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A meshfree interface-finite element method for modelling isothermal solutal melting and solidification in binary systems

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ABSTRACT

In this paper, numerical modelling of isothermal solutal melting and solidification in binary systems is done using a new meshfree interface-finite element method (MI-FEM) where the implicitly represented liquid–solid interface is allowed to arbitrarily intersect the finite elements. A meshfree radial basis functions (RBFs) method is used for solving a distance-regularized level set (DRLS) equation such that re-initialization is completely eliminated and fast marching algorithms for interfacial velocity extension are not necessary resulting in a more efficient solution with excellent volume conservation. In the proposed method, intersection points between the mesh and the zero level set are used as meshfree nodes such that at the interface-embedded elements interpolants are constructed using meshfree RBFs ensuring both the partition of unity and Kronecker-delta properties are satisfied allowing for precise and easy imposition of Dirichlet boundary conditions (DBCs) on each side of the interface. A coupling of the MI-FEM with a new meshfree automata (MA) method is used to efficiently predict the microstructural evolution during solidification. Benchmark problems with strong discontinuities were solved where very good accuracy was obtained. The solute conservation and interfacial equilibrium equations describing solutal phase transformation in binary systems were solved using the newly developed method. Mathematical formulation and implementation followed by numerical results and analysis will be presented and discussed.

1. Introduction

1.1. Solutal melting and solidification

Solutal phase transformation is an isothermal diffusion-controlled process such that under certain process parameters melting of the solid or, conversely, solidification of the liquid will occur. Maintaining equilibrium at the liquid–solid interface governs the direction and rate of its evolution. Proper understanding of the interfacial kinetics is essential since it occurs in a number of relevant industrial processes such as powder metallurgy which is an important technique for surface refurbishment and fabrication of complex components. Careful selection of bonding parameters is essential in order to avoid inferior mechanical and thermal properties of the finished product. Incomplete melting in wide-gap brazing results in porous joints with inferior mechanical properties [1]. Incomplete melting of additive powder particles during transient liquid phase bonding of single crystals results in stray grain formation which introduces grain boundaries into the single crystal along with their inherent weaknesses making the material more susceptible to grain boundary corrosion and sliding [2–5]. Careful selection of process parameters such as temperature, time and solute concentration is very important in optimizing the process and the final microstructure of the product. Therefore, it is not surprising that numerical modelling of the effect of process parameters on the interfacial kinetics during phase transformation is very essential.

Numerical modelling of phase transformation of metals and alloys remains one of the most challenging problems in materials science. This is due to the requirement of simultaneously solving a highly non-linear and coupled free boundary problem in addition to predicting the future location of the liquid–solid interface which is itself an unknown. The complex topological evolution of the interface and handling of interfacial dynamics such as merging and splitting makes numerical analysis quite challenging.

In numerical modelling of solidification and phase transformation, the interface separating two distinct phases can be assumed either diffuse (with a finite thickness) or a sharp interface (infinitesimally thin). The diffuse interface assumption is taken in phase field (PF) methods often attributed to Cahn and Hilliard [6,7]and Allen and Cahn [8]. In such methods, a phase parameter is introduced which is 1 in phase A and 0 in phase B while it varies sharply but smoothly across an interfacial region with a finite thickness. The PF method has gained considerable popularity in materials science and modelling of phase transformation due to its ability to directly incorporate the thermodynamics of phase transition into the formulation. It also

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eliminates the need to assign boundary conditions directly at the interface. Additionally, computation of interface normals and curvature is also avoided.

Traditional finite element modelling of phase transformation based on the sharp-interface assumption involves interface tracking techniques [9–16] where the interfaces are explicitly tracked by imposing marker points directly at the interface while an adaptive meshing technique is used such that the mesh is continuously updated to conform to the evolving liquid and solid topology. The main advantage of this Lagrangian approach is that imposing the Dirichlet boundary conditions (DBC) at the interface, as is often typical in sharp-interface solidification and melting numerical models, is easy since there will always be interfacial nodes that directly represent the interface. However, the main challenge with this approach is that the interfaces are represented explicitly requiring the continuous update and re-generation of the mesh which becomes very time consuming especially in 3D analysis. Explicit handling of interfacial dynamics such as merging or splitting becomes a significant challenge where interfacial nodes must be added or deleted as required to ensure an accurate solution.

Rather than explicitly tracking the sharp-interface, it can be captured using a fixed mesh while allowing it to evolve independently of the underlying mesh. Methods based on this Eulerian approach is the volume-of-fluid method developed by Hirt and Nichols [17] which is very popular in modelling computational fluid dynamics problems such as multi-phase flows. In the VOF method, a step function, f, is used to define the interface such that it is 0 in one phase and 1 in the other while the sharp-interface lies somewhere at $0<f<1$. Advantages of the VOF method include easy handling of interfacial dynamics and their excellent volume and mass conservation properties [18]. However, an extra step is often required to reconstruct the interface from the VOF solution using popular methods such as the piecewise linear interface calculation (PLIC) [19]. The overall accuracy of the method depends largely on the performance of its interface reconstruction schemes.

Another approach is to implicitly define the interface by a higher dimension, smooth, and continuous function, Φ, such as a signed distance function (SDF), where the interface is the zero level set of that function. The SDF is then evolved by solving a Hamilton–Jacobi level set equation [20]:

$$\frac{\partial \Phi}{\partial t}+\vec{V}.\vec{\nabla}\Phi+V_n^{ext}\left\|\vec{\nabla}\Phi\right\|=0 \tag{1}$$

where Φ is the level set function (LSF) value, $\vec{V}$ is the convective velocity in the domain, and V_n^{ext} is the normal velocity of the interface extended sufficiently around the interfacial area. This approach has a number of very attractive features such as easy calculation of the local normal vector to the interface, curvature, and easy handling of interface dynamics such as splitting and merging.

It is important to note that since the interfacial evolution is now independent of the underlying mesh, a finite element formulation used to calculate the field variables must account for the inter-element discontinuities where the interface may arbitrarily intersect the elements. An additional complication due to the implicit representation of discontinuities is that there are no nodes that immediately lie on the interface. As a result, it is not straightforward to impose the essential boundary conditions governing interfacial equilibrium as in the conventional finite element method (FEM).

The relatively recent generalized/extended finite element methods (GFEM/XFEM) based on the Partition of Unity method (PUM) developed by Melenk and Babuska [21] are excellent techniques for handling both weak and strong discontinuities that may arbitrarily intersect the finite elements. The (GFEM/XFEM) are practically identical methods [22] where the GFEM was adopted by the Texas school [21,23,24] and the XFEM was adopted by the Northwestern school [22,25,26]. In the GFEM/XFEM, discontinuities are allowed to intersect the element eliminating the requirement of aligning the edges of elements with the discontinuity as is typically done in conventional FEMs. A hybrid finite element-meshless approach is used where the conventional FEM is used for elements away from the discontinuity while local enrichment at nodes of elements intersected by the interface is done within the framework of the PUM [21] such that a field variable can be approximated by

$$U(\mathbf{x})=\sum_{i=1}^{n_{std}} N_i(\mathbf{x})U_i+\sum_{j=1}^{n_{enr}}\psi_j(\mathbf{x})a_j \tag{2}$$

where $N_i(\mathbf{x})$ in Eq. (2) are the standard finite element shape functions for node i, U_i are the nodal degrees of freedom, $\psi_j(\mathbf{x})$ are the enrichment functions and a_j are the nodal enrichment degrees of freedom. n_{std} and n_{enr} are the number of nodal standard degrees of freedom and nodal enriched degrees of freedom, respectively.The GFEM/XFEM is tremendously successful especially in the area of solid mechanics and modelling of crack propagation and fracture where it entertains a high degree of maturity. This is mainly due to the flexibility of the PUM for inclusion of pre-determined analytical solutions as enrichment functions which significantly facilitates handling of singularities that arise at crack tips during crack propagation analysis. Adding the well-known asymptotic singular near-tip solutions near crack fronts and dislocation cores as enrichments can significantly reduce the h-refinement required to handle such features.

The GFEM/XFEM generally involves the use of some type of enrichment functions such as Heaviside or ridge functions where the added enrichment functions correspond to added degrees of freedoms at the nodes of the original element as shown in Fig. 1. Two complications become immediately apparent. The first is that for certain types of enrichment functions, such as ridge functions, the enrichment effect may not vanish for elements adjacent to the intersected element [22]. This means that shape functions at the adjacent elements will no longer satisfy the partition of unity property since only some of the nodes of the element are enriched while others are not. Such elements are termed “blending” elements which have been shown to slow convergence if left untreated [27,28]. Specialized methods are often needed to avoid the parasitic behaviour associated with blending elements and a lot of research has been done to overcome problems associated with them [22]. The second apparent problem is that there are no degrees of freedoms that are directly associated with the interface.

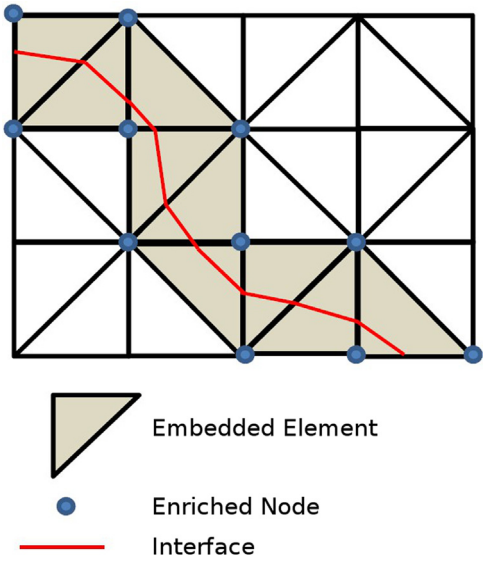

Fig. 1. Nodal enrichment in the XFEM/GFEM.