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Influence of Convection on Rod Spacing of Eutectics

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Abstract

The influence of convection on the concentration field in front of a growing rod eutectic was determined numerically for eutectic compositions of $W_e = 0.1$ and $W_e = 0.05$. The change in spacing λ between the rods with increasing intensities of convection was calculated assuming the eutectic grows at minimum interfacial undercooling. The spacing increases more or less linearly with the intensity of stirring.

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B.1 Introduction

Composites offer the unique advantage of being able to combine the properties of different components into one material. In-situ composites obtained by directional solidification of eutectics possess a high degree of thermal stability and strengths greater than their individual components.

Convection plays a significant role in determining the eutectic microstructure. MnBi-Bi [1,2] and InSb-NiSb [3] eutectics solidified in space showed a decreased spacing between the rods compared to earth processed samples grown at identical growth rates. Prior theoretical work on the effect of convection on the growth of lamellar eutectics predicted that the spacing between the lamellae increases with increasing convection [4,5]. Here we describe a three-dimensional model for the influence of convection on the microstructure of rod eutectics.

B.2 Model

The structure of a rod eutectic viewed normal to its interface is shown in figure 1. The rods are placed on the corners of a hexagon as assumed by Jackson and Hunt [6]. The computational domain is also shown. The domain is chosen to represent the smallest region which satisfies a periodicity condition.

Certain simplifying assumptions are made to reduce computational difficulties. It is assumed that the rods have a square cross-section. This facilitates the use of Cartesian coordinates to model the problem. Also, as in all prior theoretical work, it is implicitly assumed that the volumetric properties are the same in all the three phases. This results in the same numerical values for mass fraction, volume fraction and mole fraction. The interface is assumed to be planar.

The effect of convection is modelled by assuming a transverse flow U across the interface with a constant velocity gradient Gu=du/dy over the computational domain of interest. The direction of the velocity U and the domain are shown in figure 2.

Using the symbols defined at the end of the paper, the differential equation for continuity of mass at steady-state is

$$\frac{\partial^2 W}{\partial x^2} + \frac{\partial^2 W}{\partial y^2} + \frac{\partial^2 W}{\partial z^2} + \frac{V}{D}\frac{\partial W}{\partial z} - \frac{GuZ}{D}\frac{\partial W}{\partial x} = 0 \tag{B.1}$$

The boundary conditions are:

at $z = \lambda/2$, where λ is the spacing between the rods, $W = W_e$ (B.2)

at $z = 0$, and over the α phase, $D(dW/dz) = -V(W_i - W_s^\alpha)$ (B.3)

at $z = 0$, and over the β phase, $D(dW/dz) = -V(W_i - W_s^\beta)$ (B.4)

Higher values of z were tried for the far field boundary condition. With $z= \lambda$, W changed only in the 5^{th} decimal place after $z= \lambda/2$, and so we decided to use $z= \lambda/2$ for the far field boundary condition.

The computational domain represents a small section of a periodic array of rods. Thus it is assumed that the composition field repeats itself periodically in both the x and y directions,

$$W_{x=0} = W_{x=\lambda} \tag{B.5}$$

and

$$W_{y=0} = W_{y=\sqrt{3}\lambda} \tag{B.6}$$

We assume negligible solid solubility and hence $W_s^\alpha = 1.0$ and $W_s^\beta = 0.0$. The differential equation is non-dimensionalized to reduce the number of variables to two for a fixed eutectic composition. The scaling variables are similar to that used by Baskaran and Wilcox [4], $X = x/\lambda$ and $Y = y/\lambda$. The non-dimensional equation is

$$\frac{\partial^2 W}{\partial X^2} + \frac{\partial^2 W}{\partial Y^2} + \frac{\partial^2 W}{\partial Z^2} + \Lambda \frac{\partial W}{\partial Z} - \Gamma Z \frac{\partial W}{\partial X} = 0 \tag{B.7}$$

where $\Lambda = \lambda V/D$ is a rod spacing based Peclet number and $\Gamma = Gu\lambda^2/D$ is the dimensionless convective velocity gradient at the interface. The boundary conditions are:

$$\text{at } Z = 1/2, \; W = W_e \tag{B.8}$$

$$\text{at } Z = 0, \text{ over the } \alpha \text{ phase, } D(dW/dZ) = \Lambda W_i \tag{B.9}$$

$$\text{at } Z = 0, \text{ over the } \beta \text{ phase, } D(dW/dZ) = \Lambda(W_i - 1) \tag{B.10}$$

and the periodicity conditions in the x and y directions,

$$W_{X=0} = W_{X=1} \tag{B.11}$$

$$W_{Y=0} = W_{Y=\sqrt{3}} \tag{B.12}$$

A central finite difference method is used to solve the differential equation. A variable mesh size is used in the x and y directions. This is necessary to ensure that the phase boundaries coincide with a mesh line. This enables taking care of the mathematical singularity that arises at the three phase junctions. The composition of the solid phase at the phase boundary is taken to be an average composition of the α and β phases.

The parameter of importance to fiber spacing is the average concentration of the interfacial liquid over each of the solid phases. Numerically this is done by averaging the concentration at a mesh point over an area formed by traveling half the grid space in the x and y directions. The average concentration over the entire α and β phases is then calculated.

B.3 Results

A plot of the computed isoconcentration lines at the interface for an eutectic composition of $W_e = 0.1$ growing without the disturbing influence of convection is shown in figure 3a. The rods appear rectangular in these plots due to the unequal scales for the axes. Convection distorts the contours and the effect of convection with an intensity $\Gamma = 250$ is shown in figure 3b. The corresponding isoconcentration lines for an eutectic composition of $W_e = 0.05$ is shown in figures 4a and 4b.

To account for the influence of convection on the spacing between the rods, Jackson and Hunt's [6] analysis is modified to include a perturbation in the concentration field Δ due to convection. Thus the perturbation in the concentration field in the α and β phases are,

$$\Delta_\alpha = (\bar{W}_{i\alpha} - W_e)_o - (\bar{W}_{i\alpha} - W_e) \tag{B.13}$$

$$\Delta_\beta = (\bar{W}_{i\beta} - W_e)_o - (\bar{W}_{i\beta} - W_e) \tag{B.14}$$

In the absence of convection the deviation of the average interfacial composition from the eutectic is proportional to $\Lambda = \lambda V/D$,

$$(\bar{W}_{i\alpha} - W_e)_o = A_\alpha \Lambda \tag{B.15}$$

$$(\bar{W}_{i\beta} - W_e)_o = A_\beta \Lambda \tag{B.16}$$

The values of A_α and A_β from the analytical solution of Jackson and Hunt [6] for circular rods are:

$$A_\alpha = 2M \tag{B.17}$$

$$A_\beta = \frac{-2(1 - W_e)M}{W_e} \tag{B.18}$$

$$\text{where } \mathrm{M} = \sum_{n=1}^{\infty} \left(\frac{\mathrm{J}_1^2(\mathrm{n}\pi(1 - \mathrm{W}_e)^{1/2}}{\mathrm{J}_0^2(\mathrm{n}\pi)} \right) \tag{B.19}$$

In the above equation J_0 and J_1 are Bessel functions.

Further analysis is similar to that developed by Baskaran and Wilcox [4] for lamellar eutectics. Numerical results show that Δ is independent of Λ Thus

$$\Delta = \Lambda f(\Gamma) \tag{B.20}$$

The numerical solution for $\Gamma = 0$ (no convection) and $\Lambda = 0.05$ was compared with the analytical solution. The average concentration over the α phase (rods) for an eutectic composition of $W_e = 0.1$ was calculated to be 0.10049 which compares well with the analytical solution of $\bar{W}_{i\alpha} = 0.10025$, an error of 0.2%. The calculated average concentration over the β phase (matrix) is 0.09577 compared to the analytical solution of $\bar{W}_{i\beta} = 0.09775$, an error of 2%. The average composition for the other eutectic composition investigated, $W_e = 0.05$, is also very nearly identical to that calculated analytically. The difference between the calculated and analytical values of deviation from the eutectic composition, $(\bar{W}_i - W_e)$ is high. For $W_e = 0.1$ the calculated value of the deviation from the eutectic composition over the α phase is 0.00049 and the analytical value is 0.00025. Over the β phase the values of the calculated and analytical deviations from the average compositions are 0.00423 and 0.00225 respectively. This deviation from the analytical results is due to 1) assuming a square cross-section of the rods and 2) placing the rods on the corners of a hexagon rather than on a circle as done by Jackson and Hunt [6].

The change in undercooling with increasing convection was calculated using equation 14 in Chandrasekhar et al.ś paper [5]. The result is shown in figure 5. A least squares fit yields for $W_e = 0.1$:

$$g/2 = 1 - 0.000583\Gamma_o, \quad r^2 = 0.999 \tag{B.21}$$

and for $W_e = 0.05$

$$g/2 = 1 - 0.0004\Gamma_o, \quad r^2 = 0.998 \tag{B.22}$$

where r is the correlation coefficient.

The effect of convection on spacing is calculated using equation 21 from Baskaran and Wilcox's paper [4]. The result is shown in figure 6. A least square fit yields for $W_e = 0.1$:

$$\lambda/\lambda_o = 1 + 0.002404\Gamma_o, \quad r^2 = 0.999 \tag{B.23}$$

and for $W_e = 0.05$,

$$\lambda/\lambda_o = 1 + 0.001531\Gamma_o, \quad r^2 = 0.997 \tag{B.24}$$

It is interesting to compare the results of this computation with those of our earlier work [5] for lamellar eutectics. The spacing between lamellae for eutectic compositions of 0.30 and 0.50 increases with the square of the stirring intensity. For an eutectic composition of 0.10 the change in spacing of lamellae is given by [5]:

$$\lambda/\lambda_o = 1 + 8.9 \times 10^{-4}\Gamma_o^{1.32} \tag{B.25}$$

The change in spacing for a rod eutectic of the same composition, $W_e = 0.1$, is given by equation (23). A comparison is shown in figure 7.The change in spacing is less for rod eutectics than for the lamellar eutectics for a given value of Γ_o.

An important motivation for this work was to estimate the effect of natural convection on spacing of rod eutectics. The value of Γ_o computed for a typical experimental set-up [7] is 6.5×10^{-3}. For this value of Γ_o, $\lambda \approx \lambda_o$. Thus natural convection is not predicted to change the spacing by perturbing the concentration field ahead of the growing eutectic interface.

B.4 Conclusions

1. The spacing between the rods increases with an increase in convection.

2. The effect of convection on spacing decreases with decrease in the eutectic composition.

B.5 Acknowledgement

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Nomenclature

A_α, A_β	=	Constants
D	=	Diffusion Coefficient in the melt (m^2/s)
Gu	=	Gradient of transverse velocity near interface $(du/dz)_o$ $(s^{-1}$
r_α, r_β	=	Radius of the α and β phases respectively, defined by [6] (m)
U	=	Melt velocity parallel to the interface (m/s)
V	=	Freezing Rate (m/s)
W	=	Mass fraction of component A in the melt
W_e	=	Eutectic mass fraction
W_i	=	Interfacial melt composition
$\bar{W}_i$	=	Average interfacial melt composition
W_s^α	=	Composition of the α phase (the rods, assumed 1.0 here)
W_s^β	=	Composition of the β phase (the matrix, assumed 0.0 here)
x,y	=	Distances along the solid interface (m)
X,Y	=	Dimensionless distances along the solid interface, x/λ and y/λ
z	=	Distance into the melt from the interface (m)
Z	=	Dimensionless distance into the melt from the interface, z/λ
Γ	=	$Gu\lambda^2/D$, Dimensionless convective velocity at the interface
Γ_o	=	$Gu\lambda_o^2/D$
λ_o	=	Value of λ at Gu=0
λ	=	Spacing between the rods (m)
Λ	=	$\lambda V/D$ Freezing rate based Peclet number

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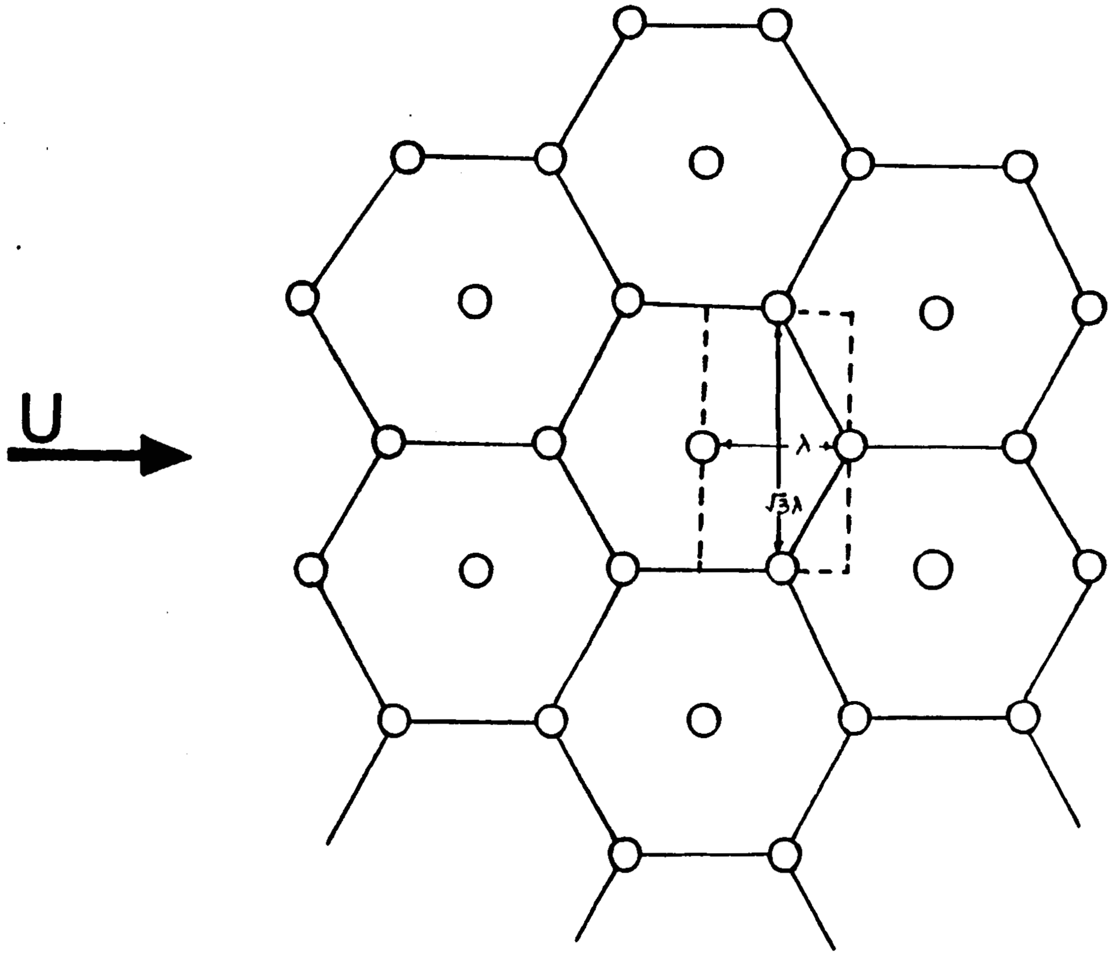
- Figure 6: The ratio of the minimum undercooling with convection to that without convection, g/2, versus $\Gamma_o = \Gamma/(\lambda/\lambda_o)^2$.

- Figure 7: The ratio of rod or lamellar spacing with convection to that without convection, λ/λ_o, versus $\Gamma_o = \Gamma/(\lambda/\lambda_o)^2$.



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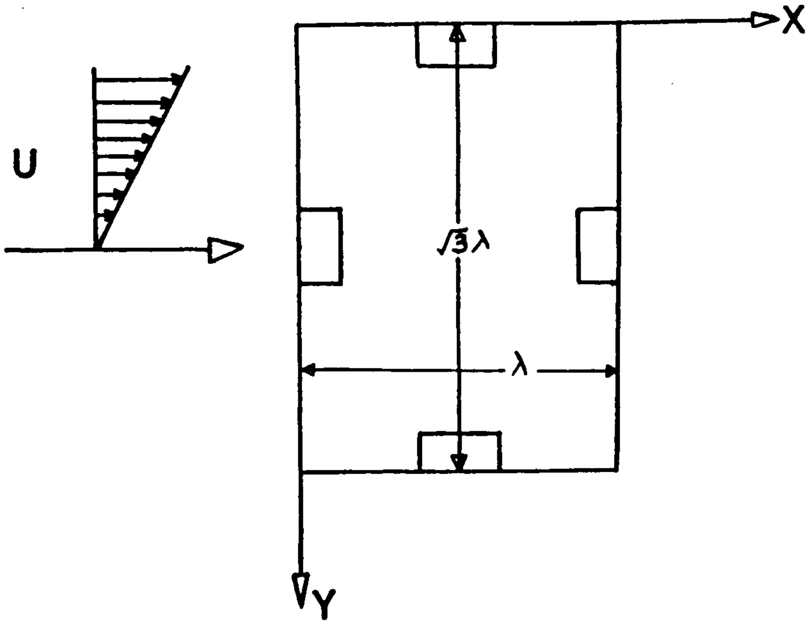

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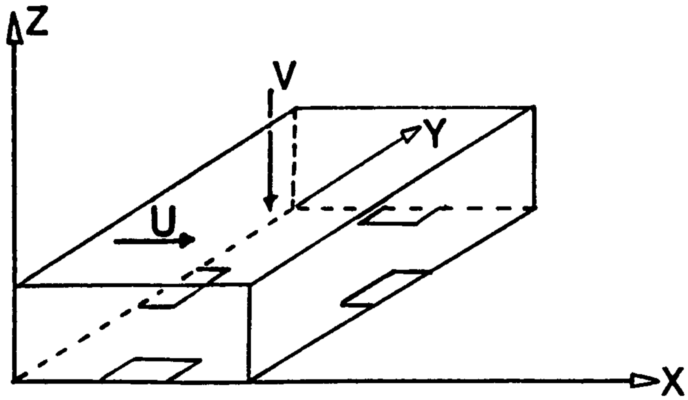

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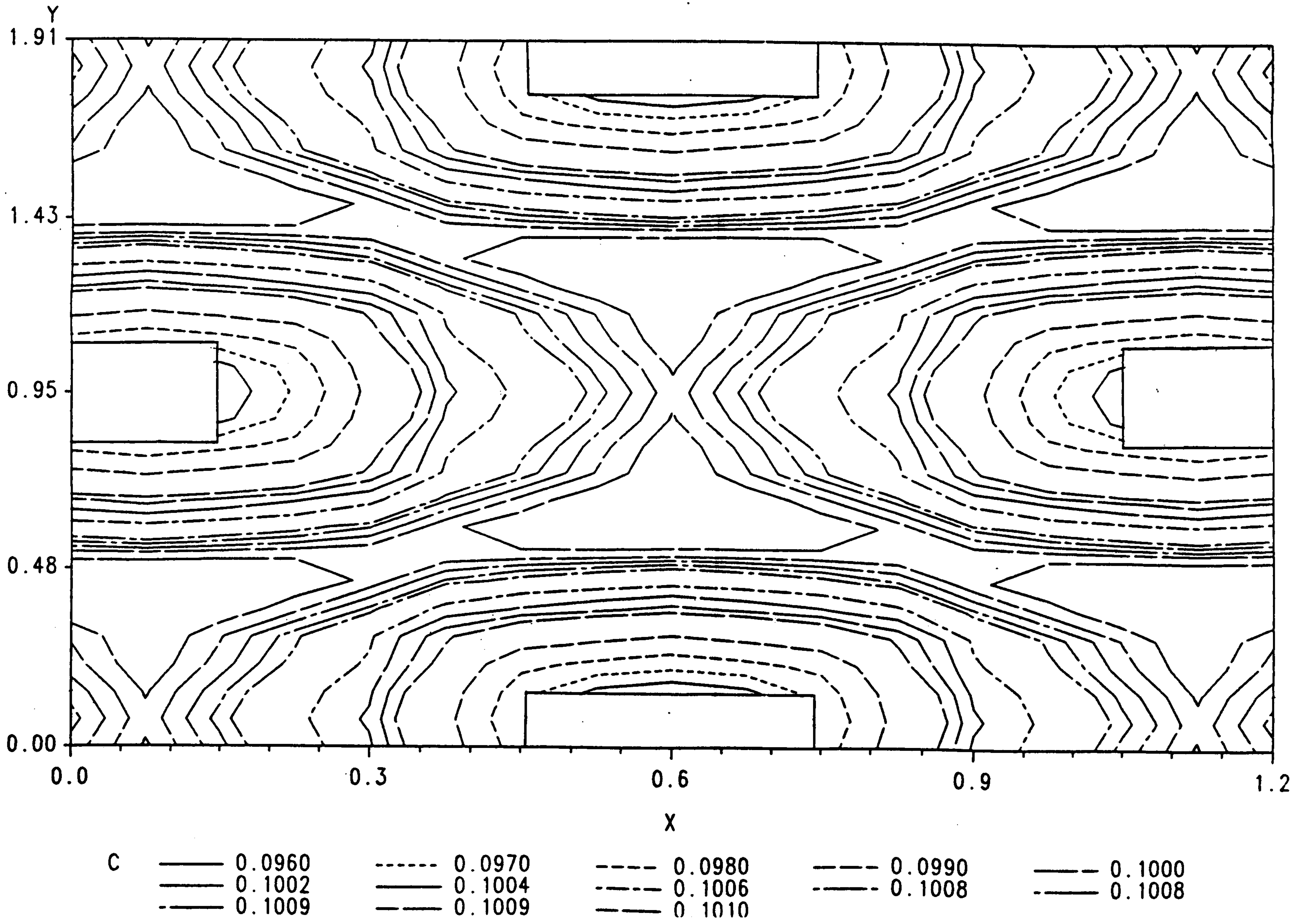
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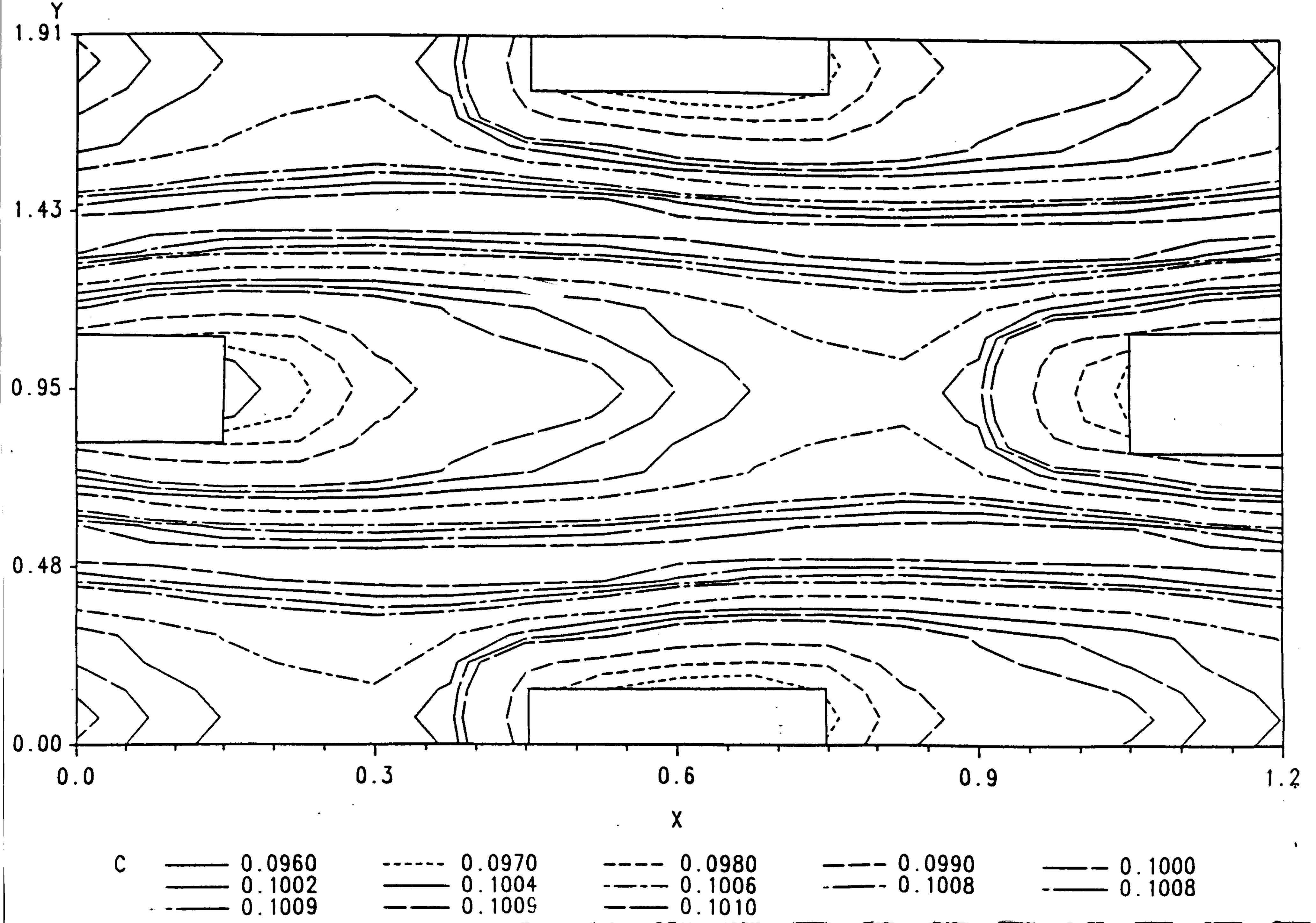

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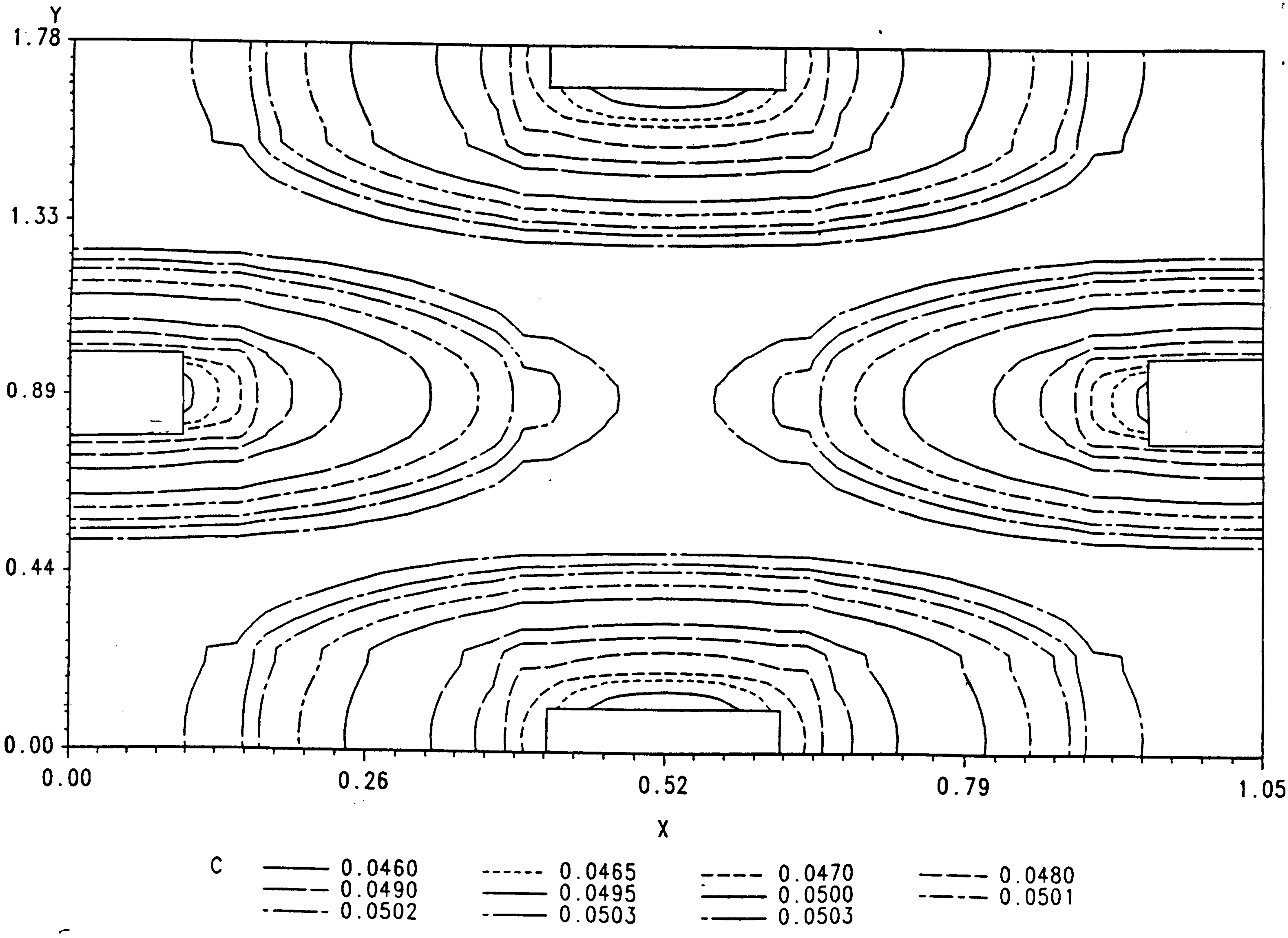
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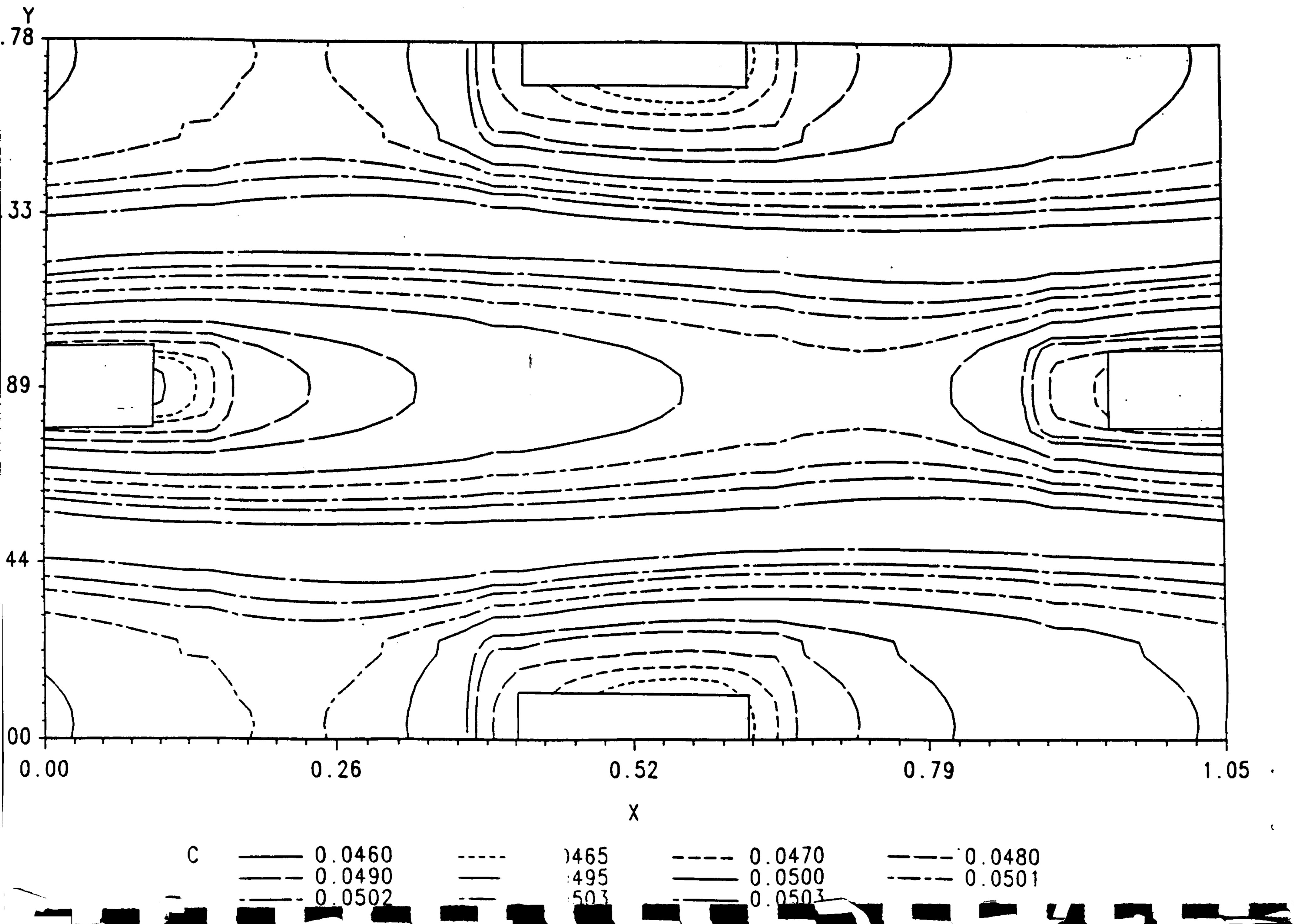

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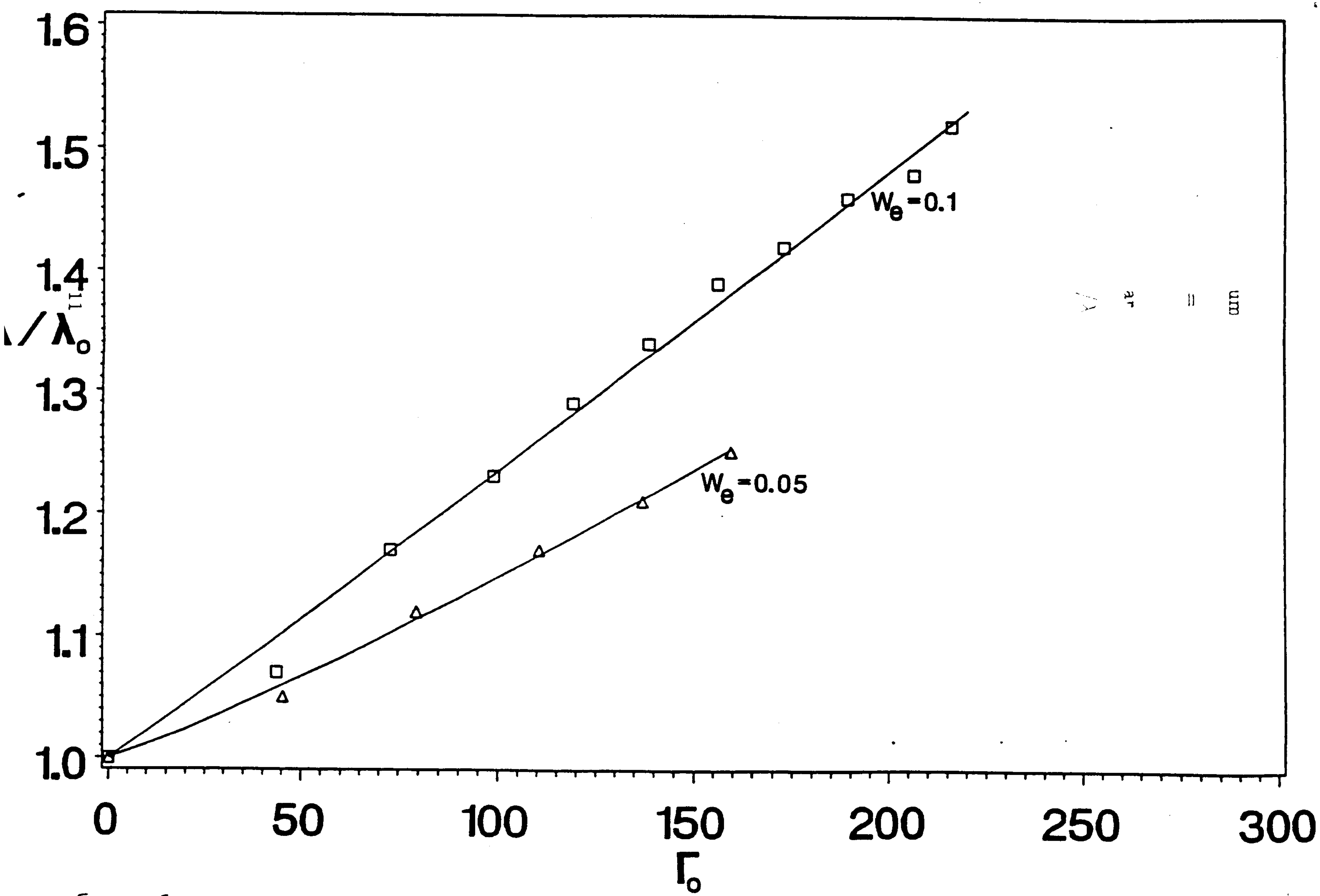

$W_e = 0.1$
$W_e = 0.05$
Γ_o
λ_o
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100
150
200
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300
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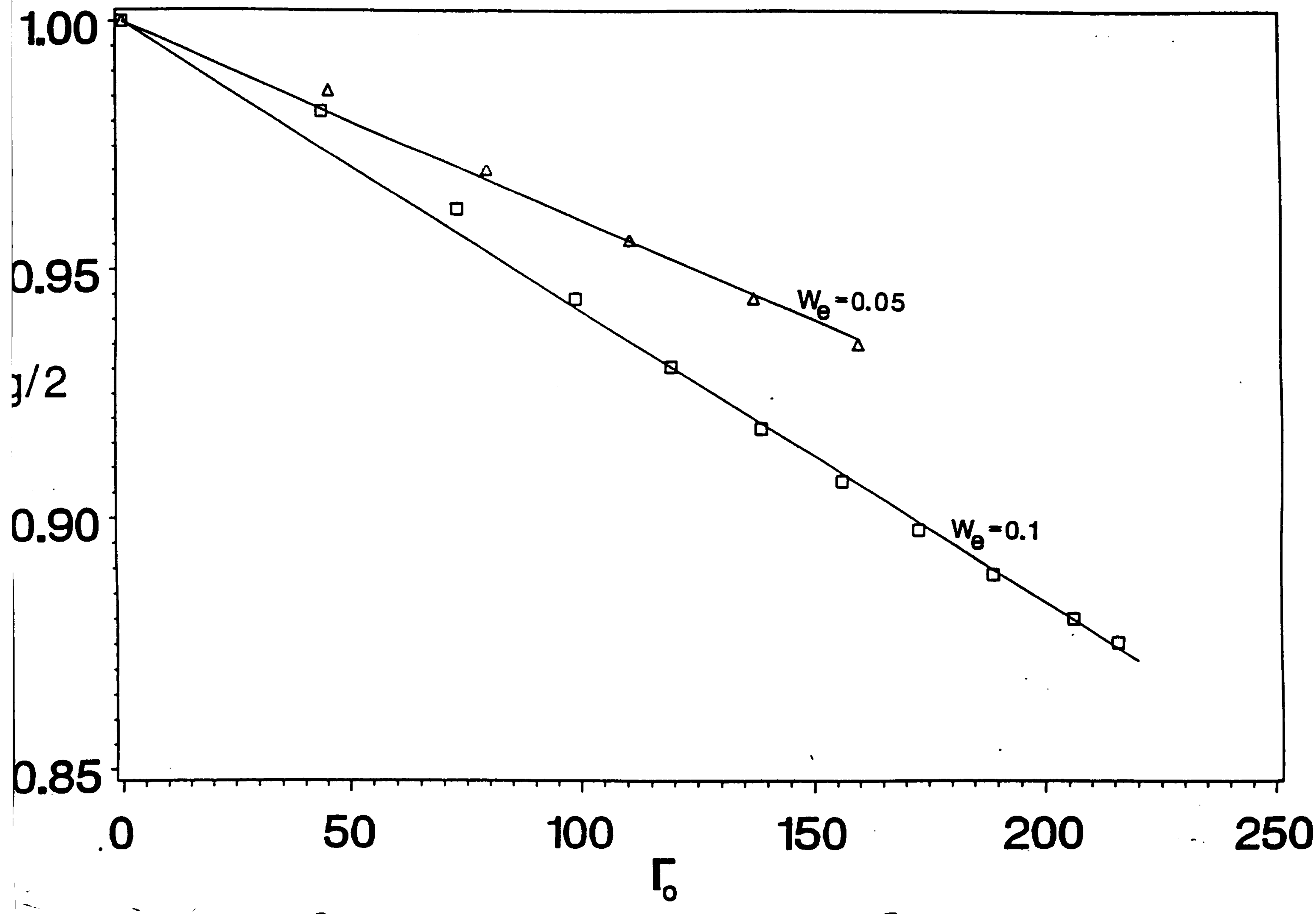
1.3
1.4
1.5
1.6

F. 5



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Γ_o
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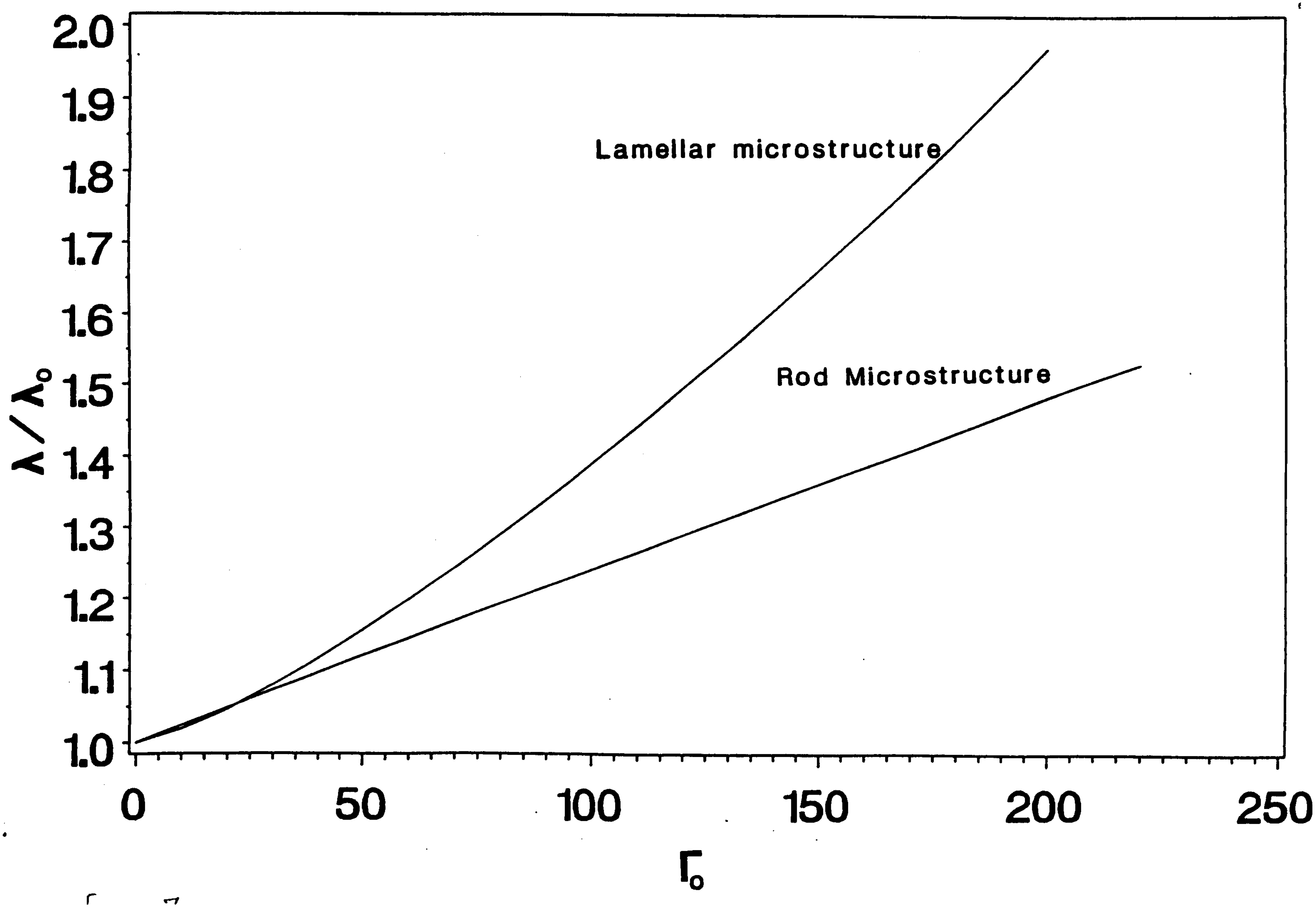
Lamellar microstructure
Rod Microstructure
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1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
λ / λ_o
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100
150
200
250
Γ_o