Journal of Computational Physics 297 (2015) 480–494

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A level set method for materials with texturally equilibrated pores

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ARTICLE INFO

Article history:
Received 24 December 2014
Received in revised form 8 May 2015
Accepted 17 May 2015
Available online 21 May 2015

Keywords:
Level set method
Textural equilibrium
Percolation
Dihedral angle
Mean curvature

ABSTRACT

Textural equilibrium controls the distribution of the liquid phase in many naturally occurring porous materials such as partially molten rocks and alloys, salt–brine and ice–water systems. In these materials, pore geometry evolves to minimize the solid–liquid interfacial energy while maintaining a constant dihedral angle, θ, at solid–liquid contact lines. We present a level set method to compute an implicit representation of the liquid–solid interface in textural equilibrium with space-filling tessellations of multiple solid grains in three dimensions. Each grain is represented by a separate level set function and interfacial energy minimization is achieved by evolving the solid–liquid interface under surface diffusion to constant mean curvature surface. The liquid volume and dihedral angle constraints are added to the formulation using virtual convective and normal velocity terms. This results in an initial value problem for a system of non-linear coupled PDEs governing the evolution of the level sets for each grain, using the implicit representation of the solid grains as initial condition. A domain decomposition scheme is devised to restrict the computational domain of each grain to few grid points around the grain. The coupling between the interfaces is achieved in a higher level on the original computational domain. The spatial resolution of the discretization is improved through high-order spatial differentiation schemes and localization of computations through domain composition. Examples of three-dimensional solutions are also obtained for different grain distributions networks that illustrate the geometric flexibility of the method.

1. Introduction

Textural equilibrium determines the solid–liquid topology in many natural materials, such as partially molten rocks [1], ice–water systems [2], salt–brine systems [3] and alloys [4], see [5] for a recent review. Textural equilibrium is the state of thermodynamic equilibrium where the interfacial area has evolved to minimize the solid–liquid surface energy density, γ_{sl} [6], and hence to constant mean curvature, κ, if the pressure is hydrostatic and the grains are isotropic. In these materials the topology and geometry of the pore network is controlled by the dihedral angle, θ, which is a function of the surface energies of the mineral grains and the pore fluid [5]. The basic theory of textural equilibrium in two-phase materials has been introduced by Smith [4,7] in the context of partially molten alloys. Texturally equilibrated pores are common in porous

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http://dx.doi.org/10.1016/j.jcp.2015.05.023
0021-9991/

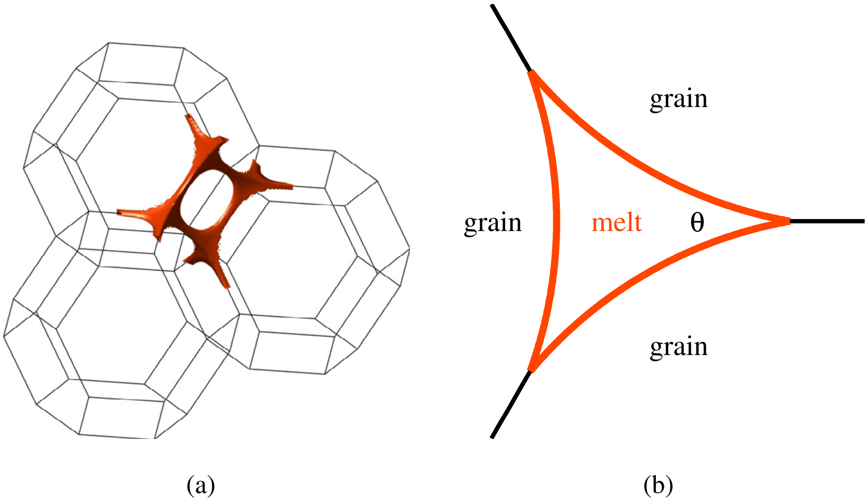

Fig. 1. (a) Wireframe of three truncated octahedron grains with a texturally equilibrated grain edge porosity of 1%. (b) Cross section of a grain-edge channel illustrating the definition of dihedral angle, θ. Images from Ghanbarzadeh et al. [5] used with permission from the American Physical Society.

materials with fast solid–liquid kinetics or in cases where long equilibration time scales are available, therefore they are common in geological systems. In most cases, solid–solid interfaces can be considered stationary on the timescale required to reach textural equilibrium of the pore network [1,5], so that the solid–solid surface energy density, γ_{ss}, is not minimized. Fig. 1(a) illustrates how these pre-existing grain–grain boundaries impose a lattice on the pore space and introduces contact lines along which solid–liquid and solid–solid interfaces meet at sharp angles (Fig. 1(b)). In a two phase material with isotropic surface energies, mechanical equilibrium at the contact line requires that

$$\gamma_{ss} = 2\gamma_{sl} \cos(\theta/2) \tag{1}$$

where θ is the dihedral angle, γ_{ss} and γ_{sl} are solid–solid and solid–liquid surface energy densities, respectively [6].

The physical principles of textural equilibrium are similar to standard wetting problems [8]. The most important difference between textural equilibrium and standard wetting problems is the role of the solid. In typical wetting problems the solid geometry is given and does not evolve. In the problems considered here the solid has a dual role. The solid–solid grain boundaries and edges do not evolve and provide a static lattice for fluid percolation. The solid–liquid grain boundaries, however, do evolve and determine the topology percolation of the pore space.

A characteristic of texturally equilibrated porous media is that the pore network percolates at any porosity for $\theta \le 60°$ while a percolation threshold exists for $\theta > 60°$ [9]. This property is specially important in comparison with the percolation theories in granular porous media where a porosity of 3% is required for connectivity of the pore space [10]. This ability of texturally equilibrated pore networks to percolate at very low porosities provides an elegant explanation for several geological observations [11,12,2]. For example, the small dihedral angle between basaltic melt and olivine explains the near instantaneous extraction of partial melts beneath mid-ocean ridges that was inferred from a number of indirect observations [9,1,13–15]. The decrease of the dihedral angle between rock salt and brine with increasing pressure and temperature [3,16] can explain how rock salt that is generally impermeable at shallow depth [17] can become permeable and stained by oil at greater depth [12].

The first models which calculated the three-dimensional shape of pore networks in textural equilibrium were developed by [18] and [1]. The former was based on interfacial surface energy minimization and the latter was developed based on the idea that at equilibrium, chemical potential of components in different phases is constant. Both models eventually reach to same *essential condition* for texturally equilibrated pores

$$\kappa = \text{const} \tag{2}$$

where κ is mean curvature of the solid–liquid interface for a two-phase system under hydrostatic pressure and with isotropic surface energies. Later, the model developed in [1] was reproduced to study the seismic wave velocities of partially molten rocks [19] and their electrical properties [20]. Recently, Wimert and Hier-Majumder [21] developed a three-dimensional micro-geodynamic model to solve for grain-melt geometry in an isotropic unit cell comprised of rhombic dodecahedral grains balancing pressure, surface tension, and viscous deformation forces.

A closed surface which minimizes the area subject to a fixed enclosed volume must have constant mean curvature, κ [22]. Therefore, in textural equilibrium, solid–liquid interface is a minimal surface subject to dihedral angle condition at boundaries. Considering a solid–liquid interface given by $z = f(x, y)$, mean curvature can be defined as

$$\kappa = \frac{(1+f_y^2)f_{xx} + (1+f_x^2)f_{yy} - 2f_x f_y f_{xy}}{2(1+f_x^2+f_y^2)^{\frac{3}{2}}} = \text{const} \tag{3}$$