

Solid–Liquid Interfaces: Molecular Structure, Thermodynamics, and Crystallization

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J. Friso van der Veen, Guest Editors

Abstract

Materials phenomena ranging from the melting or freezing of ice to biomineralization in living organisms, to lubrication and the commercial casting of superalloys, are known to be critically influenced by molecular-scale structure and processes occurring at the interfaces between the crystalline solid and liquid phases. The properties of solid–liquid interfaces have long been a topic of intense interest in materials science, primarily because of their role in governing nucleation, growth, and morphological evolution in crystal growth from the melt or solutions. This issue of the MRS Bulletin provides an overview, highlighting new developments in experiment, theory, and modeling techniques that have led to substantial recent progress in the characterization of the molecular-level structural and thermodynamic properties of solid–liquid interfaces and their consequences for a variety of crystallization phenomena.

Keywords: crystallization, molecular structure, solid–liquid interfaces, thermodynamics.

Over the past two decades, intense practical interest in vapor-phase crystal growth has motivated the development of an advanced understanding of the molecular-level structure, thermodynamics, and kinetic properties of solid–vapor surfaces. Detailed investigations of crystal surfaces have been made possible by the development and application of powerful scanning probe and electron microscopies, surface-sensitive x-ray characterization techniques, and advanced atomistic, mesoscopic, and continuum-level theoretical tools.

In contrast to the situation for solid–vapor surfaces, a molecular-level understanding of solid–liquid interfacial properties has remained substantially less developed. This situation can be attributed in part to the inherent difficulties associated with experimental characterizations of “buried” interfaces between two condensed phases. In

addition, theoretical and simulation studies of solid–liquid interfaces require as a prerequisite the ability to accurately model the structural properties of both crystalline and fluid phases; system-specific theoretical studies have remained few in number, with the most detailed work being devoted to model systems with relatively simple interatomic interactions.

Despite the inherent challenges associated with molecular-level studies of solid–liquid interfaces, over the past decade a number of developments in experimental and simulation methods have been realized that are leading to rapid progress. It is the intent of this issue of *MRS Bulletin* to present some highlights of recent work in this area, focusing in particular on issues germane to the understanding of phenomena related to crystallization from the melt or solutions across a broad class of materials systems.

Traditionally, solid–liquid interfaces are characterized by the degree of structural order that they exhibit. “Smooth,” or faceted, interfaces are characterized by an atomically abrupt change in the degree of crystalline order across the solid–liquid boundary. Such interfaces have structures that can be described by analogy to the familiar picture of low-temperature solid–vacuum surfaces, where well-defined “terraces” are separated by abrupt atomic-scale steps. Molecularly “rough” solid–liquid interfaces, by contrast, are more suitably described as being structurally diffuse, with a degree of crystalline order that varies continuously over the scale of a few atomic planes across the solid–liquid boundary. Such interfaces are characteristically highly dynamic on an atomic scale, with interface atoms rapidly fluctuating between solid- and liquid-like environments. While “smooth” solid–liquid interfaces usually possess highly anisotropic properties, giving rise to faceted growth morphologies, molecularly rough interfaces are typically weakly anisotropic and lead to the formation of intricate dendritic solidification morphologies. The articles in this issue cover phenomena associated with both smooth and rough classes of solid–liquid interfaces in a broad range of materials systems and contrast the mechanisms involved in crystallization in both cases.

In the first article, Chernov et al. provide an overview of recent developments in the theoretical understanding of step and kink dynamics for faceted solid–liquid interfaces, in the context of the crystallization of inorganic and protein crystals from solution. Interest in solution growth originates from a variety of practical applications in materials, biological, and environmental sciences. Such general interest has motivated in-depth experimental studies over the past decade that have employed *in situ* atomic force microscopy and related techniques to characterize the structure and dynamics of steps during crystal growth from solution. These detailed experimental investigations have raised a number of new fundamental questions, which have been the focus of recent theoretical work aimed at advancing the state of understanding of step dynamics on faceted solid–liquid interfaces in solution growth. These theoretical developments and an overview of the key experimental observations that have motivated them form the focus of the review by Chernov et al.

While faceted solid–liquid interfaces are typically observed in crystal growth from solutions, molecularly rough interfaces are common in the solidification of materials such as metals and colloids from their melts. Until recently, much of the most de-

tailed information related to the structural and thermodynamic properties of molecularly rough solid-liquid interfaces has been provided by atomic-scale computer simulations, as represented by the pioneering work of Broughton and Gilmer¹ for model Lennard-Jones systems (i.e., systems interacting with repulsive $1/r^{12}$ and attractive $1/r^6$ interactions, where r is the interatomic separation).

The second article in this issue, by Hoyt et al., provides an overview of the state of understanding of the thermodynamic and kinetic properties of molecularly rough crystal-melt interfaces as they have been derived from recent atomistic simulations for a variety of model systems as well as several specific metals. These studies have provided new insights into variations in interfacial free energy with crystal structure, an issue germane to the nucleation of metastable phases in deeply undercooled melts. A particular emphasis in the article is given to the degree of anisotropy in interfacial free energies and mobilities exhibited in metallic crystal-melt interfaces. While such anisotropies are generally weak for rough solid-liquid interfaces, they nevertheless have important consequences for the morphologies observed in dendritic solidification. The predictions of numerical simulations for interfacial free energy anisotropies are shown to compare favorably with recent equilibrium crystal shape measurements in metal alloy systems, which are also described. The authors discuss how these predictions have led to new insights into unusual dendritic growth morphologies observed in commercial Al-based alloy systems.

In seminal work by Turnbull² more than 50 years ago, the first measurements of solid-liquid interfacial free energies in metals were derived from nucleation studies in undercooled melts (see Figure 1). Since that time, experimental studies of nucleation have continued to provide one of the most common frameworks for investigating thermodynamic properties of solid-liquid interfaces. The article by Kelton et al. provides an overview of the current state of the art in such studies. The authors describe recent experimental work employing novel "containerless processing" (e.g., electrostatic or electromagnetic levitation) methods, which enable one to deeply undercool alloy melts. Experiments employing this technique have provided new evidence for the development of icosahedral order in undercooled melts, and the significance of this finding for the nucleation of solids is discussed. Specifically, experimental observations and theoretical analyses indicate that the solid-liquid interfacial free energy is a decreasing function of the

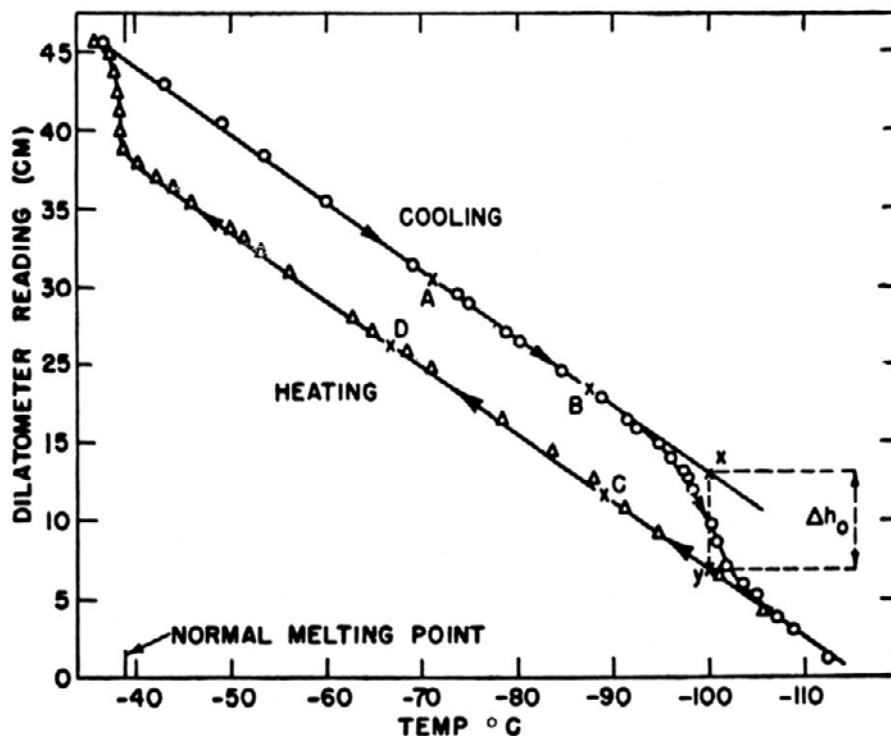


Figure 1. Turnbull's demonstration (1952) of large undercooling of liquid mercury.² Emulsification of the liquid into micron-sized droplets isolated the heterogeneous nucleants ("motes") into a small number of droplets, so that most of the liquid crystallized by homogeneous nucleation. The crystallization was observed by the change in volume, measured as a dilatometer height, Δh_0 . These experiments established that the structure of the liquid is fundamentally different from that of the crystal and inspired Frank's hypothesis of icosahedral (polytetrahedral) short-range order in simple liquids.³ Turnbull's analysis of the data with classical nucleation theory showed that the solid-liquid interfacial energy is large (equivalent to melting 61% of a monolayer) and increases with temperature.

degree of local tetrahedral and icosahedral order in the crystalline solid phase. The specific emphasis in the article is on the effects that ordering in the liquid and at solid-liquid interfaces have upon both heterogeneous and homogeneous nucleation processes in alloy melts. Thus, the article also describes experimental investigations of magnetic ordering in deeply undercooled melts of ferromagnetic alloys and the influence of substrate structure of "catalysts" on heterogeneous crystal nucleation.

The article by Wu et al. is a more detailed look at the problem of extracting a value for the solid-liquid interfacial energy from crystal nucleation experiments. Gibbs first calculated the work to form a spherical crystal nucleus in an undercooled melt by separating it into a bulk term proportional to the number of atoms in the cluster, and a surface term proportional to its surface area. Even though the approach has been remarkably successful, especially for condensation from the vapor, a number of fundamental questions remain, some of

them related to the fundamentals of nucleation and others to the specifics of the solid-liquid phase transformation. This article reviews the thermodynamics necessary for a rigorous calculation of the reversible work, as well as the assumptions commonly used to calculate a nucleation rate from this work. Aspects of the problem that complicate the Gibbsian picture include the nonspherical shape of the nucleus (which can be highly irregular for small interfacial energies, as in the crystallization of colloidal suspensions), the temperature coefficient of the interfacial energy (generally thought to be positive due to the entropy loss in the liquid near the interface), and the possible dependence of the interfacial energy on the size of the nucleus. The article shows how theory (thermodynamic, density functional), computer simulation (molecular dynamics, phase field), and experimental simulation (confocal microscopy on colloidal suspensions) can shed light on the problem.

The final two articles highlight the current state of the art in the application of

electron microscopy and x-ray scattering techniques to investigations of the structural, kinetic, and thermodynamic properties of solid-liquid interfaces.

The article by Howe and Saka describes how *in situ* transmission electron microscopy (TEM) studies allow determination of the structure, chemistry, and kinetic behavior of solid-liquid interfaces with subnanometer spatial resolution. Examples are given illustrating the applications of TEM to measurements of equilibrium ordering and compositional profiles across solid-liquid interfaces. It is also demonstrated how, through the use of calibrated heating holders, it is possible to study the dynamics of interface motion with growth velocities as low as ~ 2 nm/s. Such investigations open the way for the first direct analyses of the kinetics and mechanisms governing interface migration. The measurement of size-dependent melting temperatures in small particles provides a strategy for probing interfacial thermodynamic properties, through the well-known Gibbs-Thomson relations. Howe and Saka include as a final example the application of TEM to studies of the equilibrium melting

temperatures of small particles embedded in a crystalline matrix. They demonstrate that the melting point of such particles can be either elevated or depressed depending on the relative magnitudes of the solid-matrix, liquid-matrix, and solid-liquid interfacial free energies.

The final article, by van der Veen and Reichert, highlights recent applications of state-of-the-art synchrotron x-ray scattering measurements to the study of structural ordering at solid-liquid interfaces. The article includes a brief overview of the techniques used to probe solid-liquid interface structure with x-rays and discusses a range of applications illustrating the detailed information that can be derived from such techniques. Specifically, the article includes examples taken from recent work by the authors to water-solid interfaces, liquid-metal/solid-semiconductor interfaces and colloids in confinement between solids. In general, the solid surface is found to induce ordering within the liquid both in the perpendicular and in-plane directions. For liquid Pb on Si(100), a fivefold local symmetry was observed adjacent to the

silicon wall, evidencing the icosahedral ordering discussed in the article by Kelton et al. for metallic bulk melts. The authors also treat the effect of two opposing interfaces, which may differ substantially from that of a single interface. The most interesting example in nature is that of water sandwiched by two solids. Studies of the melting of ice in contact with silica revealed interfacial melting as a precursor of bulk melting, where the watery layer was found to have an anomalously high density.

How freezing and melting phenomena are influenced by the presence of interfaces may be predicted by consideration of interfacial free energies and classical nucleation, but these depend strongly on local atomic-scale ordering effects, about which we have only recently begun to gain more knowledge.

References

1. J.Q. Broughton and G.H. Gilmer, *J. Chem. Phys.* **79** (1983) p. 5105.
2. D. Turnbull, *J. Chem. Phys.* **20** (1952) p. 411.
3. F.C. Frank, *Proc. Roy. Soc. London, Ser. A* **215** (1952) p. 43. □

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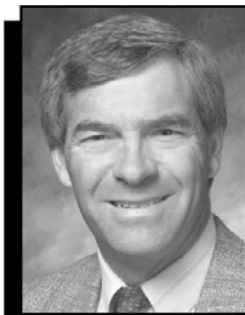
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