IOP Conference Series: Materials Science and Engineering

PAPER • OPEN ACCESS

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To cite this article: P Soar *et al* 2020 *IOP Conf. Ser.: Mater. Sci. Eng.* **861** 012054

IOP Conf. Series: Materials Science and Engineering **861** (2020) 012054 doi:10.1088/1757-899X/861/1/012054

The integration of structural mechanics into microstructure solidification modelling

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Abstract. *In situ* structural mechanics are an often neglected area when modelling alloy microstructure during solidification, despite the existence of practical examples and studies which seem to indicate that the interaction between thermal or mechanical stresses and microstructure can have a significant impact on its evolution and hence the final properties at a macroscopic level. A bespoke structural mechanics solver using the finite volume method has been developed to solve the linear elasticity equations, with design choices being made to facilitate the coupling of this solver to run *in situ* with an existing solidification model. The accuracy of the structural mechanics solver is verified against an analytic solution and initial results from a fully coupled system are presented which demonstrate in a fundamental example that the interaction between structural mechanics and a solidifying dendrite can lead to a significant change in growth behaviour.

1. Introduction

When casting metal alloys, the material properties at the macroscopic level are dependent on the underlying morphology of the microstructure as defined by the arrangement of the dendrites that form as the liquid metal solidifies. Consequently, the ability to understand and manipulate the development of dendrites by controlling the environment in which the solidification occurs has the potential to allow for the creation of alloys that possess superior material properties. There are numerous practical experiments and numerical models which demonstrate the utility of these principles, the understanding of which has been a subject of research for decades as highlighted in the review of the field by Asta *et al.* [1]. More recent work by Kao *et al*. [2] explores the use of magnetic fields to induce fluid flow to further understand defect formation and alter dendritic development.

Numerical models simulating the process of solidification at the microstructure level can currently consider many of the parameters influencing the growth behaviour of the dendrites. However, one area of the modelling seemingly neglected so far is the impact of including *in situ* structural mechanics as a factor influencing dendritic growth. This *in situ* interaction requires that the deformation and accumulation of stress under external forces is modelled at the same time as the solidification itself, with the processes interacting throughout. Asta *et al*. [1] identified the interaction between structural mechanics and the microstructure solidification causing casting defects as being one of the open questions requiring further research, with numerous experimental examples further underlining the importance of this currently neglected area. Reinhart *et al.* [3] demonstrate in an experiment at ESRF

that stress and gravity cause defects to occur and the dendrite arms to be impacted mechanically. More recently an experiment undertaken by He *et al*. [4] investigated the impact of pulling, directional solidification and temperatures on the microstructural development and mechanical properties of a solidified aluminium alloy, finding it to impact both the microstructure and defect formation. A further example of structural mechanics behaviour influencing the microstructure has been identified by experiments run on a solidifying Gallium 25wt% Indium alloy by N. Shevchenko and S. Eckert from Helmholz-Zentrum Dresden-Rossendorf, where the experimental radiograph in figure 1(a) shows that the dendrites begin by growing in a seemingly fixed straight orientation, but figure 1(b) shows that later in the experiment the highlighted dendrite has deformed under its own weight, leaving it with a clear deviation in growth orientation when compared to the start. Any attempts to model this scenario using current methods which neglect mechanical effects would ignore this behaviour, leading to the dendrite continuing to grow along the initial orientation with no deformation, consequently causing a significantly different microstructure.

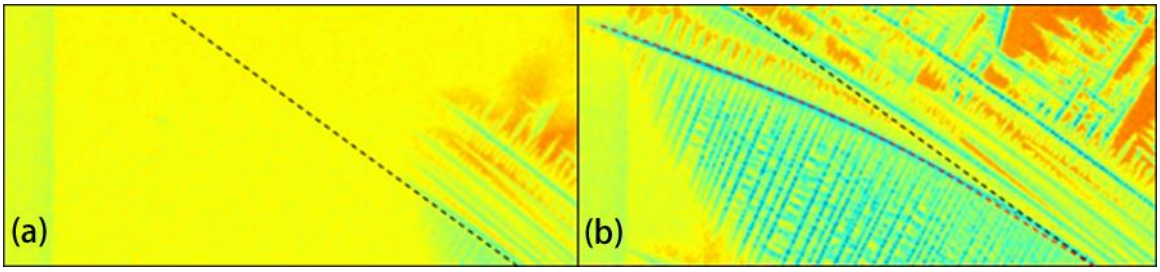

Figure 1. Dendrite growth showing structural mechanics impact.

The impact of mechanical interaction during the solidification process has been identified as an important modelling consideration in many studies, however many such cases take a post processing approach where the stresses will have no effect on the development of the solidification of the cast structure [5, 6]. Furthermore, the modelling that does consider these interactions largely restrict themselves to macroscopic models where the only mechanical behaviour considered is temperature driven [7, 8]. A solidification model created by Fackeldey, Ludwig and Sahm [9] considers these *in situ* effects, however this is achieved by modelling the process macroscopically and accounting for the microstructure in a more general sense using parameters to describe the primary and secondary arm spacing and eutectic fraction within a region of the macrostructure, as opposed to directly modelling the dendrites comprising the microstructure as this research intends.

Numerical models developed within this research group by Kao *et al*. [10] have been used to investigate how external parameters such as fluid flow and electromagnetics can be used to control the microstructural evolution. This work can be expanded further with the introduction of structural mechanics as an additional parameter in the microstructural solidification process, with the potential to lead to more accurate simulations of the dendritic growth behaviour.

The aim of this research will be to design a structural mechanics model that can be coupled with the ThermoElectric Solidification Algorithm (TESA), a bespoke code developed in house by CSEG which runs large scale simulations of microstructural growth in parallel [11]. This code has been designed to simulate the processes of solidification, fluid flow and electromagnetics within a single model capable of solving complex multi-physics phenomena such as casting [2], freckle defect formation [12] and undercooled growth [13]. However, to avoid some of the complications of coupling straight to this complex code, a more straightforward solidification code using the enthalpy method [14] was utilised for the initial coupling to demonstrate the fundamental changes in behaviour from the *in situ* interaction.

2. Numerical modelling

2.1. Solidification model

The solidification model that has been chosen for the initial tests of coupling with *in situ* structural mechanics is the enthalpy based method described by Voller [14]. This approach to solidification introduces the order parameter f to formulate an enthalpy-based method for a diffuse interface, where f represents the liquid fraction where $f = 1$ is fully liquid and $f = 0$ is fully solid.

The governing equations for this approach relate f to the volumetric enthalpy H, by defining H as the sum of the latent heats:

$$H = c_{\mathrm{p}}T + fL \tag{1}$$

where c_p is the specific heat, T is the temperature and L is the latent heat of the volume. With the conservation of enthalpy being given by

$$\frac{\partial H}{\partial t} = \nabla.(K\nabla T) \tag{2}$$

which assumes that the thermal conductivity K is constant. The interface is undercooled to the temperature T^i:

$$T^i = T_{\mathrm{m}} - \frac{\Gamma(\theta)}{L} T_{\mathrm{m}}\kappa \tag{3}$$

where κ is the curvature, T_m is the melting temperature and the surface stiffness is defined via an often utilised fourfold symmetry model:

$$\Gamma(\theta) = d_0(1 - 15\epsilon_4 cos(4\theta)) \tag{4}$$

The numerical approach Voller took was to convert this equation set into a dimensionless system which was discretised onto a Cartesian grid. In this paper the same approach was taken, so for the sake of brevity the detail of this approach has not been repeated.

2.2. Governing equations & assumptions for structural mechanics

Due to the fundamental nature of the research being undertaken, it was decided the linear elasticity equations would make for an appropriate choice of material model. This describes the behaviour of materials where the following assumptions are true: the deformations are 'small', there is a linear relationship between the stress and the strain and that the results of the problem show no plastic behaviour. Furthermore, as the model is currently only working in two dimensions, plane strain has been assumed. These simplifying assumptions will not hold for all solidification problems, but due to the paucity of existing published work exploring this phenomenon, it makes intuitive sense to begin by ensuring the most fundamental material model provides meaningful results. For example, effects such as thermal contraction and solidification driven density changes would introduce shrinkage flows, but the inclusion of these hydrodynamical effects is currently beyond the scope of the work. The material properties also have temperature dependence, but aside from interfacial undercooling the dendrite can be considered predominantly isothermal at the melting temperature with little spatial variation in material properties.

The equations for linear elasticity in two dimensions are described as follows:

$$\rho\frac{\partial^2 u_x}{\partial t^2} = \frac{\partial \sigma_x}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + F_x \tag{5}$$

$$\rho\frac{\partial^2 u_y}{\partial t^2} = \frac{\partial \sigma_y}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + F_y \tag{6}$$

where ρ is the density of the material, u_x and u_y the displacements in the x and y directions respectively, σ_x and σ_y the stresses in the x and y direction, τ_{xy} is the shear stress and F_x or F_y represent the x and y components of a body force acting upon the material.

The target application of his work is ultimately directional solidification in casting, where growth velocities are typically on the order of 10μm/s, with computational grid sizes of 10μm and time steps of 1ms giving a characteristic solidification length of 0.01μm per time step. For structural mechanics to have any noticeable effect the displacements per time step should be on a similar order of magnitude or notably longer, allowing the structural mechanics to be treated as a quasi-stationary process for a broad range of problems. This assumption simplifies the implementation, however as each solution is steady state the force component is changed from the full body force components to ΔF_x and ΔF_y, representing the change in the force exerted between the current time and the last timestep the structural mechanics was resolved.

Using Hooke's law equations (5) and (6) can be transformed into a displacement formulation, leading to the following pair of partial differential equations which are then solved simultaneously:

$$(2\mu + \lambda)\frac{\partial^2 u_x}{\partial x^2} + (\lambda + \mu)\frac{\partial^2 u_y}{\partial x \partial y} + \mu\frac{\partial^2 u_x}{\partial y^2} + \Delta F_x = 0 \tag{7}$$

$$(2\mu + \lambda)\frac{\partial^2 u_y}{\partial y^2} + (\lambda + \mu)\frac{\partial^2 u_x}{\partial x \partial y} + \mu\frac{\partial^2 u_y}{\partial x^2} + \Delta F_y = 0 \tag{8}$$

where μ and λ are the two Lamé constants defined as follows:

$$\lambda = \frac{vE}{(1 + v)(1 - 2v)}; \mu = \frac{E}{2(1 + v)} \tag{9}$$

defining E and v are respectively as the Young's Modulus and Poisson's ratio of the material.

2.3. Structural solver development

When solving structural mechanics problems, it is generally taken for granted that the Finite Element Method (FEM) will be the most appropriate choice of model. However, the process of meshing the structure intrinsic to the FEM approach can present a problem in the framework of coupled solidification with structural mechanics since every change in the structure due to solidification, would require computational power to constantly be diverted to re-meshing the structure to remain accurate. Furthermore, FEM generally models the geometry using unstructured grids, presenting a complication in coupling to TESA as the interpolation required to pass information between solvers to the Cartesian grid would increase complexity.

Instead a Finite Volume Method (FVM) approach has been taken as it synergises with solidification processes that are typically represented as a change in volume on a fixed grid, this change in volume providing the mechanical model with a straightforward means of calculating the change in forces exerted as solidification progresses. FVM is often associated with Computational Fluid Dynamics due to the volume conserving approach. However this is mere convention, as the attainable accuracy of results is comparable when modelling structural mechanics problems, as shown by Oñate, Cervera and Zienkiewicz [15] where for a simple structure under constant loads both the FEM and FVM produce the same results, with other groups supporting this position by finding modelling using the FVM to be in good agreement with analytic solutions [16, 17].

The FVM can be found applied to structural mechanics in many existing multi-physics problems such as fluid-structure interaction, both in a general sense [18] and how it can be related to solidification fronts [19] and welding [20]. In this related area, while models using different numerical schemes can certainly be coupled together, it is generally more straightforward and efficient for a similar numerical method to be used for both the fluid and solid equations.

For the purposes the future coupling to TESA, the FVM employed uses a Cartesian grid, which simplifies the discretisation of the governing equations down to relatively straightforward numerical schemes, which synergise well with the staggered grid Finite Difference approach being used to model solidification. As both approaches store material properties in the volume centred nodes with displacements and velocities on the corresponding cell faces due to the staggered mesh, meaning that

less work is required to pass any quantities required by both solvers between the corresponding grids without requiring any complicated interpolations.

In order to validate the accuracy of the structural mechanics solver, a problem was set up that could be modelled by the Euler Bernoulli Beam theory, which provides an analytic solution for the deflection of a beam with a point load applied to the end of a cantilever beam. The results of this validation can be observed in figure 2 and show the FVM is returning results in close agreement with the analytic solution, clearly within the 3% interval beam theory is held to be accurate for.

However, as some assumptions of the Euler-Bernoulli beam theory limit the scenarios that can be modelled, this validation was further verified by modelling several 2D scenarios violating these assumptions. Here the FVM results were found to be in close agreement with solutions obtained using the commercial code COMSOL. This is reassuring to see as COMSOL, aside from being used widely both in academia and industry, also uses the FEM to obtain its answers, so the close agreement that can be found here seems to further support that the use of FVM to solve structural mechanics will not have any negative implications on the accuracy of the model.

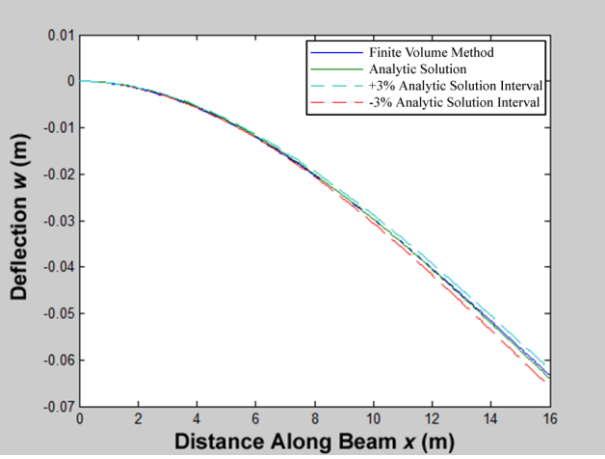

Figure 2. Comparison of deflections calculated using beam theory analytic solution and finite volume structural mechanics solver along 16m×4m×4m cantilever beam with a -1N Point load applied at the free tip using grid spacing $\Delta x = 0.1$m and material properties $E = 1000$Pa, $\nu = 0.33$ and $\rho = 8960\text{kgm}^{-3}$.

2.4. Advection of solid material

After the displacements are obtained, an advection-based process is used to account for changes in the solid fraction profile after the change in external forces have been accounted for. This process can be represented by the following equation:

$$\Delta f + \nabla \cdot \boldsymbol{u} f = 0 \tag{10}$$

where Δf is the change in solid fraction and $\boldsymbol{u}$ is the vector of displacement values obtained from the structural mechanics code. To avoid the results showing a bias caused by a dependence on the order of the x and y sweep, an operator split scheme was written to discretise this equation. The scheme implemented utilises a Volume of Fluid (VOF) method with a Simple Line Interface Calculation (SLIC) approach as described by Noh and Woodward [21] to reconstruct the interface so that unrealistic diffusion of the solid material from the advection process is avoided.

2.5. In situ coupling process

In order to bring the previously outlined elements together in a loosely coupled solver they must be able to pass information between them. This begins by identifying which areas of the domain, represented by a liquid fraction profile f are to be considered solid by marking areas with a sufficiently low f value. Once the solid domain is identified, the structural mechanics code runs to obtain $\boldsymbol{u}$ which contains the displacements in x and y at the faces of each cell for the current timestep. These displacements are then used to drive an advection process causing solidified material to move into the surrounding cells to generate an updated profile for f. This f can then be used as an initial condition for the solidification solver, itself producing an updated f after a period of solidification has occurred. This represents a

complete iteration of the coupled solver, which can be repeated for as many steps as the scenario being modelled requires with the final f profile after solidification acting as the initial condition for the next iteration of the structural mechanics solver. As the structural mechanics solver is steady state, the displacement is calculated on the difference between the previous force and the updated force from f. With the body force is dependent on f, if no solidification occurs the solution would remain the same as the previous calculation as it remains in steady state. However, as f is modified by the solidification solver, the change in force gives a new displacement. The magnitude of the change in force is dependent on the time interval between successive calls to the structural mechanical solver. Frequent calls give small displacements, while less frequent calls will give larger displacements. Thus, while the structural mechanical solver is steady state, this inherently introduces a time scale dependent on solidification.

3. Results

To understand the behaviour of the fully coupled model a simple test case of columnar growth with a body force applied to the solid cells was conducted. In this problem set up all of the domain boundaries are considered adiabatic, with the top surface where solidification initiates being a solid wall and the other boundaries considered to be Neumann conditions which allow no flux. A dimensionless approach is taken where the variables $\Delta x = \rho = E = 1$ which are scaled using base SI scaling factors to obtain the values in m, kg and s allowing the system to be governed by the dimensionless force. A consequence of this approach is that for a given set of material properties i.e. ρ and E, the dimensionless force scales with the meter SI unit. The dimensionless temperature is scaled by $T^* = (T - T_m)/(L/c)$, where L is the latent heat of fusion, c the specific heat and T_m the melting temperature. The initial conditions of the domain area assume dimensionless undercooling of ΔT = -0.643. In this context, high undercooled growth gives very small dendrites with high solidification velocities, while conversely in low undercooled growth the dendrites are much larger and grow more slowly. However, dendrites exhibit self-similarity across a wide range of undercooling and so while the real force required to influence solidification will vary significantly, this dimensionless force should be similar in magnitude.

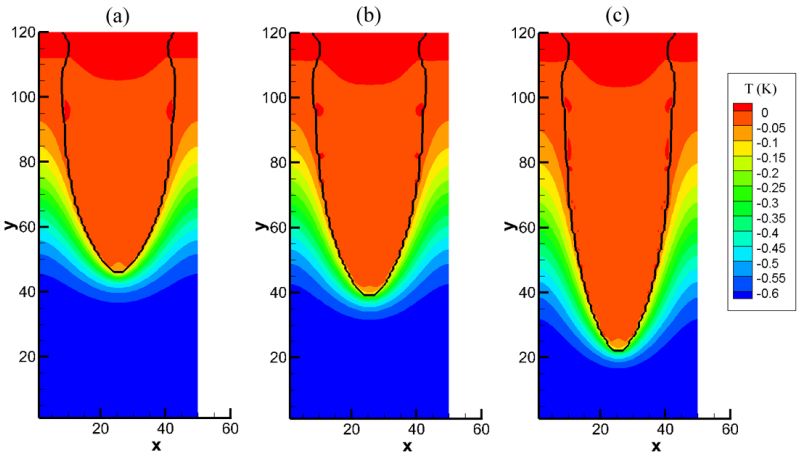

Figure 3. Dendrite behaviour under forces with thermal field T. (a) Positive force opposing growth direction, (b) no force, (c) negative force in growth direction.

In figure 3 there are three cases displaying the solid fraction and thermal field behaviour under different body force conditions. The cases considered are zero force, a body force acting in the direction of solidification and a body force acting against the direction of solidification. These cases were chosen as large deformations tangential to the growth direction will modify the preferential growth of the dendrite, which is behaviour currently unaccounted for in the solidification model.

Using the no force case in figure 3(b) as a reference, it is clear that when the force is applied in the direction of solidification as in figure 3(c) the dendrite arm is extended, while conversely when the body force is applied against the direction of solidification as in figure 3(a) the structure becomes shorter and

wider. The components of the normal and shear strains which accumulate during the *in situ* solidification occurring under these positive and negative force conditions have been provided in figure 4 and figure 5 respectively. For growth under the positive force, it can be observed in figure 4 that for all types of strain the largest component seems to be running through the centre of the dendrite, caused as the tip of the dendrite is the region of the highest growth of new solid material, meaning that this is the region where the largest deformations occur with each run of the structural mechanics solver. In the negative force case in figure 5, while there is a corresponding high strain region running through the centre for the same reasons, the largest components of the strain can be found near the wall which is accumulating strain due to being stretched throughout the process by a dendrite increasing in solid mass at a greater rate.

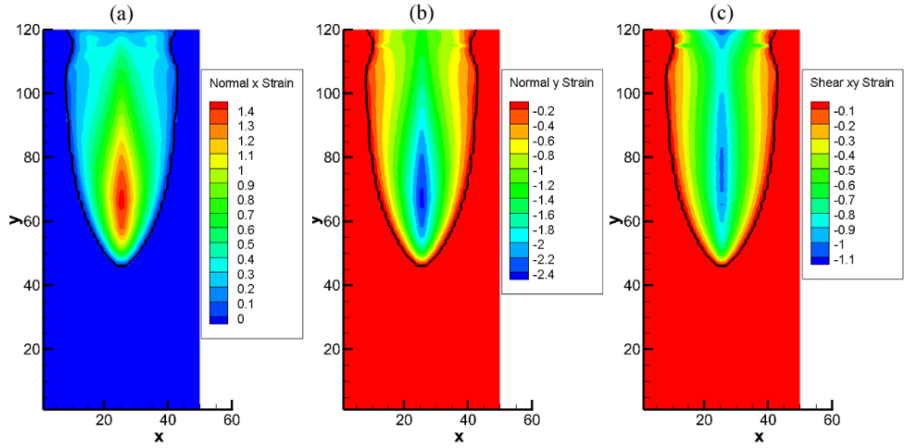

Figure 4. Accumulated strains in dendrite grown under positive body force. (a) Normal x strain, (b) normal y strain and (c) shear xy strain.

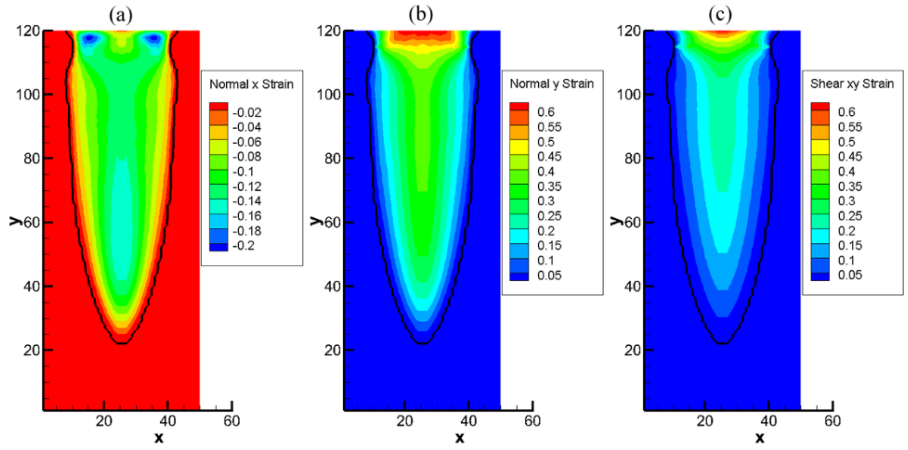

Figure 5. Accumulated strains in dendrite grown under negative body force. (a) Normal x strain, (b) normal y strain and (c) shear xy strain.

Although the cases represent the unrealistic situation of high undercooled growth and large body forces, these results are consistent with expectations and provide further qualitative understanding of the potential mechanisms for more realistic systems. When the force is in the direction of solidification structural deformations cause the dendrite to extend into the bulk. The deformation per unit time, which represents an added velocity allows the dendrite tip to extend further into the melt condensing isotherms which provides additional heat transfer. Conversely, the resisting force in figure 3(a), has the opposite effect where the slowing of the tip allows the thermal boundary to extend decreasing heat transfer. In more realistic casting situations of alloys, structural mechanics will have much less effect on the thermal problem compared to the solute problem, where mass transfer has very similar mechanisms, except there is a large disparity in both time and length scales, with a typical Lewis number on the order of 10000. However, with the focus on understanding the coupling of structural mechanics to solidification this simplified problem removes the necessity to also consider advection of solute through the displacement field, but requires very large forces to have a significant morphological change.

4. Conclusion

In summary, a coupled system modelling microstructure solidification while considering *in situ* structural mechanics was described which utilised a FVM approach due to constraints endemic to the nature of solidification modelling. This was done by creating a purpose-built structural mechanics solver to allow for coupling with the existing numerical code TESA, which was then validated against an analytic solution and coupled to an enthalpy-based solidification model. This coupled system was used to explore the fundamental case of a dendrite growing under the influence of a body force, both following and opposing the growth orientation of the dendrite. This demonstrates the behaviour that would be intuitively expected and is supported by observations of the analogous case of crystal growth under flow, where complementary forces induce comparatively elongated and slender dendrites, whilst opposing forces induce dendrites which appear compressed. Two key aspects still requiring inclusion are to account for the spatial variation as the dendrite deforms which alter the growth orientation and for implementing for alloy systems a similar advective process capable of redistributing f within a partitioned solute. These promising results highlight that the *in situ* effect of structural mechanics on the solidification process can be captured using the described approach and act as proof of concept, justifying the further development, where the structural mechanics code will be ultimately be fully coupled to the main TESA code enabling studies to be run which allow the impacts of these interactions to be better understood.

Acknowledgments

Peter Soar gratefully acknowledges the financial assistance offered by the University of Greenwich VC scholarship for his PhD studies.

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