures that have an approximate packing efficiency of 68%. The least dense are simple cubic structures, with a packing efficiency of only 52%. Packing efficiency is also dependent on the size and shape of the atoms or ions. In ionic crystals, the radius of cation to anion is called the ratio or radius ratio, with which the ions fit into the lattice. Tight packing with higher density is achieved with the optimal radius ratios, whereas suboptimal ratios result in the voids in the lattice to render the packing efficiency at a lower value. Packing efficiency can also be affected by defects, such as vacancies, or dislocations, within the crystal structure. A higher density of defects reduces the effective packing in the material, and thus the density of the material. Also, factors external like temperature and pressure are involved as well. Higher temperatures will expand the lattice and thereby decrease packing efficiency, whereas higher pressures will compress the lattice and increase efficiency and density, and crystal packing efficiency is vital to design materials with desired densities. In the latter application, lower efficiency can be desirable in order to achieve an increase in weight or porosity where desired, for example, in catalysts or lightweight structures.

### **Hardness**

In material science, hardness, that measures the resistance of a material to deformation, indentation or scratching is a critical physical property. Evaluation of a material for a given application demands its measurement. Hardness is quantified by several standardized tests. Materials are ranked by the Mohs scale, a qualitative method, from 1 (softest, talc), 2, ... 10 (hardest, diamond) by their property to scratch or being scratched by other materials. Vickers hardness test tests like the material's resistance to hardness by applying a specific amount of loading using a diamond shaped indenter. Hardness value in Vickers Hardness Number (VHN) is calculated from the size of the indentation. The Brinell hardness test determines the size of the indentation made by a steel or tungsten carbide ball indenter and expresses its size as the Brinell Hardness Number (BHN). These techniques deliver information regarding the strength and wear resistance of materials crucial for their industrial applications.

A material's atomic bonding and lattice structure play a strong part in what hardness is achieved. Ionic bonded materials, such as NaCl, have moderate hardness because of strong

electrostatic forces, but they are brittle. Strong directional, localized bonds and a rigid lattice structure produce very hard coefficients, including diamond and silicon carbide, which are covalently bonded materials. In iron and other such metals, the metallic bonds characterized by the delocalized electrons give moderate hardness along with malleability. Moreover, crystal defects and impurities also have important roles. The lattice is weakened by vacancies, dislocations, and grain boundaries all of which reduce hardness. Nevertheless, in certain instances, controlled addition of defects including alloying or doping can actually increase the hardness by preventing dislocation motion.

Carbide inserts and diamond tipped drills, which find applications in applications requiring high hardness, are cutting tools that require extreme resistance to wear and deformation. In the machinery and construction industries, the wear resistant materials, such as tungsten carbide, or hardened steel, play a critical role. Protective coatings, abrasives and armor also make use high hardness materials. With the understanding and the optimization of hardness scientists can fine tune material properties to meet demands of durability, wear resistance and strength.

### **Melting Points**

By equilibrium between solid and liquid phases we mean melting point, the temperature at which a solid transforms into a liquid under atmospheric pressure. A material's melting point represents a fundamental property in material science, giving an indication of the temperature at which a material's structural integrity begins to decrease, and the material's thermal stability. This is important because the operational limits of materials used for high temperature environments are set by this, and therefore the selection of materials for materials applications such as aerospace components, industrial furnaces, electronic devices, etc. A high melting point indicates that material has strong internal bonds, and is therefore less prone to being distorted or failing under thermal stress. The ability to predict the melting points of materials is important since controlled melting is required for processing techniques such as casting, welding and sintering in material fabrication and joining.

A number of factors determine the melting point of binary crystals, including bond strength and lattice energy, coordination number and atomic interactions. Bond strength is the force which holds the atoms or ions together in the crystal lattice; stronger bonds take more energy to break, so have higher melting points. The lattice energy is the energy released when gaseous ions form an ionic solid, and is thus largest for compounds with the greatest ionic character; compounds with higher lattice energy have higher melting points. The packing

efficiency and stability of the crystal lattice is affected by its coordination number, the number of nearest neighbor atoms or ions surrounding a given atom or ion. However, the coordination number is usually higher and results in a more tightly packed structure with more atomic interactions so that the melting point is higher. Together, these factors increase the thermal stability of a material, making it appropriate for use in high temperature applications where structural integrity must be retained. However, by understanding the influences and manipulating them, material scientists can engineer materials with tailored melting points to fulfill specific industrially relevant applications, such as the synthesis of heat resistant alloys and ceramics for use in hostile environments.

### **Applications of Binary Crystals**

Binary crystals, composed of two distinct atomic or ionic species, have wide-ranging applications due to their unique physical, chemical, and electronic properties. Their adaptability and structural diversity make them indispensable across various industries and scientific fields. Below are some key applications:

#### **1. Electronics and Semiconductors**

- Binary crystals like silicon carbide (SiC), gallium arsenide (GaAs), and indium phosphide (InP) are pivotal in the electronics industry.
- These materials are used in the fabrication of semiconductors, which are essential for transistors, diodes, and integrated circuits.
- They enable the development of high-performance electronic devices such as power amplifiers, solar cells, and LEDs due to their excellent electrical and thermal properties.

#### **2. Optical Devices**

- Binary crystals like zinc sulfide (ZnS) and calcium fluoride (CaF<sub>2</sub>) are utilized in optical applications for their transparency and refractive properties.
- They are used in lenses, prisms, and infrared optics in instruments like cameras, microscopes, and telescopes.
- GaAs and other optoelectronic materials are vital for laser technology and fiber optics communication.

#### **3. High-Strength Materials**

- Materials like SiC and boron nitride (BN) exhibit exceptional hardness and thermal stability, making them suitable for cutting tools, abrasives, and wear-resistant coatings.
- Their resilience under extreme conditions makes them valuable in aerospace and automotive industries for components like turbine blades and heat shields.

#### **4. Energy and Catalysis**

- Binary crystals like titanium dioxide ( $\text{TiO}_2$ ) are used in photocatalysis for environmental cleaning and hydrogen production.
- Lead iodide ( $\text{PbI}_2$ ) and cesium lead halides are employed in perovskite solar cells for efficient energy conversion.
- Catalysts in industrial chemical processes often utilize binary oxides or sulfides.

#### **5. Biomedical Applications**

- Calcium phosphate-based binary crystals are used in bone grafts and dental implants due to their biocompatibility.
- Binary fluorides and oxides are applied in medical imaging and radiation therapy.

Binary crystals' versatility and tailored properties continue to drive advancements in technology, addressing challenges in energy, healthcare, and sustainability. Their exploration and development remain critical for innovation in modern material science.

#### **Advances in Characterization and Modeling**

Binary crystals have been revolutionized by advances in characterization and modeling techniques, such that their properties can be precisely determined, and their behavior under different conditions predicted. However, with the advent of modern characterization methods, like X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM), it is possible today to perform detailed analysis of crystal structures, lattice parameters and defects. XRD is accurate for atomic arrangement and phase identification, SEM and TEM reveal surface morphology and atomic scale nature. Raman spectroscopy and Fourier-transform infrared spectroscopy (FTIR) are techniques that provide information on bonding and vibrational modes (which are key to understanding material properties). Phase transitions and thermal stability important for high temperature



applications are studied by thermal analysis methods such as differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA).

On the modeling side, the computational tools density functional theory (DFT) and molecular dynamics simulations have dramatically increased the extent to which properties of binary crystals can be predicted and optimized. Electronic structures, bonding, and energy states are insights into DFT which allow materials to be designed with tailored electronic or optical properties. Atomic interactions, defect dynamics and mechanical behavior under stress are modeled from molecular dynamics simulations. By reducing the need for extensive trial-and-error in material synthesis, these methods complement experimental techniques. We outline how machine learning and data driven approaches are emerging as powerful tools to predict properties and discover novel binary crystals from analysis of large datasets. Advanced characterization and modeling methods have recently enabled accelerated material discovery, resulting in the synthesis of binary crystals with optimized properties for semiconductors, optoelectronic, and high strength materials applications. These developments are essential to meeting the demands of energy efficiency, sustainability, and technological innovation in the fast developing materials science arena.

## Results and Discussion

**Table 1: Physical Properties and Applications of Selected Binary Crystals**

Binary Crystal	Density (g/cm <sup>3</sup> )	Hardness (Mohs)	Melting Point (°C)	Key Characteristics/Applications
Sodium Chloride (NaCl)	2.17	2.5	801	Common salt, used in food processing and chemical industry.
Silicon Carbide (SiC)	3.21	9-9.5	2,730	Abrasives, cutting tools, and high-temperature ceramics.
Gallium Arsenide (GaAs)	5.32	6.5	1,238	Semiconductors, solar cells, and optoelectronic devices.
Zinc Sulfide (ZnS)	4.10	3.5-4	1,185	Optical materials for lenses, IR windows, and LEDs.

Tungsten Carbide (WC)	15.63	8-9	2,870	Wear-resistant materials, cutting tools, and drills.
Aluminum Oxide (Al <sub>2</sub> O <sub>3</sub> )	3.95	9	2,072	Refractories, abrasives, and electrical insulators.
Calcium Fluoride (CaF <sub>2</sub> )	3.18	4	1,418	Optical lenses, spectroscopy windows, and lasers.
Titanium Dioxide (TiO <sub>2</sub> )	4.23	6-6.5	1,843	Photocatalysts, pigments, and solar energy devices.

Key physical properties, density, hardness and melting points of the selected binary crystals are summarized and highlighted on their important applications. Sodium Chloride (NaCl) is less dense (2.17 g/cm<sup>3</sup>), harder (2.5 Mohs), and melts at 801°C, and is applied chiefly for food processing and in the chemical industry. Silicon Carbide (SiC), an abrasive having an exceptionally high hardness (9-9.5 Mohs) and high melting point (2,730°C), is extensively used in cutting tools and high temperature ceramics. A key material in semiconductors, solar cells, optoelectronic devices, Gallium Arsenide (GaAs) has a density of 5.32 g/cm<sup>3</sup>, a melting point of 1,238°C. Zinc Sulfide (ZnS) has moderate hardness (3.5-4 Mohs) and a melting point of 1,185°C and is used for its optical applications such as IR windows and LEDs. Tungsten Carbide (WC) has very high density (15.63 g/cm<sup>3</sup>) and hardness (8–9 on the Mohs scale), and is used in wear resistant tools and drill bits. Aluminum Oxide (Al<sub>2</sub>O<sub>3</sub>), with hardness of 9 Mohs and with a melting point of 2,072°C, is used in refractories and as an abrasive. Optics and solar energy use Calcium Fluoride (CaF<sub>2</sub>) and Titanium Dioxide (TiO<sub>2</sub>) because of the moderate density and thermal stability. The versatility of binary crystals can be observed from the applications in the technological and industrial areas as shown in this table.

**Table 2: Comparative Physical Properties of Binary Crystals for Advanced Applications**

Binary Crystal	Density (g/cm <sup>3</sup> )	Hardness (Mohs)	Melting Point (°C)	Key Characteristics/Applications
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Magnesium Oxide (MgO)	3.58	6	2,852	Refractories, electrical insulators, and thermal barriers.
Boron Nitride (BN)	2.25-3.48	9.5	2,973	Abrasives, lubricants, and high-temperature ceramics.
Lead Iodide (PbI <sub>2</sub> )	6.16	2.5	402	Radiation detection, perovskite solar cells.
Calcium Oxide (CaO)	3.34	3	2,572	Cement production, steelmaking, and environmental cleanup.
Zirconium Carbide (ZrC)	6.73	8.5	3,500	High-temperature ceramics, aerospace, and nuclear reactors.
Iron Sulfide (FeS)	4.75	4	1,191	Catalysts, pigments, and magnetic materials.
Silicon Dioxide (SiO <sub>2</sub> )	2.65	7	1,710	Glass manufacturing, semiconductors, and optical fibers.
Potassium Bromide (KBr)	2.75	2.5	734	Optical materials, spectroscopy, and chemical synthesis.

The physical properties (density, hardness, melting point) of the binary crystals tabled here indicate the wide applications of these crystals. Magnesium Oxide (MgO) (density 3.58 g/cm<sup>3</sup>, hardness 6 Mohs, high melting point 2,852°C) is widely used in refractories, electrical insulators and thermal barrier. Boron Nitride (BN) is exceptional for its hardness (9.5 Mohs) and melting point (2,973°C) and used in abrasives, lubricants and high temperature ceramics. Lead Iodide (PbI<sub>2</sub>) is a basic material, with a density of 6.16 g/cm<sup>3</sup>, and a relatively low melting point (402°C), and is used in radiation detection and perovskite solar cells. Calcium Oxide (CaO), of moderate hardness (3 Mohs) and exceptionally high melting point (2,572°C), is used in cement production, steel making and environmental remediation. Zirconium Carbide (ZrC) is an ideal high temperature ceramic and aerospace component with the properties of density (6.73 g/cm<sup>3</sup>), melting point (3,500°C. Iron Sulfide (FeS) is

interesting as a catalyst, pigment, and magnetic material because of moderate density (4.75 g/cm<sup>3</sup>) and hardness (4 Mohs). Glass, semiconductors and optical fibres use Silicon Dioxide (SiO<sub>2</sub>); it is hard (7 Mohs) and melts at high temperature (1,710°C). Potassium Bromide (KBr) used in spectroscopy and chemical synthesis has a density of 2.75 g/cm<sup>3</sup> and melting point of 734°C. The variety shown by binary crystals for satisfying technological and industrial needs is illustrated in this table.

### **Conclusion**

Binary crystals are fundamental in material science and industrial applications due density, hardness, and melting points, which define the structural and functional characteristics of binary crystals. Density is a measure of the mass per unit volume (mass-to-volume ratio), and depends on atomic mass, volume, and packing efficiency, which affects the crystal's mechanical strength and stability. Hardness (resistance to deformation) is governed by atomic bonding, lattice structure and the presence of defects or impurities and is of critical importance to wear resistant and high strength applications. Melting points tell us something about the thermal stability of a material, and is based on the strength of the bonds (e.g., lattice energy), the atomic coordination (number of ways one can make a bond with other atoms in a structure) and the ability of the crystal structure to stand high temperatures. The interplay between these properties is revealed in their influence on a wide range of material performance in different fields. For electronic, aerospace, refractory and tool cutting applications where durability, or thermal resistance, is critical, high density materials with the highest attainable hardness and melting point are required. Characterization techniques have been greatly advanced and computational modeling deepened our understanding of these properties, allowing the design of binary crystals with specific needs in mind. The potential of binary crystals in the context of innovative technologies is continually expanded by the study of structure, bonding and physical properties relationships. The understanding and optimization of density, hardness, and melting points still are indispensable for the progress of material science, because they make binary crystals one of the pillars of modern engineering and industry.

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