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A new method for calculating thermoelectric current during the solidification of alloys

Y.F. Fan^{1,2a}, Y. Fautrelle^{2,3b}, Z.M. Ren^{1c}, O. Budenkova^{2,3d}, C.J. Li¹, W.L. Ren¹

¹ Department of Material Science and Engineering, Shanghai University, 200072 Shanghai, PR China

² Univ. Grenoble Alpes, SIMAP/EPM, F-38000 Grenoble, France

³ CNRS, SIMAP/EPM, F-38000 Grenoble, France

^afyfshu@shu.edu.cn, ^bYves.Fautrelle@simap.grenoble-inp.fr; ^czmren@staff.shu.edu.cn,

^dolga.budenkova@simap.grenoble-inp.fr

Abstract

A continuous liquid-solid interface model is introduced to calculate thermoelectric current. For comparison, the governing equations are solved by both a home-made code based on finite difference scheme and a commercial code COMSOL. The results are well in agreement with analytical calculation. The reliability of the model and the method are proved through a computation of some examples.

Key words: modeling, thermoelectric magnetic force, phase field, dendritic growth

Introduction

During solidification of metallic alloys, internal thermoelectric currents may form at a liquid-solid interface due to the Seebeck effect [1]. There are two necessary conditions. The first is the existence of the temperature gradient across the interface and the second is a difference of thermoelectric power between the liquid and solid phases. To quantify the Seebeck effect, a thermoelectric term has to be added to the classical forms of Ohm's laws, and the thermoelectric current across the discontinuous liquid-solid interface must satisfy special boundary conditions. Shercliff [1] sets up the conditions at the interface as the following:

$$J_{nL} = J_{nS} \quad (1)$$

$$\frac{J_{tL}}{\sigma_L} - \frac{J_{tS}}{\sigma_S} = (S_S - S_L) \delta T / \delta \tau \quad (2)$$

where n and s refer to directions normal and tangential to the interface respectively. In this paper, we introduce a continuous liquid-solid interface, where there is no need to introduce any boundary condition. The results obtained with our home-code allow a quantitative comparison both with those obtained with the COMSOL software and analytical calculations. In [2] an attempt of a similar approach is made, however, the coupling between the thermal and electrical problem is significantly simplified.

Governing Equations

The current density is calculated according to Ohm's law [1].

$$\frac{\mathbf{J}}{\sigma} = \mathbf{E} - S \nabla T \quad (3)$$

Here, the additional term $S \nabla T$ accounts for the Seebeck effect, \mathbf{E} represents the electrical field ($\mathbf{E} = -\nabla \psi_E$), σ is the electrical conductivity, \mathbf{J} is the current density and S is the thermoelectric power of the material. The electrical current density must satisfy the zero divergence condition:

$$\nabla \cdot \mathbf{J} = 0 \quad (4)$$

Thus the equation (3) becomes:

$$\nabla(\sigma \nabla \psi_E) = -\nabla(\sigma S \nabla T) \quad (5)$$

To make the liquid-solid interface continuous, we define a function $p(\phi)$ where ϕ is a continuous function defined as $\phi=0$ in the solid and $\phi=1$ in the liquid. The smoothing function $p(\phi)$ is defined as follows:

$$p(\phi) = \phi^3(10 - 15\phi + 6\phi^2) \quad (6)$$

Let S_S and S_L be the Seebeck coefficients for the solid and liquid fractions respectively, and σ_S and σ_L be the electric conductivities. Then intermediate values may represent the mushy zone, and be given as

$$S = S_S + p(\phi)(S_L - S_S) \quad (7)$$

$$\sigma = \sigma_S + p(\phi)(\sigma_L - \sigma_S) \quad (8)$$

The temperature field is governed by the heat equation (9), namely

$$\nabla \cdot (\lambda \nabla T) = 0 \quad (9)$$

A single thermal conductivity λ may be introduced by means of the function $p(\phi)$ as in (7) or (8). In the present case the solid and liquid phases are treated as homogeneous in thermal conductivity. Then, the temperature field T is the solution of a Laplace equation:

$$\Delta T = 0 \quad (10)$$

Results

The calculation of thermoelectric current density is carried out using a 2D square box size of 0.1m with grid point numbers 1000×1000 , and a circular equiaxed grain with a radius r_0 was placed in the centre of the domain. Material properties are provided in Table 1. Fig. 1 shows the geometry and boundary conditions, among which the electric potential boundary conditions which are constructed in a way to assure no electric current through the walls. In the whole domain the liquid-solid phase function distribution is based on eq.(11) [3]:

$$\phi(x, y) = \frac{1}{2} \left[1 + \tanh\left(\frac{\sqrt{x^2 + y^2} - r_0}{2\sqrt{2}}\right) \right] \quad (11)$$

Fig. 2 shows the profile of solid-liquid interface and the smoothing function near the interface.

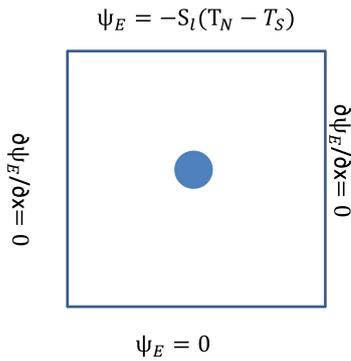


Fig. 1: Sketch of the geometry and the boundary conditions.

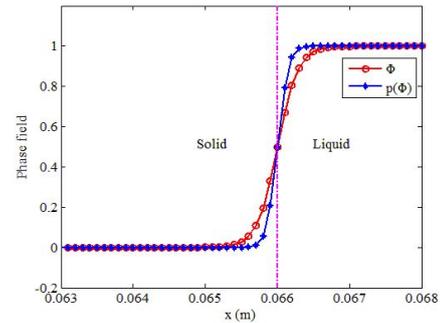


Fig. 2: One-dimensional phase-field variable profile over the solid/liquid interface where .

Tab.1. Materials properties for the thermoelectric current simulation

Parameter	Symbol	Value
Electric conductivity of the solid	σ_S	3.8×10^6 S/m
Electric conductivity of the liquid	σ_L	3.8×10^6 S/m
Absolute thermoelectric power of the solid	S_S	-1.1×10^{-6} V/K
Absolute thermoelectric power of the liquid	S_L	-1×10^{-7} V/K
Temperature gradient	G	5400K/m

We present results for which the temperature gradient is supposed to be constant and prescribed.

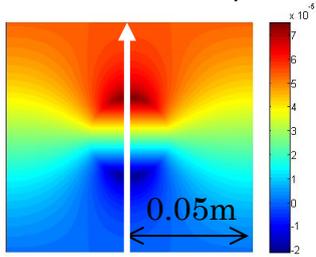


Fig. 3: Two-dimensional thermoelectric potential generated by a constant thermal gradient of 5400K/m

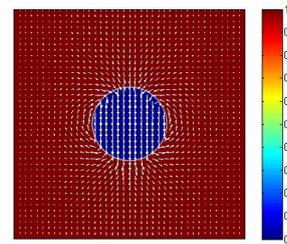


Fig. 4: Two-dimensional Phase-field and thermoelectric current whose flowing direction is indicated by white arrows.

Fig. 3 shows the computed thermoelectric potential generated by a constant thermal gradient of 5400K/m. Fig. 4 suggests that inside the sphere electric current density is almost uniform, whereas outside the equiaxed grain it decreases rapidly with the distance away from the grain. The latter behavior satisfies the far field conditions and can validate this simulation method to a certain extent.

Fig. 5 shows the densities of thermoelectric current computed with different programs under at the same condition and plotted along the vertical line which is indicated by the white arrow in Fig. 3. The flat segments of each curve correspond to the thermoelectric current within the solid. Results obtained by finite difference scheme agree with those obtained by COMSOL very well. Though the analytical calculation result is slightly different, it remains within the permitting range of error.

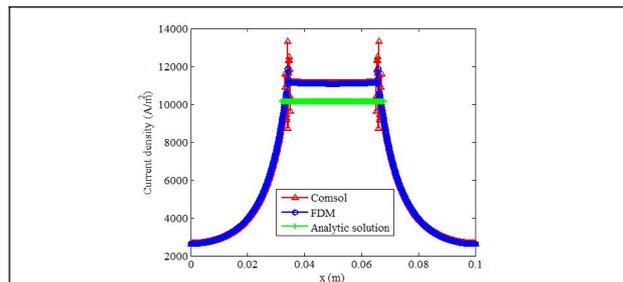


Fig.5: Electric current density magnitude along y axis: comparison between numerical simulations and analytical calculations

Combine the results shown in Fig. 3, Fig. 4 and Fig. 5, it can be concluded that thermoelectric current within the solid is distributed uniformly, and the finite difference scheme is reliable. So the validity of this simulation method is verified.

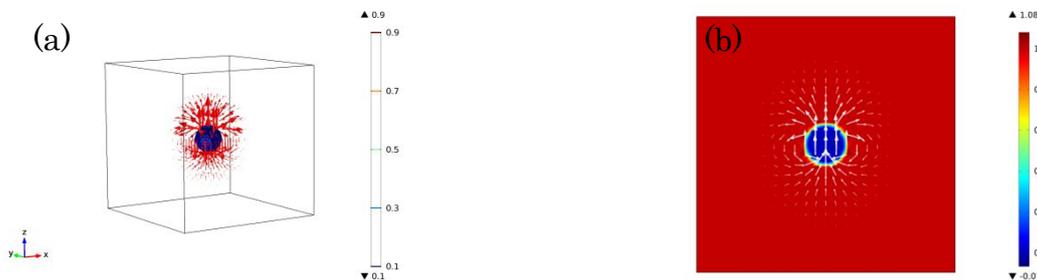


Fig. 6: The calculations are achieved by COMSOL, (a) three-dimensional phase-field ($\phi=0.5$) and thermoelectric current flowing direction indicated by red arrows; (b) three-dimensional phase-field in the $x-z$ plane and thermoelectric current flowing direction indicated by white arrows.

The calculations have been also performed in the 3D-case in the same conditions both with COMSOL and our home-code. The results are shown in Fig. 6. In Fig. 6(a) a spherical grain is taken into consideration and the thermoelectric current flowing direction is indicated by red arrows. In Fig. 6(b) $x-z$ plane phase-field and thermoelectric current

flowing direction is indicated by white arrows. These two figures together display that thermoelectric current is nearly zero at the boundary, which satisfies the far field conditions and validates that this simulation method can be extended to three dimensional.

Conclusions

A new method for calculating thermoelectric current is tried and verified. Through numerical experiment, the computed values are proved to agree with theoretical value within the permitting range of error. It validates definitely the simulation method used here, which consist to use a phase function.

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