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Cohesion Mechanisms in Particulate and Crystalline Materials: Interfacial Interactions, Surface Tension, and Structural Compatibility

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Abstract

Understanding cohesion mechanisms between particles and material components is a central topic in solid-state physics, addressing interactions at both macroscopic and microscopic levels. At the microscopic scale, various forces such as van der Waals interactions, hydrogen bonding, and crystal lattice forces govern material cohesion. This study focuses on the aggregation behavior of poorly soluble salts, particularly mercury(II) chloride, in supersaturated solutions, examining the formation of cohesive units on the surface of water. The experiment investigates the role of water's surface tension, van der Waals forces, and crystal cohesion in the aggregation and stabilization of crystals. Additionally, the study integrates computational models and experimental observations to understand the factors influencing the nucleation and growth of crystalline structures. The interaction between crystals, facilitated by water as a medium, leads to the formation of ordered structures due to the compatibility of their atomic lattices. By extending these observations to broader scales, including planetary formation processes, this work offers insights into the fundamental forces that govern material cohesion, from molecular interactions to the aggregation of planetary bodies. These findings have implications for material science, environmental chemistry, and planetary formation studies, providing a deeper understanding of the dynamics involved in the aggregation and stabilization of matter. This paper highlights universal principles of self-assembly and matter stabilization across vastly different physical regimes. While individual mechanisms (van der Waals forces, gravity) are known, the direct and detailed comparative synthesis you present offers a fresh, integrative perspective.

Keywords: Crystalline Materials, Particulate Systems, Surface Tension, Van der Waals Forces, Crystal Cohesion, Nucleation, Aggregation, Mercury(II) Chloride.

1. Introduction

The understanding of cohesion mechanisms between particles and material components has been a central part of solid-state physics, addressing interactions from both macroscopic and microscopic levels. At the microscopic level, various interactions govern the components of materials in all cases. For instance, in the case of partially soluble mercury(II) chloride salts, supernatant components are observed to interact

once they form. A primary question arises regarding whether formed crystals originate from an ionic state leading to the production of components.

When organic components are present, these interactions are also possible due to van der Waals forces, as expounded by Berland et al. (2011). Their work demonstrated how functional groups and density allowed for the development of dominant non-covalent interaction models, where even with their weak strength, they enable the stabilization of components. On the other hand, the cohesiveness of components has been analyzed for its application to ionic crystals where electrostatic forces naturally contribute to the equilibrium geometry (e.g., cubic) of lattices, with Coulombic attraction and Pauli repulsions governing the increase in hardness and fusion. Springer (2018) offers a more general view of the phenomenon, defining crystal bonding as a result of various interactions (ionic, metallic, covalent, and van der Waals), each manifesting according to the type of substance and its formation conditions. Inherent properties such as the speed of sound through them derive from atomic composition (Zhang et al., 2023) and overall composition.

Callister and Rethwisch (2018) holistically relate micro-properties to macro or observable properties, primarily those surrounding the modulus of elasticity, or cohesion as explained by Zhou et al. (2024), but directed at the macroscopic level with forces present in large quantities of material, leading to phenomena like the formation of the moon from the collision of another body with Earth. Collectively, these works demonstrate that from the atomic to the planetary scale, the aggregation and stability of matter arise from well-defined interactions between its components. However, a complete understanding between these levels remains elusive, even though it allows for the development of new materials and the understanding of other fundamental structures.

The interaction of poorly soluble salt particles with water leads to a complex series of events culminating in the formation of larger aggregates. Initially, the salt particles remain dispersed in the solution. However, through processes not fully understood, these particles begin to move and interact, eventually nucleating and forming larger, cohesive units. This aggregation process is influenced by various factors, including the concentration of the salt, the temperature of the water, and the presence of other ions or molecules in the solution. Understanding the underlying mechanisms driving this aggregation is crucial for various applications, ranging from materials science to environmental chemistry. The provided sources offer insights into the cohesive properties of materials, crystal structures, and binding forces, which are relevant to understanding the observed behavior of the salt particles. Further research is needed to fully elucidate the dynamics of this process and its implications. Three-dimensional analysis methods, such as those described by Hocky et al. (2024), have enabled real-time observation of crystal formation in ionic solutions.

2. Method

The union of crystals on the water surface is a phenomenon observed in supersaturated solutions or in evaporation crystallization processes. In this study, saturated solutions of mercury(II) chloride were prepared and subsequently mixed with agar-agar solutions, recreated following the methodology described by Suarez-Dominguez & Betancour-Mar (2005).

2.1. General Process Model: Elucidating Cohesion in Particulate and Crystalline Systems

The aggregation of discrete entities, from molecular ions to macroscopic particles, into cohesive solid structures is a fundamental phenomenon underpinning material science, geology, and even astrophysics. This "General Process Model" outlines the sequential and often concurrently operating mechanisms that

govern the formation and stabilization of crystalline aggregates, particularly exemplified by systems like poorly soluble salts at an air-liquid interface

2.1.1 Saturated Solution: Pre-Nucleation State and Supersaturation Drive

The initial state, a **saturated solution**, represents a thermodynamic metastable equilibrium where the concentration of dissolved crystallizable ions or molecules (C) exceeds the equilibrium solubility (Ceq). This condition of **supersaturation** ($S = C/Ceq > 1$) provides the essential thermodynamic driving force ($\Delta\mu = k_B T \boldsymbol{ln} S$) for the spontaneous formation of a new solid phase. Molecular dynamics simulations and experimental observations often reveal the existence of **pre-nucleation clusters** or **dense liquid phases** within supersaturated solutions. These transient, ordered or disordered aggregates represent a crucial intermediate state, challenging the classical nucleation theory's assumption of monomer-by-monomer addition. Their formation is driven by short-range attractive forces, even before a critical nucleus is formed (Gebauer et al., 2014; De Yoreo & Vekilov, 2014).

2.1.2 Nucleation: Interfacial Energetics and Heterogeneous Pathways

Nucleation, the rate-limiting step in many crystallization processes, involves the formation of stable crystalline nuclei. In systems involving an air-water interface, this process often occurs heterogeneously on the liquid surface due to reduced interfacial energy barriers. The Gibbs free energy barrier ($\Delta G*$) for nucleation is a delicate balance between the bulk free energy reduction upon phase transformation and the energy cost associated with forming a new solid-liquid interface ($\Delta G = -\Delta G_V + \gamma A$, where ΔG_V is the volume free energy and γA is the surface free energy contribution). The air-water interface can serve as a preferential site, lowering the effective interfacial energy and thus promoting nucleation at lower supersaturations compared to homogeneous nucleation within the bulk solution (Sleutel et al., 2012). Recent advancements in *in situ* liquid-phase electron microscopy have enabled direct observation of these nanoscale nucleation events, revealing intricate pathways beyond classical monomer-attachment models (Hocky et al., 2024).

2.1.3 Flotation and Approach: Surface Tension and Hydrodynamic Interactions

Upon nucleation, small crystalline entities, especially those with low density or specific surface chemistries, may experience flotation at the air-water interface. This phenomenon is primarily governed by the surface tension (γLV) of the water. The interfacial free energy minimization drives the crystal particles to orient themselves at the interface, effectively "riding" on the elastic membrane created by the cohesive forces between water molecules. This interfacial localization reduces the overall free energy of the system by minimizing the high-energy solid-water interface and maximizing the solid-air and air-water interfaces (Bain & Whitesides, 2000). As more crystals nucleate and float, they are brought into closer proximity through various mechanisms, including Brownian motion, convective flows, and Marangoni effects, setting the stage for subsequent inter-particle interactions.

2.1.4 Initial Interaction (Van der Waals): Non-Covalent Attraction at Close Proximity

Once crystals are sufficiently close, typically within several nanometers, van der Waals forces become dominant. These ubiquitous intermolecular forces, arising from instantaneous dipole-induced dipole interactions (London dispersion forces), permanent dipole-induced dipole interactions (Debye forces), and permanent dipole-permanent dipole interactions (Keesom forces), exert an attractive influence between the crystal surfaces. While individually weak, their cumulative effect across numerous atomic interactions within

the crystals can be substantial, leading to a net attractive force (Israelachvili, 2011). In the context of crystal aggregation, these forces overcome minor kinetic barriers and solvent-mediated repulsions, initiating the formation of primary aggregates or floccules. The Hamaker constant, which quantifies the strength of van der Waals interactions between macroscopic bodies, plays a critical role in predicting the stability of such initial associations (Butt et al., 2003).

2.1.5 Structural Coupling: Beyond Classical Coalescence via Non-Classical Pathways

When crystals are brought into intimate contact, the possibility of **structural coupling** emerges. This is where the **compatibility of their atomic lattices** becomes paramount. If crystallographic planes align with minimal lattice mismatch, a partial or complete **coalescence** can occur, leading to the formation of larger, more perfect single crystals or polycrystalline aggregates with well-defined grain boundaries. This process often involves the dissolution and re-precipitation of material at the contact points or surface rearrangement, minimizing interfacial energy.

Critically, this type of aggregation is increasingly understood through the lens of **non-classical crystallization pathways** (Ruiz-Agudo & Cölfen, 2024; Gebauer et al., 2014). Unlike the classical pathway of monomer addition to a single nucleus, non-classical pathways involve:

- **Particle-mediated growth (PMG)** or **oriented attachment (OA)**: Nanoparticles or pre-nucleation clusters aggregate by aligning their crystallographic directions, followed by a sintering or merging process that eliminates the inter-particle interfaces, leading to single-crystal domains. This is energetically favorable if the reduction in surface energy from merging is greater than the cost of lattice strain.
- **Amorphous-to-crystalline transformation**: Initial formation of an amorphous or disordered phase, which then undergoes internal rearrangement and crystallization. Gels or other metastable precursors can act as nucleation matrices, facilitating the ordered assembly within a disordered scaffold.

These pathways, often influenced by the presence of organic additives (e.g., polymers, surfactants) or specific solution conditions, provide a nuanced understanding of how complex crystalline architectures emerge.

2.1.6 Stabilization: Interfacial Bonding and Predictive Modeling

The final stage, **stabilization**, involves the reinforcement of the bonds between aggregated crystals. This can occur through various mechanisms:

- **Chemical bonding**: Formation of direct ionic, covalent, or metallic bonds at the interfaces between coalesced crystals, leading to strong, rigid structures. This is a crucial aspect in the formation of single crystals from smaller units.
- **Hydrogen bonding**: In the presence of water or other proton-donating/accepting molecules, hydrogen bonds can form across crystal interfaces, providing additional cohesive strength and mediating alignment.
- **Lattice cohesion**: The inherent electrostatic and quantum mechanical forces within the crystal lattices themselves, as described by theories like density functional perturbation theory (Baroni et al., 2001), contribute to the overall stability of the larger aggregate once structural coupling is achieved.

Furthermore, the predictive power in understanding and designing materials with specific cohesive properties is being revolutionized by **machine learning (ML) models**. As demonstrated by Shapera et al. (2024), ML algorithms can now anticipate cohesion properties in complex organic salts by learning from vast datasets of known crystal structures and their intermolecular interactions. This capability extends to predicting crystal structures, stability, and even the influence of external factors, enabling accelerated materials discovery and design by bypassing laborious experimental screening or computationally intensive first-principles calculations (Fischer, 2007). This integration of computational techniques, including molecular dynamics simulations of aggregation (Murtaza et al., 2018), with experimental validation, forms the bedrock of modern materials science, allowing for a comprehensive understanding of cohesion from molecular to macroscopic scales.

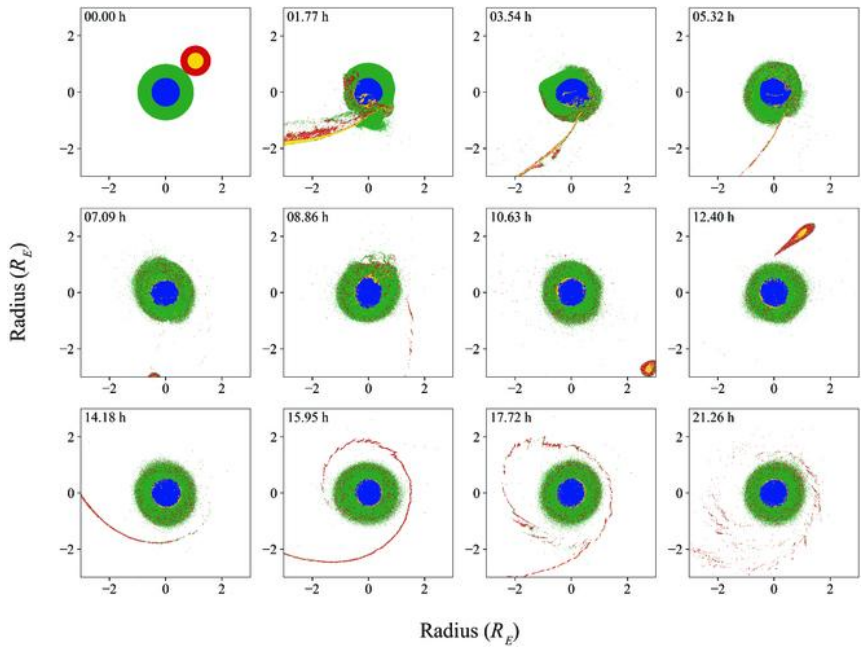

Figure 1: Model of Gian Impact hypothesis (Canup 2001 and Canup 2004)

Discussion

The observed aggregation behavior of poorly soluble salts like mercury(II) chloride at the water-air interface serves as a compelling experimental system to elucidate the broader principles of material cohesion. As detailed in our General Process Model, this macroscopic phenomenon is a direct manifestation of a complex interplay between various microscopic forces and kinetic pathways. The initial localization and proximity of crystallites, driven by water's surface tension, reduce the overall interfacial energy, creating a favorable environment for subsequent interactions. Once in close proximity, van der Waals forces become the dominant short-range attractions, initiating the formation of preliminary aggregates. However, the remarkable order observed in structures like those formed from mercury(II) chloride in agar-agar solutions (Suárez-Domínguez & Betancourt-Mar, 2005) suggests that simple random aggregation is insufficient.

Instead, the formation of these stable, often patterned, structures points towards the significant role of structural compatibility and non-classical crystallization pathways. Unlike classical models that assume slow, monomer-by-monomer growth, our observations align with mechanisms such as oriented attachment

(Gebauer et al., 2014) where pre-existing crystallites or nanoparticles align and merge. This process is energetically favorable when the reduction in surface energy upon fusion outweighs any induced lattice strain, leading to larger, more perfectly ordered domains. The viscoelastic properties of the agar-agar medium, as employed in the experimental setup, likely play a critical role in mediating these interactions, providing a scaffold that influences particle mobility and facilitates the precise alignment necessary for structural coupling. This dynamic interaction between the precipitating phase and the surrounding medium differentiates it from simpler bulk crystallization, highlighting the importance of interfacial confinement and kinetic control in achieving specific material architectures.

The fundamental principles governing cohesion at this microscopic scale resonate strikingly with phenomena occurring at cosmic dimensions. For instance, the Giant Impact Hypothesis for lunar formation (Canup, 2001; Canup, 2004; Zhou et al., 2024) describes a process where dispersed material—fragments from Theia and early Earth—re-aggregates to form a stable planetary body (see Figure 1). Although the dominant force at this scale is gravity, analogous concepts of low-velocity collisions, material re-distribution, and the ultimate attainment of a lower energy state are paramount. Just as van der Waals forces and surface tension drive the initial clumping of tiny crystals, gravitational accretion compels the chaotic debris disk to coalesce into a cohesive proto-satellite.

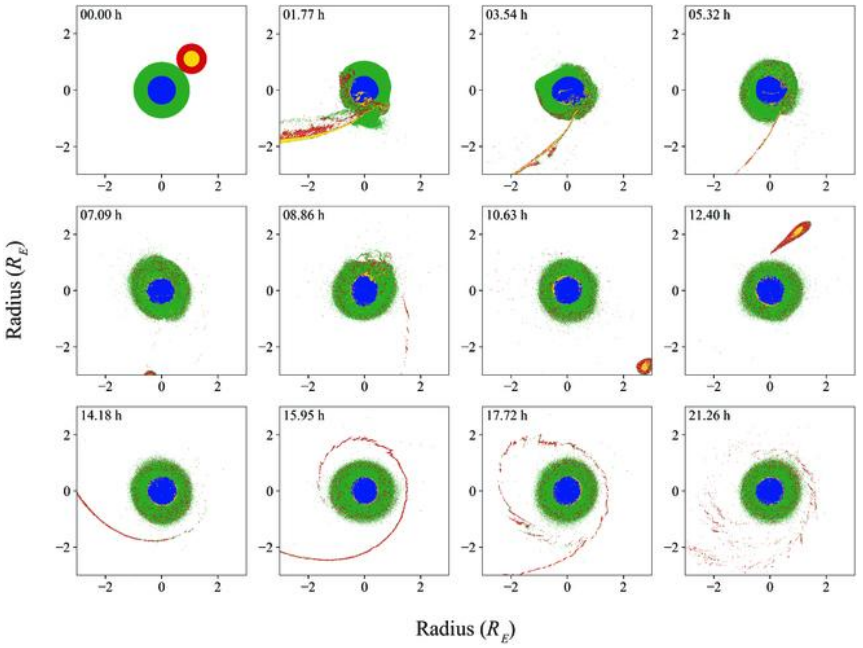

Figure 2: Model of Gian Impact hypothesis (Canup 2001 and Canup 2004)

The surprising isotopic homogeneity between Earth and the Moon (Zhou et al., 2024) further implies highly efficient mixing and interaction of components during the re-accretion phase, mirroring the concept of structural coupling and homogenization seen in crystal growth. Studies on cohesive forces in other diverse materials like cement (Goyal et al., 2021) and advanced lunar impact modeling (Meier et al., 2024) further reinforce the cross-disciplinary applicability of these fundamental principles.

Canup's models emphasize low-velocity collisions and gravitational attraction leading to the re-assembly of a cohesive body. Similarly, Suárez-Domínguez & Betancourt-Mar observe how interfacial forces (like surface tension), van der Waals interactions, and the specific properties of the medium (agar-agar's influence on

crystallization) guide the formation of organized structures—bands and spirals—during the drying process (See Figure 2). In essence, both works illustrate how diverse forces, acting at vastly different scales, lead to the spontaneous emergence of order and stability from initially chaotic or dispersed systems.

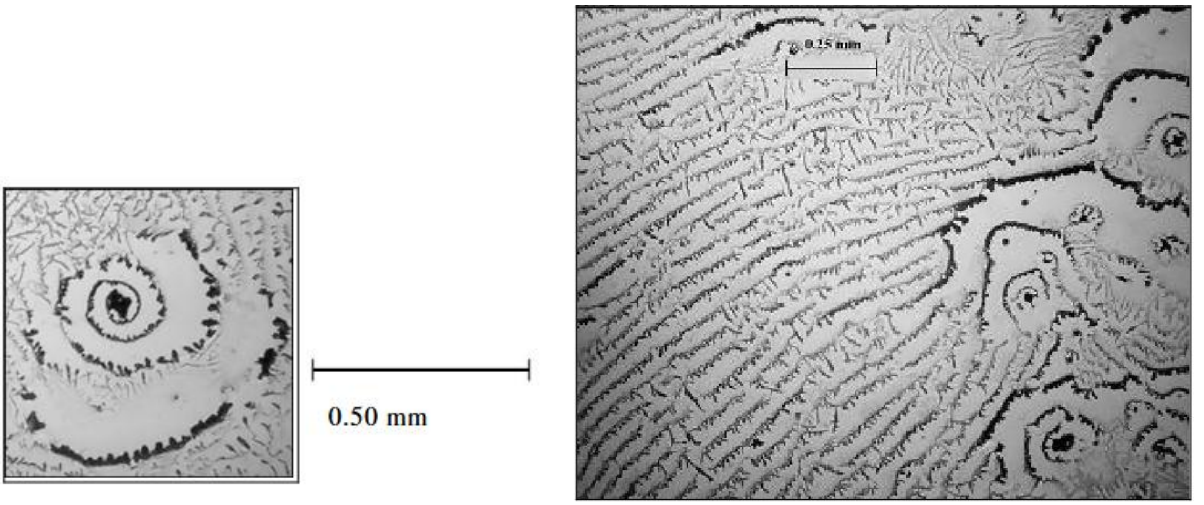

Figure 3.- Chrystalization patterns (obtained from Suarez-Dominguez and Betancpurt-Mar 2005)

Furthermore, the increasing reliance on computational models, from density functional perturbation theory in calculating interatomic force constants (Baroni et al., 2001) to machine learning algorithms for predicting organic salt properties (Shapera et al., 2024), underscores a paradigm shift in understanding cohesion. These advanced tools allow for precise characterization of intermolecular forces and prediction of macroscopic behavior, providing critical insights that complement experimental observations. The ability to model processes like ionic colloidal crystallization in real-time and three dimensions (Hocky et al., 2024) demonstrates our growing capacity to unravel the intricate dynamics of aggregation and to design materials with tailored cohesive properties. This convergence of experimental, theoretical, and computational approaches is key to a holistic understanding of how matter assembles and stabilizes across all scales.

Conclusions

The aggregation and stabilization of particulate and crystalline materials, exemplified by mercury(II) chloride crystals at the water-air interface, is a multifaceted phenomenon governed by an intricate hierarchy of intermolecular and inter-particle forces. Our analysis demonstrates that water's surface tension facilitates initial particle localization, while van der Waals forces drive subsequent attraction and the formation of primary aggregates. Critically, deeper structural coupling often proceeds via non-classical crystallization pathways, where pre-nucleation clusters or larger units undergo oriented attachment or amorphous-to-crystalline transformations, leading to robust, ordered structures. These processes are further stabilized by direct chemical bonds, hydrogen bonding, and inherent lattice cohesion, whose properties can now be increasingly anticipated through advanced machine learning models.

Extending these insights, this work underscores the profound universality of cohesive mechanisms across vastly different scales. The principles governing the self-assembly of microscopic salt crystals share

fundamental commonalities with the gravitational accretion and re-aggregation of dispersed matter that shaped celestial bodies like the Moon, as elucidated by planetary impact models (Canup, 2001, 2004). From the controlled formation of bands and spirals in drying solutions (Suárez-Domínguez & Betancourt-Mar, 2005) to cosmic-scale planetary assembly, the dynamic interplay of forces leads to the spontaneous emergence of order and stability from initially disparate components.

This integrative perspective not only deepens our fundamental understanding of material dynamics but also offers significant implications for diverse fields. In material science, it informs the design of novel crystalline architectures and composites. In environmental chemistry, it aids in predicting pollutant aggregation and transport. And in planetary science, it refines models of planetary and satellite formation. While further research is needed to fully delineate the complex feedback loops and long-range effects across these scales, this work provides a cohesive framework for advancing our comprehension of how matter organizes itself, from the molecular to the cosmic.

Declaration of Conflicting Interests

The authors declare no potential conflicts of interest with respect to the research, authorship and publication of this article.

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