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A SIMILARITY SOLUTION FOR A BINARY ALLOY SOLIDIFICATION MODEL WITH A SIMPLE MUSHY ZONE

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Abstract

It is shown that there exists at least one exact solution of the Neumann type for the binary alloy solidification problem, with a simple mushy zone model. Also, some numerical results are presented.

Resumen

Se demuestra la existencia de al menos una solución exacta del tipo Neumann para el problema de solidificación de una aleación binaria, con un modelo simple con zona pastosa. Se presentan también algunos resultados numéricos.

Key words: Stefan problem, binary alloy solidification, similarity variable, Neumann solution, phase-change problem, free boundary problems, exact solutions, mushy zone.
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I. Introduction

In Stefan problems [3, 9, 15], it is generally assumed that the phase change takes place at a unique temperature called melting temperature and that there exists a sharp phase change boundary called freezing front. On one side of the freezing front there exists a stable solid phase and on the other side exists a stable liquid phase.

This assumption considerably simplifies the problem, but it is true strictly for pure metals. Generally, some impurities are also present and so it seems more appropriate to consider solidification/liquidification of alloys.

In the solidification of binary alloys [6], both heat and mass diffusion take place and solidification of dilute binary alloy

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is governed by the equilibrium phase diagram as shown in fig. 1. The temperature and concentration of any one phase can not be independent of another at the freezing front and they are governed by the phase diagram.

Let the temperature and concentration of a small volume element in the concentration and temperature plane be denoted by (C, T). If the point (C, T) lies to the right of the liquidus line, then the volume element is in a stable liquid phase. If the point (C, T) lies to the left of the solidus line then the volume element is in a stable solid phase. If the point (C, T) lies in between the solidus and liquidus lines then the volume element is supposed to be in the mushy phase and for the stability of the mushy phase it is essential that the volume element contains both solid and liquid phases. The temperature and concentration of this volume element in the mushy phase can be determined from the knowledge of the phase diagram [6].

The occurrence of mushy region is commonly observed during alloy solidification and sometimes mushy region develops after a short time itself.

In [10, 14, 15, 16] an exact similarity solution has been obtained for a binary alloy solidification problem by assuming that a sharp freezing front separating the solid and liquid regions exists.

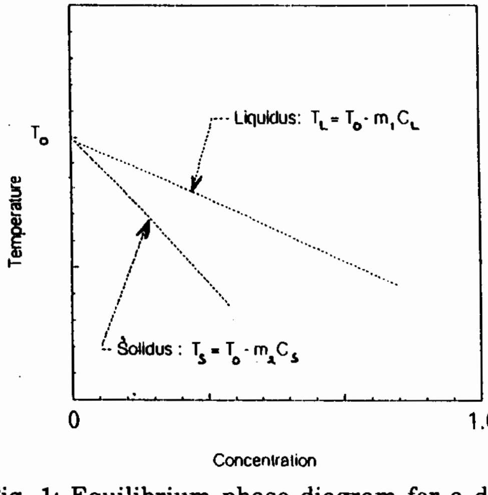

Fig. 1: Equilibrium phase diagram for a dilute binary alloy

In [4, 8, 15] it has been recently shown that for the sharp freezing front model of alloy solidification, in the so called liquid region, there are volume elements for which the points (C, T) lie in the mushy phase. A review on the mathematical formulation of the mushy zone is given in [5].

In the present study an exact similarity solution for a one-dimensional alloy solidification has been constructed. The solid and liquid regions are separated by a mushy region, following the simple model developed for the one-phase [11, 12] and two-phase [7, 13] Stefan problems. As far as we know, no exact solution in which all the three regions are present exists in the literature. It is hoped that this type of analytical solutions may provide some guidelines. These solutions can be used for checking analytical and numerical solutions of more complicated problems of alloy solidification.

II. Model of the problem

We shall consider the following problem: find the boundaries $x = s(t)$ and $x = r(t)$, defined for $t > 0$ with $s(t) < r(t)$ and $s(0) = r(0) = 0$, the temperature $\theta = \theta(x, t)$ and the concentration $C = C(x, t)$, defined for $x > 0$ and $t > 0$, by the expressions

$$\theta(x,t) = \begin{cases} \theta_1(x,t) > T_{cr}(t) & \text{if } 0 < x < s(t),\ t > 0, \\ T_{cr}(t) & \text{if } s(t) \le x \le r(t),\ t > 0, \\ \theta_2(x,t) > T_{cr}(t) & \text{if } r(t) < x,\ t > 0, \end{cases} \qquad (1)$$

and

$$C(x,t) = \begin{cases} C_1(x,t) & \text{if } 0 < x < s(t),\ t > 0 \\ C_m(x,t) & \text{if } s(t) \le x \le r(t),\ t > 0 \\ C_2(x,t) & \text{if } r(t) < x,\ t > 0, \end{cases} \qquad (2)$$

respectively, such that they satisfy the following conditions (the subscripts 1, 2 and m refer to solid, liquid and mushy regions, respectively):

$$\alpha_1 \theta_{1_{xx}} = \theta_{1_t}, \quad 0 < x < s(t), t > 0, \qquad (3)$$

$$D_1 C_{1_{xx}} = C_{1_t}, \quad 0 < x < s(t),\ t > 0, \qquad (4)$$

$$\theta_1(0,t) = T_B \quad t>0, \tag{5}$$
$$C_{1x}(0,t) = 0 \quad t>0, \tag{6}$$
$$\theta_1(s(t),t) = T_{cr}(t) \quad t>0, \tag{7}$$
$$\alpha_2\theta_{2_{xx}} = \theta_{2t}, \quad r(t)<x,\ t>0, \tag{8}$$
$$D_2C_{2_{xx}} = C_{2t}, \quad r(t)<x, t>0, \tag{9}$$
$$\theta_2(x,0)=\theta_2(+\infty,t)=T_0, \qquad x>0, \tag{10}$$
$$C_2(x,0)=C_2(+\infty,t)=C_0, \qquad x>0, \tag{11}$$
$$\theta_2(r(t),t)=T_{cr}(t) \qquad t>0, \tag{12}$$
$$k_1\theta_{1_x}(s(t),t)-k_2\theta_{2_x}(r(t),t)= =\rho\lambda[(1-\varepsilon)\,\dot r(t)+\varepsilon\,\dot s(t)],\ t>0, \tag{13}$$
$$\theta_{1_x}(s(t),t)(r(t)-s(t))=\gamma,\ t>0, \tag{14}$$
$$D_1C_{1_x}(s(t),t)-D_2C_{2_x}(r(t),t)= =[C_2(r(t),t)-C_1(s(t),t)]\cdot [(1-\varepsilon)\dot r(t)+\varepsilon\,\dot s(t)],\ t>0, \tag{15}$$
$$T_{cr}(t)=T_A-m_1C_1(s(t),t) \qquad t>0, \tag{16}$$
$$T_{cr}(t)=T_A-m_2C_2(r(t),t) \qquad t>0, \tag{17}$$
$$s(0)=r(0)=0, \tag{18}$$

where $\lambda > 0$ is the latent heat of fusion, $\rho > 0$ is the mass density which is taken equal in both solid and liquid phases, $k_i > 0$, $c_i > 0$, $\alpha_i = a_i^2 = \frac{k_i}{\rho c_i}$, D_i are the thermal conductivity, the specific heat, the thermal diffusion coefficient and the mass diffusion coefficient for the phase i (i = 1: solid phase, i = 2: liquid phase) respectively. Coefficients ε and γ are real numbers ($0 < \varepsilon < 1$, $\gamma > 0$) which characterizes the mushy zone [9, 10, 11]. Further, the initial temperature T_0, the boundary temperature T_B and the critical temperature T_{cr} satisfy the relation $T_B < T_{cr}(t) < T_0$, for all $t > 0$. Without loss of generality, we suppose that $T_B > 0$. Moreover, $T = T_A - m_1C$ and $T = T_A - m_2C$ are the solidus and liquidus curve (see figure 1) and we assume that $C_m = C_1 + \varepsilon(C_2 - C_1)$. The concentration C_m of the mushy region is obtained by using law of mixtures and the fact that for the equilibrium of any volume element in the mushy phase, it must contain both solid and liquid phases with their concentrations as C_1 and C_2.

Following the Neumann method we propose the functions

$$\theta_1(x,t)=A_1+B_1\,f\left(\frac{x}{2a_1\sqrt{t}}\right), \quad 0<x<s(t),\quad t>0, \tag{19}$$
$$\theta_2(x,t)=A_2+B_2\,f\left(\frac{x}{2a_2\sqrt{t}}\right), \quad r(t)<x, \qquad t>0, \tag{20}$$
$$C_1(x,t)=M_1+N_1\,f\left(\frac{x}{2\sqrt{D_1t}}\right), \quad 0<x<s(t),\quad t>0, \tag{21}$$
$$C_2(x,t)=M_2+N_2\,f\left(\frac{x}{2\sqrt{D_2t}}\right), \quad r(t)<x, \qquad t>0, \tag{22}$$
$$s(t)=2\,\sigma_1a_1\sqrt{t}, \qquad t>0, \tag{23}$$
$$r(t)=2\,\sigma_2a_1\sqrt{t}, \qquad t>0, \tag{24}$$

which satisfy conditions (3), (4), (8) and (9), where

$$f(x)=\mathrm{erf}(x)=\frac{2}{\sqrt{\pi}}\int_0^x \exp\left(-t^2\right)dt \tag{25}$$

is the error function.

If we impose conditions (5)-(7), (10)-(12) and (16)-(17) we obtain that the coefficients A_i, B_i, M_i, N_i (i = 1, 2) are given, as functions of parameters σ_1 and σ_2, as follows:

$$A_1=T_B, \qquad B_1=\frac{T_{cr}-T_B}{f(\sigma_1)} \tag{26}$$
$$M_1=\frac{T_A-T_{cr}}{m_1}, \qquad N_1=0 \tag{27}$$
$$A_2=\frac{T_{cr}-T_0f(\delta\sigma_2)}{1-f(\delta\sigma_2)} \qquad B_2=\frac{T_0-T_{cr}}{1-f(\delta\sigma_2)} \tag{28}$$

$$M_2 = C_0 - \frac{T_{cr} - T_A + m_2 C_0}{m_2(1 - f(\nu\sigma_2))}$$

$$N_2 = \frac{T_{cr} - T_A + m_2 C_0}{m_2(1 - f(\nu\sigma_2))} \quad (29)$$

where $\delta = \frac{a_1}{a_2} = \sqrt{\frac{k_1 c_2}{c_1 k_2}}, \nu = \frac{a_1}{\sqrt{D_2}} = \sqrt{\frac{\alpha_1}{D_2}}$ and $T_{cr}(t)$ results a constant, i.e. $T_{cr}(t) = T_{cr}$ for all $t > 0$.

Taking into account conditions (13)-(15) we obtain the following system of three equations for the unknowns σ_1, σ_2 and T_{cr}:

$$\sigma_2 = \sigma_1 + \frac{1}{2} \frac{\gamma\sqrt{\pi}}{T_{cr} - T_B} f(\sigma_1) \exp(\sigma_1^2), \quad (30)$$

$$k_1 \frac{T_{cr} - T_B}{\sqrt{\pi}\, a_1 f(\sigma_1)} \exp(-\sigma_1^2) -$$

$$- k_2 \frac{T_0 - T_{cr}}{\sqrt{\pi}\, a_2(1 - f(\delta\sigma_2))} \exp[-(\delta\sigma_2)^2] =$$

$$= \rho\lambda a_1[(1 - \varepsilon)\sigma_2 + \varepsilon\sigma_1] \quad (31)$$

$$\sqrt{\frac{D_2}{\pi}} \frac{T_{cr} - T_A + m_2 C_0}{1 - f(\nu\sigma_2)} \exp[-(\nu\sigma_2)^2] =$$

$$= \frac{T_A - T_{cr}}{m_1}(m_2 - m_1) a_1[(1 - \varepsilon)\sigma_2 + \varepsilon\sigma_1] \quad (32)$$

In order to facilitate the calculations we combine the several constants of the problem into the following dimensionless parameters:

$$\mu = \frac{m_2 - m_1}{m_1} > 0, \quad \varsigma = \frac{(1-\varepsilon)\gamma}{T_B} \frac{\sqrt{\pi}}{2} > 0, \quad (33)$$

$$K_1 = \frac{k_1 T_B}{\rho\lambda a_1^2 \sqrt{\pi}} = \frac{c_1 T_B}{\lambda\sqrt{\pi}},$$

$$K_2 = \frac{k_2 T_B}{\rho\lambda a_1 a_2 \sqrt{\pi}} = \frac{T_B}{\lambda} \sqrt{\frac{k_2 c_1 c_2}{\pi k_1}}, \quad (34)$$

$$\beta = \frac{\varsigma}{1-\varepsilon} = \frac{\sqrt{\pi}}{2} \frac{\gamma}{T_B}, \quad (35)$$

$$E = \frac{m_2 C_0}{T_B}, \quad D = \sqrt{\frac{D_2}{\pi\alpha_1}} = \frac{1}{\nu\sqrt{\pi}} \quad (36)$$

Let the real functions

$$F_1(x) = \frac{\exp(-x^2)}{1 - f(x)}, \quad F_2(x) = \frac{\exp(-x^2)}{f(x)} \quad (37)$$

defined for $x \geq 0$ and

$$\omega = \frac{(T_{cr} - T_B)}{T_B} F_2(\sigma_1), \quad (38)$$

then we can rewrite equations (30)-(31)-(32) as:

$$\sigma_2 = \sigma_1 + \frac{\beta}{\omega}, \quad (39)$$

$$K_1\omega - K_2\left[\frac{T_0}{T_B} - 1 - \frac{\omega}{F_2(\sigma_1)}\right] F1\left(\delta(\sigma_1 + \frac{\beta}{\omega})\right) =$$

$$= \sigma_1 + \frac{\varsigma}{\omega}, \quad (40)$$

$$D\left[\frac{\omega}{F_2(\sigma_1)} - \frac{T_A}{T_B} + 1 + E\right] F_1\left(\nu(\sigma_1 + \frac{\beta}{\omega})\right) =$$

$$= \mu\left(\frac{T_A}{T_B} - 1 - \frac{\omega}{F_2(\sigma_1)}\right)\left(\sigma_1 + \frac{\varsigma}{\omega}\right) \quad (41)$$

Equations (40) and (41) are equivalent to:

$$G_1(\omega, \sigma_1) = 0$$
$$G_2(\omega, \sigma_1) = 0 \quad (42)$$

where functions G_1 and G_2 are defined by

$G_1(x, y) =$

$$= D\left[\frac{x}{F_2(y)} - \frac{T_A}{T_B} + 1 + E\right] F_1\left(\nu(y + \frac{\beta}{x})\right) +$$

$$+\mu\left(\frac{x}{F_2(y)} - \frac{T_A}{T_B} + 1\right)\left(y + \frac{\varsigma}{x}\right), \qquad (43)$$

$$G_2(x,y) = y + \frac{\varsigma}{x} - K_1 x +$$

$$K_2\left[\frac{T_0}{T_B} - 1 - \frac{x}{F_2(y)}\right] F_1\left(\delta(y + \frac{\beta}{x})\right) \qquad (44)$$

In the next section we prove that system (42) has at least one solution and as a consequence we can assert that problem (1), (18) has at least one solution.

III Existence of an exact solution

The analytical solution of this problem is complete if the unknowns coefficients σ_1 and ω can be determined with the help of the equations (40) and (41). σ_2 can be determined from equation (39) and the critical temperature T_{cr} from equation (38), as follows

$$T_{cr} = T_B\left(1 + \frac{\omega}{F_2(\sigma_1)}\right) \qquad (45)$$

Taking into account that functions F_1 and F_2 verify the following properties:

$$F_1(0^+) = 1, \quad \lim_{x\to+\infty} F_1(x) = +\infty,$$
$$F_1'(x) > 0, \ \forall x > 0, \qquad (46)$$

$$F_2(0^+) = +\infty, \quad \lim_{x\to+\infty} F_2(x) = 0,$$
$$F_2'(x) < 0 \ \ \forall x > 0 \qquad (47)$$

we can easily prove:

Lemma 1: If $\frac{T_A}{T_B} > 1 + E$ then we have

a) for each fixed $y > 0$,

$$\lim_{x\to 0^+} G_1(x,y) = -\infty \qquad (48)$$

$$\lim_{x\to+\infty} G_1(x,y) = +\infty, \qquad (49)$$

moreover

$$G_1(x, 0^+) = H_1(x) \qquad (50)$$

where

$$H_1(x) = -D\left[\frac{T_A}{T_B} - 1 - E\right] F_1\left(\nu\,\frac{\beta}{x}\right) -$$

$$-\frac{\mu\varsigma}{x}\left(\frac{T_A}{T_B} - 1\right) < 0, \ x > 0$$

is an increasing function and

$$\lim_{x\to 0^+} H_1(x) = -\infty \ ,$$

$$\lim_{x\to+\infty} H_1(x) = -D\left[\frac{T_A}{T_B} - 1 - E\right] < 0$$

b) for each fixed $x > 0$,

$$\lim_{y\to 0^+} G_2(x,y) = H_2(x) \qquad (51)$$

$$\lim_{y\to+\infty} G_2(x,y) = -\infty \qquad (52)$$

where

$$H_2(x) = \frac{\varsigma}{x} - K_1 x + K_2\left[\frac{T_0}{T_B} - 1\right] F_1\left(\delta\frac{\beta}{x}\right), x > 0$$

is a decreasing function and

$$\lim_{x\to 0^+} H_2(x) = +\infty \quad \lim_{x\to +\infty} H_2(x) = -\infty$$

c) $G_{1y}(x, y) > 0, \ \forall x > 0, \forall y > 0,$ (53)

$G_{2x}(x, y) < 0, \ \forall x > 0, \forall y > 0,$ (54)

so it is possible to define implicitly the functions $y = y_1(x)$ from $G_1(x, y) = 0$ and $x = x_2(y)$ from $G_2(x, y) = 0$.

Lemma 2: The curve $y = y_1(x)$ defined implicitly from $G_1(x, y) = 0$, verifies:

i) $$\lim_{x\to 0^+} y_1(x) = +\infty \quad (55)$$

Moreover

$$y_1(x) \cong \sqrt{\log\left(\frac{d_1}{x}\right)} \quad \text{as } x \to 0^+$$

with $d_1 =$

$$= \frac{\left[\frac{T_A}{T_B} - 1 - E\right] D\nu\beta\sqrt{\pi} + \mu\varsigma\left[\frac{T_A}{T_B} - 1\right]}{D\nu\beta\sqrt{\pi} + \mu\varsigma} > 0 \quad (56)$$

ii) $$\lim_{x\to +\infty} y_1(x) = 0 \quad (57)$$

Proof:

i) From $F_1(z) \cong \sqrt{\pi}\, z$ as $z \to +\infty$ [1], we obtain (55) by contradiction. Moreover, since $(F_2(z) \cong \exp(-z^2)$ as $z \to +\infty$ [1], after some manipulation, from $G_1(x, y) = 0$, we obtain that,

$$\lim_{x\to 0^+} x y_1(x) = 0, \quad \lim_{x\to 0^+} x \exp\left(y_1(x)^2\right) = d_1 \quad (58)$$

and therefore [56]

ii) When $x \to +\infty$ in the expresion $G_1(x, y) = 0$ we obtain

$$x = \frac{D\left[\frac{T_A}{T_B} - 1 - E\right] F_1(\nu y) + \left[\frac{T_A}{T_B} - 1\right]\mu y}{D F_1(\nu y) + \mu y} F_2(y),$$

for $x \to +\infty$ and $y = y_1(x)$. (59)

From (59) we can easily obtain that $\lim_{x\to+\infty} y_1(x)$ is not a finite positive number. If we suppose that $\lim_{x\to+\infty} y_1(x) = +\infty$ then we have a contradiction because $F_2(+\infty) = 0$ and

$$\lim_{y\to+\infty} \frac{D\left[\frac{T_A}{T_B} - 1 - E\right] F_1(\nu y) + \left[\frac{T_A}{T_B} - 1\right]\mu y}{D F_1(\nu y) + \mu y} =$$

$$= \frac{D\left[\frac{T_A}{T_B} - 1 - E\right]\sqrt{\pi} + \frac{\mu}{\nu}\left[\frac{T_A}{T_B} - 1\right]}{D\sqrt{\pi} + \frac{\mu}{\nu}} > 0.$$

Therefore we have necessarily (57).

Lemma 3: The curve $x = x_2(y)$, defined implicitly from $G_2(x, y) = 0$, verifies:

i) $$\lim_{y\to 0^+} x_2(y) = x_0 > 0, \quad (60)$$

where x_0 is the unique solution of the equation

$$x = \frac{1}{K_1}\left(\frac{\varsigma}{x} + K_2\left(\frac{T_0}{T_B} - 1\right) F_1\left(\delta\frac{\beta}{x}\right)\right), \ x > 0. \quad (61)$$

Moreover $x_0 > \frac{K_2}{K_1}\left(\frac{T_0}{T_B} - 1\right)$;

ii) $$\lim_{y\to+\infty} x_2(y) = 0. \quad (62)$$

Proof:

i) From $F_2(z) \cong \frac{\sqrt{\pi}}{2}\frac{1}{z}$, as $z \to 0^+$ and $G_2(x, y) = 0$ we obtain (60).
ii) Taking into account that $F_2(z) \cong \exp(-z^2)$ and $F_1(z) \cong \sqrt{\pi}z$ as $z \to +\infty$, from $G_2(x, y) = 0$ we obtain necessarily (62) to avoid any contradiction.

Theorem 4: If $\frac{T_A}{T_B} > 1 + E$ then there is at least one solution for the binary alloy solidification model (1)-(18).

Proof: By contradiction, we suppose that there is not any solution for system (42). Then, as a consequence of Lemma 1, Lemma 2 and Lemma 3 it must occur that for all (x, y) where $G_2(x, y) > 0$ it would be $G_1(x, y) < 0$. If we choose (x^*, y^*) so that $x^* = \left(\frac{T_A}{T_B} - 1\right) F_2(y^*)$ then we have $G_1(x^*, y^*) > 0$, for all $y^* > 0$ and $G_2(x^*, y^*) > 0$ for all $y^* > \tilde{y}$, where $\tilde{y}$ is the unique solution of the equation

$$H(x) = K_1(T_A - T_B)\, F_2(x), \quad x > 0,$$

where function H is defined by

$$H(x) = x + \frac{\varsigma}{(\frac{T_A}{T_B} - 1)F_2(x)} + K_2\left[\frac{T_0 - T_A}{T_B}\right] F_1\left(\delta\left(x + \frac{\beta}{(\frac{T_A}{T_B} - 1)F_2(x)}\right)\right),$$

which is an absurd. So, we can infer that there is at least one solution for system (42) and therefore the thesis holds.

III. Numerical results and discussion

The equations (40) and (41) are highly nonlinear and can be solved only numerically. For solving system of nonlinear equations, several iterative methods and their modifications are available in the literature [2]. The major difficulty with most of them is that we must know some good approximate value of the root. It is extremely difficult to find such an approximate root in the present problem. Further, iterative methods for non linear systems require complicated computer programs. In the absence of availability of such computer programs/packages a simple numerical procedure was adopted, which was found very effective also.

For a fixed value of σ_1, equation (40) can be solved for ω. By giving different values to σ_1, a curve in the (σ_1, ω) plane can be plotted. Similarly, another curve can be plotted for the equation (41). The intersection of these two curves gives the root of the nonlinear system consisting of equations (40) and (41). It may be noted $F_2(\sigma_1)$ could be very large if σ_1 is small and therefore it is advisable to multiply both the

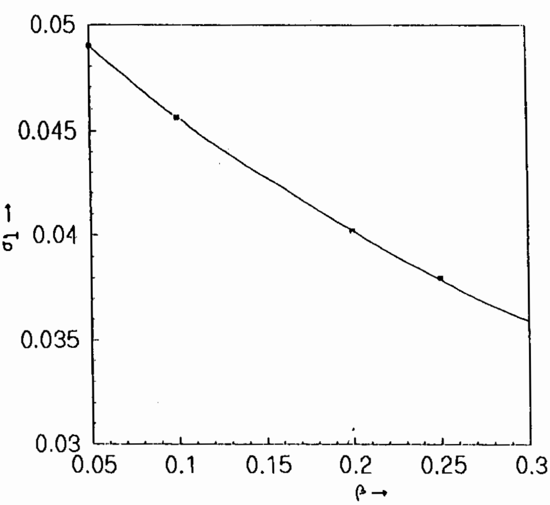

Fig. 2: σ_1 vs β. The parameters values are $\delta = 0.01$, $\varepsilon = 0.1$, $\nu = 1.0$, $m_1 = 0.4$, $m_2 = 0.6$, $C_0 = 0.1$, $D = 0.001$, $K_1 = 0.012$, $K_2 = 0.02$, $T_0 = 1.1$, $T_B = 0.8$

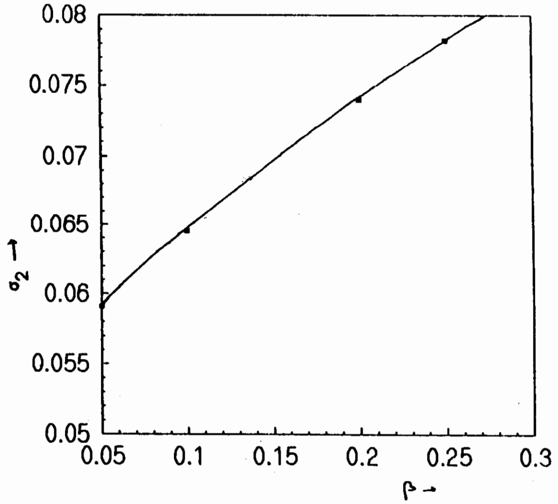

Fig. 3: σ_2 vs β. All parameters values as in fig. 2

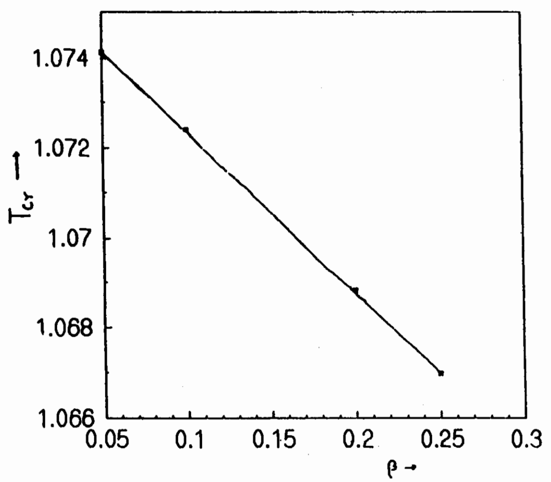

Fig. 4: T_{cr} vs β. All parameters values as in fig. 2

equations by $F_2(\sigma_1)$ before finding the roots. For finding the root of a single nonlinear equation, once again several iterative methods are available [2]. In the present work bisection method [2] was found to be very effective.

In figures 2, 3 and 4 we plot σ_1, σ_2 and T_{cr} as a function of the parameter $\beta = \gamma \frac{\sqrt{\pi}}{2}$. We observe that σ_1 and σ_2 are decreasing and increasing functions of the variable β respectively, i.e. the width of the mushy region is an increasing function of the variable β (or γ).

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