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Influence of the shape of the particles in the solidification of composite materials

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Abstract

The shape of a solidifying interface is generally affected when it encounters foreign inert particles. The degree of deformation depends on the morphology and physical properties of the particles, the melt, the solid and the external fields, affecting the pushing and capture process of the particles. The particle can be trapped by the interface at slower solidification velocity than that predicted by simple models which do not include any deformation of the interface. In all cases this interaction strongly determines the segregation of particles in the microstructure and therefore affecting the physical and physicochemical properties of the final material. In the present report the interaction between particle and interface is analyzed by means of a mathematical model employing the finite element method. The effect on interface shape of different particle shapes and relative thermal conductivities between particle and melt was studied. Thermal field results show that when the particle is more conductive than the melt, the interface is concave. Comparing the concave interfaces for different particle shapes it is observed that, when the particle is not spherical the separation particle-interface at the edge of the particle is the smallest. As a consequence of this phenomenon, which occurs in non-spherical particles, there is a remaining amount of melt between particle and solid which is the last in solidify.

Keywords: Solidification, FEM, composite material, crystal growth.

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1. Introduction

Solidification studies of materials containing particles have shown an interaction between the particle and the solid-liquid interface. One of the possible interactions is the repulsion of the particle. This phenomenon is observed in materials such as metal alloys with native particles, in metal matrix composites reinforced with ceramics, and during the crystallization of semiconductor, optical, optoelectronic and biological materials. The presence of the particle ahead of the solidification front with different values of thermal conductivity between the particle and the solid affects the thermal field in the vicinity of the particle, which affects the shape of the interface.

This phenomenon has been studied by several authors. Two dimensional models were developed to obtain the shape of the interface using numerical techniques, considering that the particle is a cylinder of infinite length. Bolling et al. 1971 and Zubko et al. 1973 considered this effect qualitatively as a criterion for entrapment or repulsion of particles. However, they did not find direct experimental evidence of the dependence of trapping and the thermal conductivities. More recently Garvin et al. (2004, 2005, 2007) performed two dimensional numerical simulations of the interaction of the solidification front with particles, accounting for the effect of the curvature of the interface due to the thermal conductivities.

Agaliotis *et al* 2008-2009 developed axi-symmetric models and numerical simulations of the particle repulsion process, decoupling the process and building the model in steps of increasing complexity. The first stage started with the temperature field, the second stage included the fluid flow for planar and not planar interfaces and spherical particles. These fields are then coupled to analyze the conditions under which there is particle pushing. This phenomenon is governed by a dynamic balance between drag and repulsion forces. In these models the strongest interactions are taking into account as follows: the repulsive force considered is the Lisfshitz force and the attractive force considered is the drag force. Other interactions such as inertia, gravity or surface tension were not considered. The model results were adjusted to the experimental results, which would indicate that the interactions considered are sufficiently strong to fit the experimental results published for the critical velocities. The results obtained show that when the particle has lower thermal conductivity than the fluid the resulting interface is convex. When the particle has greater conductivity than the fluid the resulting interface is concave, and when fluid and particle have the same thermal conductivity the resulting interface is flat.

In the present report results obtained with a numerical model of the pushing phenomenon are presented. The temperature field of the particle-interface system is analyzed in order to determine the influence of the particle shape on the shape of the interface, for particles with higher thermal conductivities than the matrix.
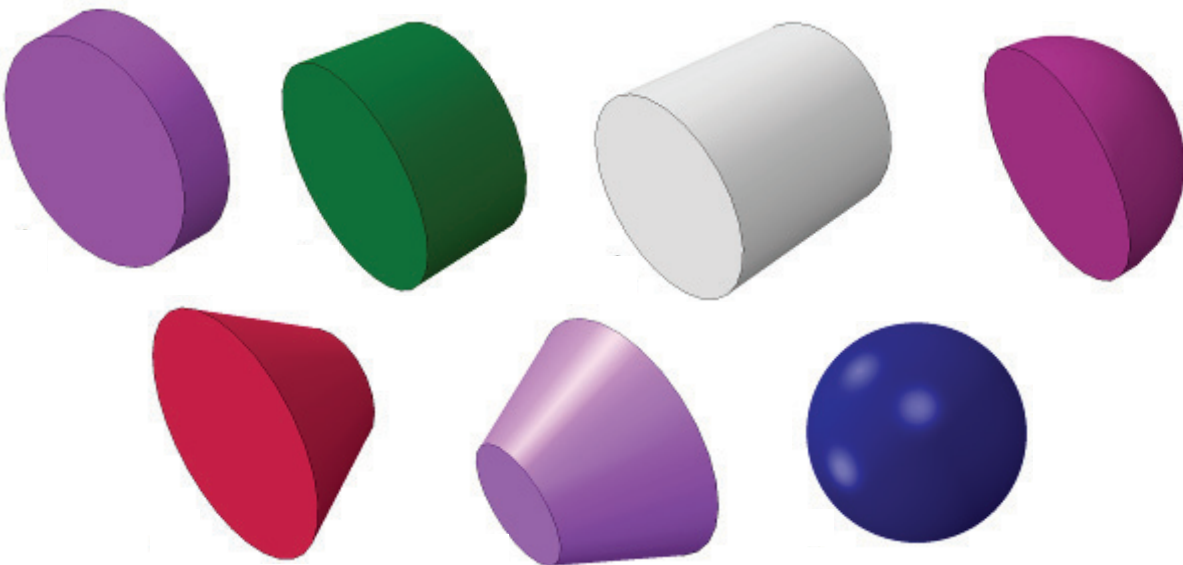

Fig. 1. Isometric perspective views of the particles considered in the model. In all cases the interface approaches the particle from the left in the direction of the axis of symmetry of the particle.

2. Methods

2.1. Description of the model

The physical model which is mathematically modelled consists of a solid particle immersed in the liquid phase of a matrix that is solidifying. The particle shapes considered are: spherical, cylindrical, conical and hemispherical as shown in Figure 1, the last three particles with the flat side towards the interface. The dimensions are parameterized by the sphere radius, R, equal to 50 microns. The cylinders are of radius R and height R/2, R and 2R, the hemisphere is of radius R, the truncated cones dimensions are height equal to the radius, major radius is equal to R and minor radius equal to R/2.
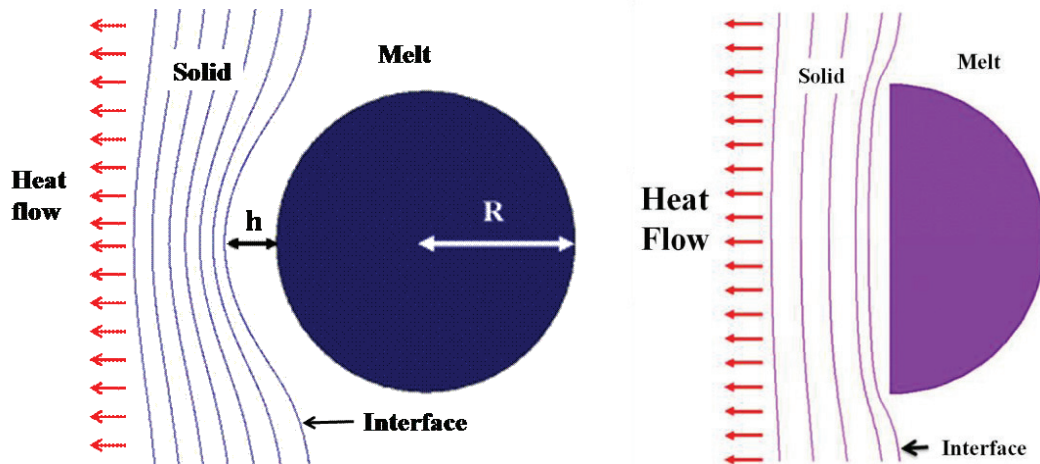

Fig. 2. Scheme of the thermal model. The shape of the interface at different particle-interface distances is shown.

The temperature field is solved using the finite element method. The thermal field generated by the cooling process which simulates solidification is dynamically modeled.

The heat extraction is considered unidirectional in the direction of the advance of the interface which causes the solidification of the matrix, as shown in Figure 2.
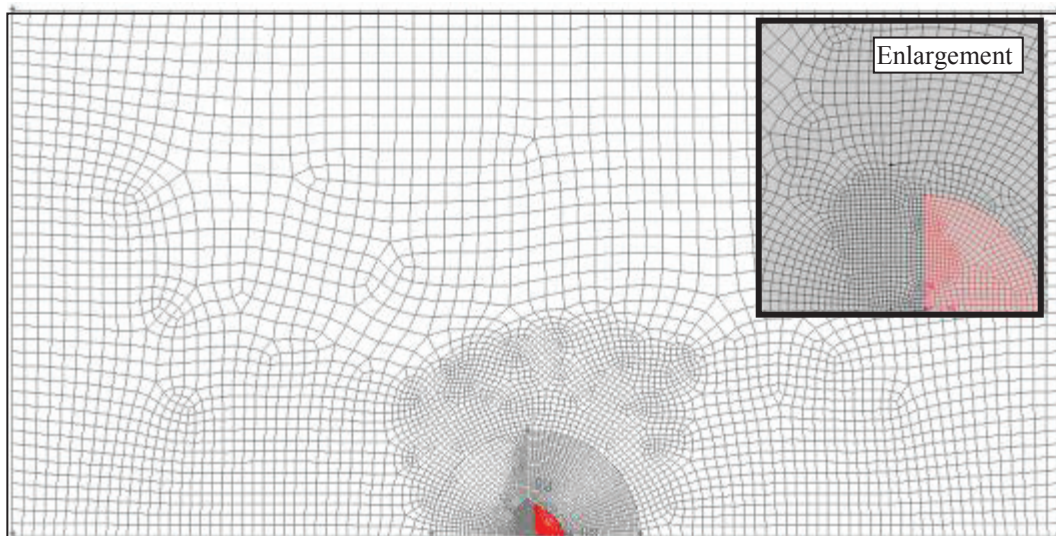

Fig. 3 Mesh used in the thermal axi-symmetrical model and hemispherical particle.

The properties are assumed to be independent of temperature. The other borders are isolated. The calculation is done on an axi-symmetrical model time-dependent. The resolution of the problem includes the equations of conservation of mass and energy dynamically. The domain was discretized using 50.000 quadrilateral elements with first order interpolation functions for the temperature field. The model was refined in the vicinity of the particle for a better detail of the curvature of the interface, as shown in Figure 3.

The shape of the interface is calculated by simulating the thermal field, at different particle-interface distances. The thermal field is determined by the values of the thermal conductivities of the particle, the liquid and solid, modifying the shape of the interface in the vicinity of the particle.

The numerical solutions were obtained using a Newton-Raphson method with a tolerance of 0.01%. The dynamic time dependant part was solved employing the Crank-Nicholson method with a variable time step adjusted by the Adams-Bashforth method (Chapra et al. 2005, Hurtado et al 2002).

The domain employed in the calculations consists of a solid particle with a thermal conductivity kp, immersed in a melt with a thermal conductivity km. Different meshes are constructed for each particle shape. The relative thermal conductivities between particle and melt kp/km employed in the calculations was 10, which corresponds to a copper/lead system (Perry et al. 1992). The solid phases were modeled as materials with high viscosity (10^6 times the viscosity of the melt).

The heat extraction rate used is 12500 J/m^{2}s. The shape and position of the interface is determined using the isotherm of solidification of pure aluminum: 933 K.

3. Results and discussion

3.1. Spherical and hemispherical particles

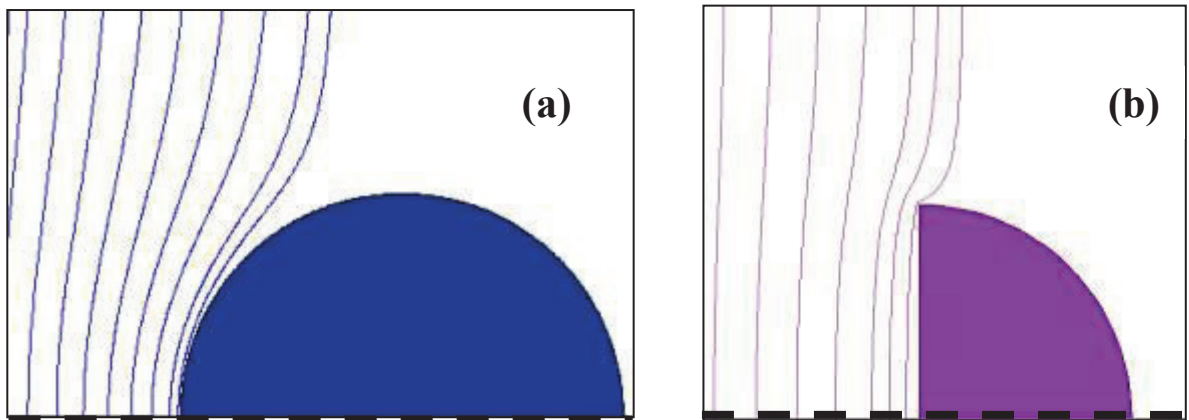The results of the simulation for spherical and hemispherical particle are shown in Figure 4.

Fig. 4. Shape of the interface at different distances.(a) conductive and spherical particle (b) conductive and hemispherical particle.

For hemispherical particles it is observed that when the particle is more conductive than the melt, the interface is flat at large distances, as the boundary condition imposed, however, as it approaches to the particle it becomes concave, enveloping the particle. When the particle is spherical, the minimum separation particle-interface is located on the axis of symmetry as shown in Figure 4 (a). In contrast, the lower separation in non-spherical particles is on the edge of the flat face, which faces the interface as is shown in Figure 4 (b). Because of this phenomenon, which occurs in non-spherical particles, remaining liquid is found between the particle and the solid as shown in Figure 4 (b).
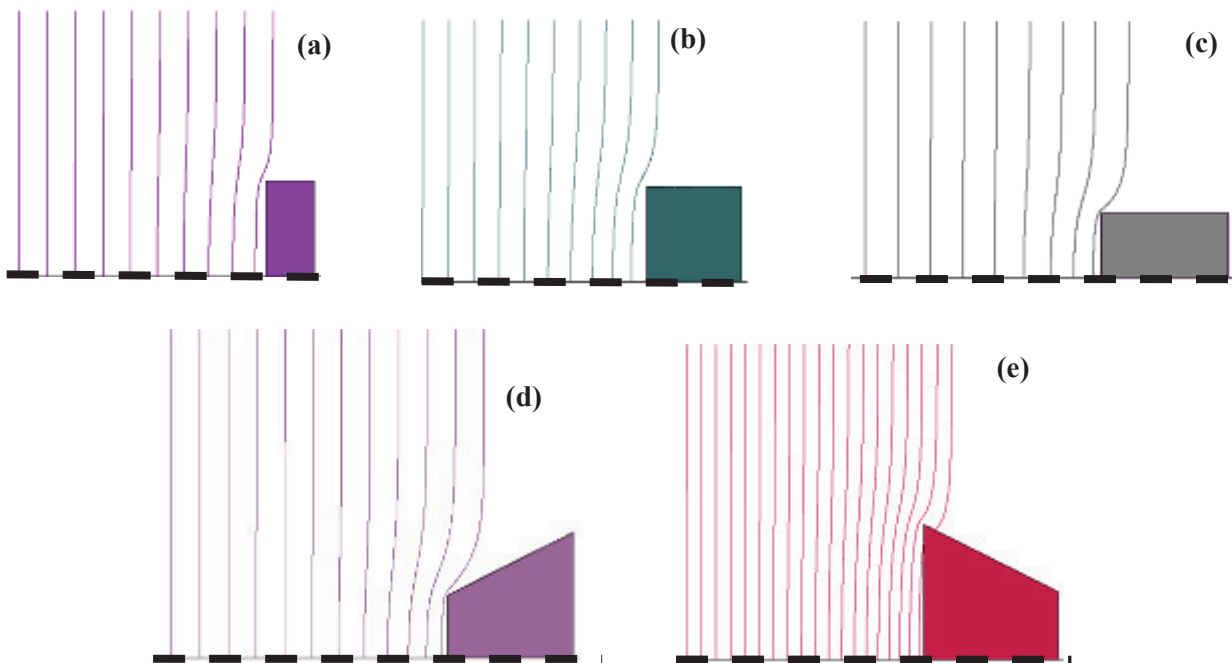
3.2. Cylindrical and conical particles

Fig. 5. Shape of the interface at different distances.(a) (b) and (c) cylinders of different heights (d) and (e) truncated cones.

The results for cylindrical and conical particles when kp / km = 10, are shown in Figure 5. It is observed how the interface shape changes as a function of distance from the particle. At distances greater than the height of the particle, the interface is practically flat and as the particle approaches the interface it gradually becomes concave.
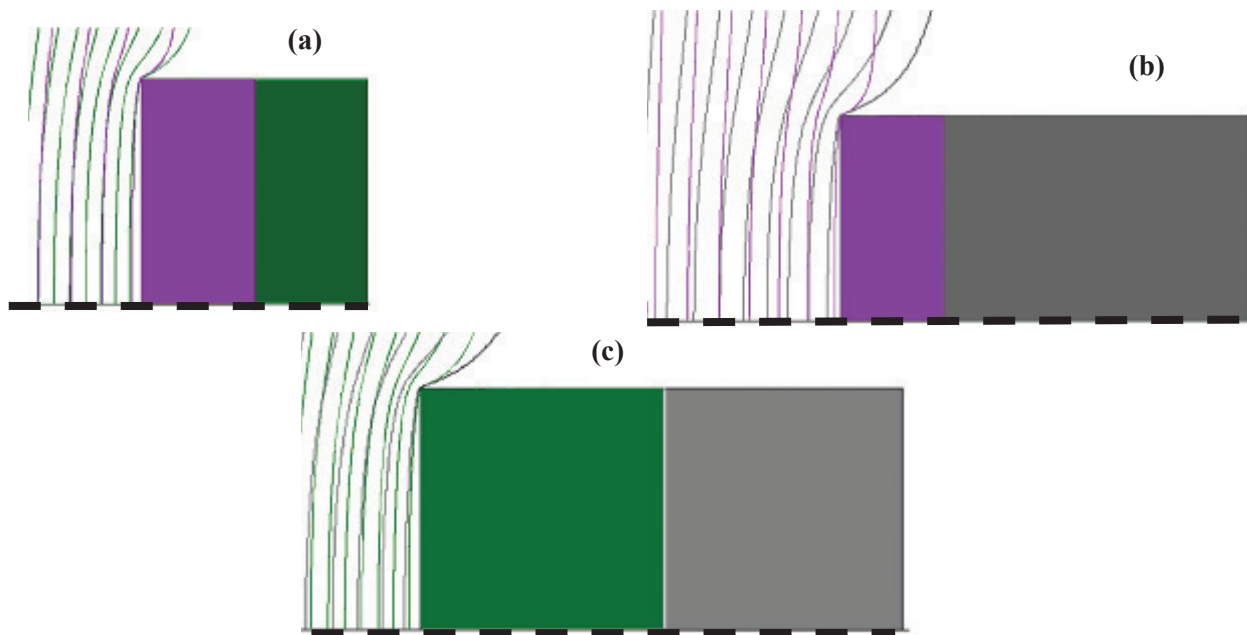

Fig. 6. Superposition of the interfaces between cylindrical particles of different heights.

By comparing the cylindrical particles of equal diameter but different heights, it is observed that the larger the height the greater the deformation of the interface and, therefore, the distance particle-interface is larger, as shown in Figure 6. In the case of cylindrical particles of large height, the amount of remaining liquid will be larger. This effect would indicate that there may be remaining liquid between the particle and the solid front even after the particle has started to be captured by the solid.

4. Conclusions

The shape and relative thermal conductivity of the foreign particles influences the shape of the solid interface at short particle-interface distances.

When the particle has larger thermal conductivity than the melt and shows a non-spherical shape that has a flat face towards the growing interface, the interface becomes concave as it approaches the particle. As a result, the first contact between interface and particle takes place at the edge of the flat face. Therefore, short after the solid has started to engulf the particle, a remaining portion of liquid can be found between the flat face of the particle and the solid. The amount of liquid remaining in cylindrical particles of large aspect ratio will be larger than that found on cylindrical particles of lower aspect ratio.

Acknowledgements

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