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Effects of mass transfer coefficient on pore shape in solid

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ABSTRACT

The shape of a pore resulting from a nucleated bubble entrapped by a solidification front for different mass transfer coefficients is predicted in this work. Mass transfer coefficient associated with different reference concentrations is used to determine different characteristics of solute transfer rate across the cap of the pore or bubble responsible for the pore shape in solid. Pore formation and its shape in solid influence contemporary issues of biology, engineering, foods, geophysics and climate change, etc. This work extends previous models, accounting for mass and momentum transport of solute across a selfconsistently determined shape of the bubble cap whose surface is satisfied by physico-chemical equilibrium beyond the solidification front, to study different mechanisms for pore formation. Mechanism of pore formation can be Case 1, which is subject to solute transport from the pore across an emerged cap through the concentration boundary layer on the solidification front into surrounding liquid in the early stage. Cases 2a and 2b are referred to opposite directions of solute transport across a submerged cap in the concentration boundary layer. In contrast to the former, the latter exhibits stronger effects of pore volume expansion on solute gas pressure in the pore than solute transport. The results show that an increase in mass transfer coefficient decreases pore radius and time for bubble entrapment in Case 1. An isolated pore cannot be found in Cases 2a and 2b, since solute concentration at the cap increases and decreases rapidly in the late stage, respectively. The predicted pore shape in solid agrees with experimental data. Mass transfer coefficient associated with solidification rate can be used to control the pore shape, which strongly depends on directions and magnitudes of solute transport.

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1. Introduction

A study of pore formation in solid is a challenging topic for materials, manufacturing, engineering, biological, geophysics and climate change technologies and sciences [1–12]. Porosity is susceptible to stress concentration, degrading the mechanical properties and impeding efficiency or functional properties of products. Substances containing a number of pores can be utilized as lightweight materials, catalysts, electrodes, vibration, acoustic energy absorption, impact energy absorption materials, food preservation and sterilization, and the scaffold for tissue ingrowth. Porosity of sea ices influences the surface elevation of ice sheets, resulting in differences in sun albedo, atmospheric heat and mass transfer, brine, and nutrients transport [4,13].

Mass transfer across the cap of a bubble or pore beyond a solidification front is responsible for morphologies of the pore in solid [14]. Solute rejected by the solidification front accumulated in liquid near the interface until concentration was high enough for

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http://dx.doi.org/10.1016/j.ijheatmasstransfer.2016.07.081 0017-9310/© 2016 Elsevier Ltd. All rights reserved. bubbles to nucleate [15–17]. The growth or shrink of the bubble depends on solute transport across the cap. It has been known that during fast growth there was less time for diffusion and the bubble decreased in cross section. More systematically speaking, enhanced mass transport to the cap from surrounding liquid and gas pressure in the bubble led to a decrease of cap radius in order to satisfy balances of pressures at the cap [18,19]. After nucleation, bubbles experience spherical growth, solidification rate-controlled elongation, disappearance of the bubbles, and formation of the pores in solid [20].

Solute gas transport through the bubble cap can be determined by solving transport equation of concentration in details. Zhdanov et al. [21] numerically calculated a steady-state solute concentration field ahead of the hemispherical portion of a single cylindrical gas bubble entrapped in a growing crystal. Mass transfer across the bubble cap was evaluated by introducing a mass transfer coefficient and a referenced concentration determined by satisfying Young-Laplace equation at the cap with a constant contact angle at each time. Solute concentration decreased along the cap surface toward the axisymmetric axis. Solute concentration increased and decreased in the directions away from the cap. Lotus-type porous metals that contain aligned long columnar pores have recently

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Ac	cap surface area $A_c = ilde{A}_c/ ilde{R}_0^2 pprox 2\pi R^2(0)(1-\cos\phi_B)$	V_w	pore volume below solidification front
Во	Bond number, $Bo \equiv \rho g \dot{R}_0^2 / \sigma$	<i>Z</i> ′	cylindrical coordinate, $z' \equiv \tilde{z}/\tilde{R}_0$
C_{∞}	initial solute concentration, $C_{\infty} = \tilde{C}_{\infty} \tilde{R}_u \tilde{T} / \rho g \tilde{R}_0$	Z_B	cap height
D	solute diffusivity		
h_B	liquid depth, as illustrated in Fig. 1(a)	Greek letter	
h_D	mass transfer coefficient, $h_D = h_D \hat{R}_0 / \hat{D}$	σ	surface tension
Κ	Henry's law constant, $K = \tilde{K}/\tilde{R}_u \tilde{T}$	ϕ	inclination angle
k_p	equilibrium partition coefficient	,	C
L	bubble radius at 90°	Subscripts	
п	moles of solute gas in pore	а	atmosphere
Ν	dimensionless variable, $N \equiv h_D \pi r_B^2 / V K$	B	base
р	pressure, $p \equiv \tilde{p}R_0/\sigma$	c	bubble cap
r	cylindrical coordinate, $r \equiv \tilde{r}/R_0$	g	gas
R	radius, $R \equiv R/R_0$	Ő	initial state
R(0)	radius of curvature at bubble apex	∞	location far from solidification front
R_u	universal gas constant		
S	solidification front location	Supers	crints
t	time, $t = tD/R_0^2$	Supers	dimensional quantity
U	solidification rate = ds/dt	/0	unicisional qualitity
V	volume, $V = V/R_0^3$		

been functionally fabricated, due to lightweight, low thermal and electrical conductivities, and high specific tensile strength in the direction parallel to the pore axis [11]. Solute transport in the gasar eutectic growth in a directional solidification can be analytically found by Liu et al. [22] subject to a flat top bubble. A more elaborate steady state solution of concentration field around a selfconsistent shape of the bubble cap in gasar eutectic growth in a directional solidification was also provided by Li et al. [23] using multiple scale expansion and matching method for a small Peclet number, defined as the ratio between a half of inter-pore spacing and distance for solute diffusion. This analytical study presented a rather complete model for predicting solute concentration and cap shape accounting for Gibbs-Thomson condition at the solidliquid interface, and solute mass balance conditions at the solidliquid and gas-liquid interfaces, and Young's law at the triple phase line.

Similar to evaluation of heat transfer by introducing heat transfer coefficient, solute gas transport across the bubble cap can be effectively evaluated by introducing a mass transfer coefficient. Physically speaking, solute gas concentration in the pore can be influenced by either solute gas concentration in the liquid ahead of the solidification or that away from the solidification front. Depending on which is dominant factor affecting pressure in the pore, the modeling of mass transfer rate can be different. The bubble is initiated from heterogeneous nucleation due to solute supersaturation. As a consequence, solute gas is transferred from the bubble to surrounding liquid in the early stage. Solute transfer rate governed by mass transfer coefficient is therefore based on difference in concentrations between the locations far from the solidification front and bubble cap surface [24]. On the other hand, solute transfer rate across a submerged bubble cap is due to the difference in concentrations between the cap surface and liquid far from the solidification front [18,19,25,26]. Lee et al. [26] describe that at the solid-melt interface away from the bubble, solute gas is rejected into the liquid as solidification progresses. When solidification occurs at the intersection of the solid-melt interface and the rim of the bubble, the solid again first rejects gas solute to the liquid side at the bubble surface. The gas is quickly released from the melt into the bubble in compliance with Henry's law. Therefore, the solute gas concentration in the pore is determined by solute gas concentration in liquid ahead of and away from the solidification front. This case, for example, is applicable to the solidification of lotus-type porous metals that contain aligned long columnar pores [11,21–23,27–29], or a submerged bubble cap into a thick concentration boundary layer along the solidification front.

In this work, the effects of mass transfer coefficients in different cases on the shape of a pore resulting from a bubble entrapped by a solidification front are predicted. The model accounts for nucleation, and mass and momentum transport of solute gas and physico-chemical equilibrium at a self-consistent determined cap of a bubble, leading to a realistic pore shape in solid, are included. Rigorous understanding of mass transfer rates to control the growth of the pore shape is obtained.

2. System model and analysis

A pore in solid, resulting from an entrapped bubble by a solidification front, is illustrated in Fig. 1(a). Since contact angle determines the pore shape in solid [13,19], the Young–Laplace equation governing balance between gas, capillary and liquid pressures is required to predict the shape of the bubble cap beyond the solidification front. Solute gas pressure in the pore is determined by solute transport across the cap in different directions and magnitudes, as illustrated in Fig. 1(b) and (c) and discussed previously. The former, Case 1, is referred to solutes transport from the pore across an emerged cap through the concentration boundary layer on the solidification front into liquid in the early stage, whereas the latter, Case 2, is applicable to solute transport from the concentration boundary layer across a submerged cap into the pore. The major assumptions made are the following:

- 1. The model system is axisymmetric.
- 2. The bubble is characterized by a small Bond number, so that perturbation solutions can be used to predict a nearly spherical cap shape of a tiny bubble [30,31]. Bond number is much less than unity, based on a typical bubble radius smaller than 10^{-4} m.
- 3. The system is static. Tangential and normal viscous stresses in the liquid are therefore neglected. Liquid pressure is hydrostatic pressure.
- 4. The pore shape in solid is delineated by tracing contact angle of the cap.

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