A B 59, B 1 B A 199

Molecular-dynamics simulation of dire wth of binary mixtures

Departamento de Física, Instituto de Ciências Exatas, Un eral de Juiz de Fora, Juiz de Fora, MG,
CEP 36036-

Departamento de Física, ICEx, UFMG, Be MG, CP 702, 30123-970, Brazil
( )

. [0163-1829(9]

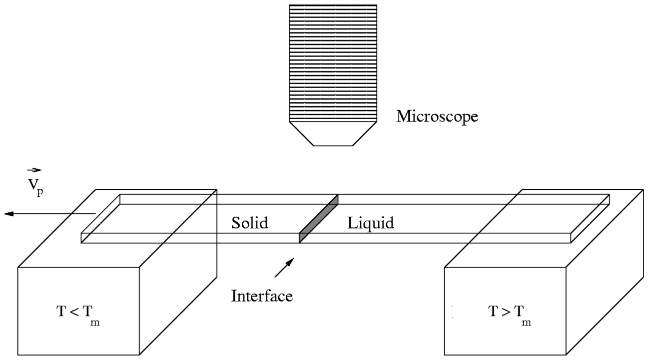
I. INTRODUCTION

. , . . , , . A . .[1,2] , - . , . .[3] A (, ,) , ( ), , , , . : ( ) ; ( ) ; ( ) . , . , . - B . ,

(-), - .[4,5] - . . A - ( ) . .[6] - , .[1,2] - - (a) (b) - ( ) . : $\Phi_{a,a}$, $\Phi_{b,b}$, $\Phi_{a,b}=\Phi_{b,a}$ . . B , ( ) - . , - ( ) 0.1. - - , . - . . . . . . , . - .

II. DIRECTIONAL GROWTH OF BINARY MIXTURES

- .[7] , , ,



. 1. B (-). . T_m .

, - -

, .[4,5]

. 1.

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, $2d$

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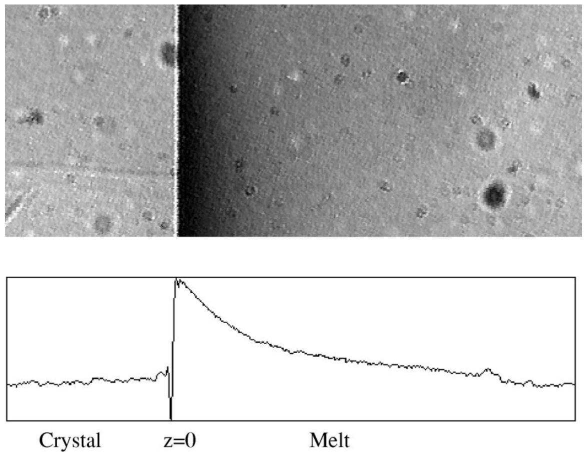

. 2. -

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A. Binary phase diagram

A ( ) -

( ) , ,

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( )

. K

(c_S) (c_L),

$K = c_S / c_L < 1$.

σ_{ab} , -

,

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σ_{ab}

σ_{ab} K.

$K<1$. 3.

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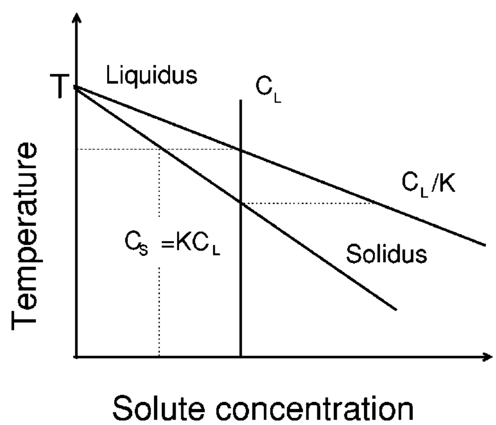
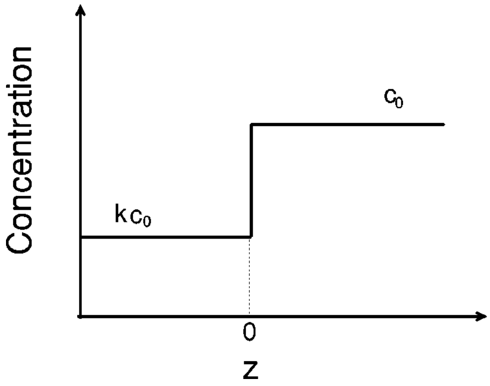


. 3. -

, $K<1$.



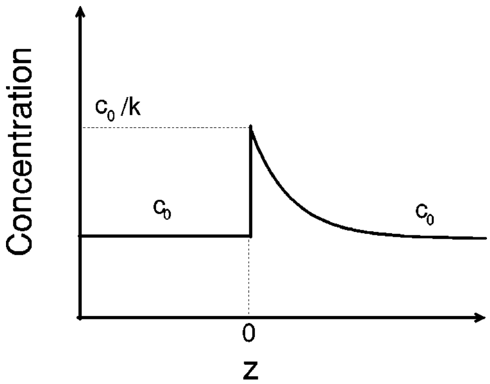
. 4. - , c_0 $K<1$.

- , . m m', , K $K=m/m'$.[2] . 4 - - c_0 - $c_S=Kc_0$. , . - (. 5), .

B. Solute transport

- , x z, , t z.

, - - , (V_s) (V_p) . - - - -



. 5. - - - $K<1$.

, . , - . , (V_s) (V_f). , , , $J_s=\rho_s\times V_s$ $J_f=\rho_f\times V_f$ $J_s=J_f$, $V_f=V_s\times\rho_s/\rho_f$, J_s,ρ_s J_f,ρ_f , . A $V_s=V_p$

$$V_f=V_p\times\rho_s/\rho_f. \tag{1}$$

, . , . - (V_s) (c_f) :[7]

$$\frac{\partial c_f}{\partial t}=D\frac{\partial^2 c_f}{\partial z^2}+V_f\frac{\partial c_f}{\partial z}, \tag{2}$$

D V_s V_f . (2) : ( ) $c_f=c_0$ z = , ( ) $(1-K)V_fc_f=-D\,dc_f/dz$ $z=0$. - ( ) . A V_s V_f $V_s=V_p$. :

$$c_L(z)=c_0\left[1-\left(\frac{1-K}{K}\right)\quad\left(-\frac{V_fz}{D}\right)\right]$$
$$=c_0\left[1-\left(\frac{1-K}{K}\right)\quad\left(-\frac{V_p\rho_sz}{\rho_fD}\right)\right], \tag{3}$$

. (1). A , c_0. . 5 - .

. 2. - . . A $l_D=D\rho_f/V_p\rho_s$. - ( ) , z l_D.

III. SIMULATION

- .

$$\Phi_{i,j}(r_{i,j})=\begin{cases}\phi_{i,j}(r_{i,j})-\phi_{i,j}(r_c)-\left(\dfrac{d\phi_{i,j}(r_{i,j})}{dr_{i,j}}\right)_{r_{i,j}=r_c}(r_{i,j}-r_c) & r_{i,j}<r_c\\ 0 & r_{i,j}>r_c,\end{cases}$$

$\phi_{i,j}(r_{i,j})$ (12-6) :

$$\phi_{i,j}(r_{i,j})=\epsilon_{i,j}\left[\left(\frac{\sigma_{i,j}}{r_{i,j}}\right)^{12}-\left(\frac{\sigma_{i,j}}{r_{i,j}}\right)^{6}\right]. \quad (4)$$

i j $\mathbf{r}_i$ $\mathbf{r}_j$, , $0\leqslant i,j\leqslant N$, N $r_{i,j}=|\mathbf{r}_i-\mathbf{r}_j|$. A $r_c=2.5\sigma_{aa}$ - .

,

N. - .

$\phi(r_c)$. A $(d\phi/dr)_{r=r_c}(r-r_c)$. , $2N$

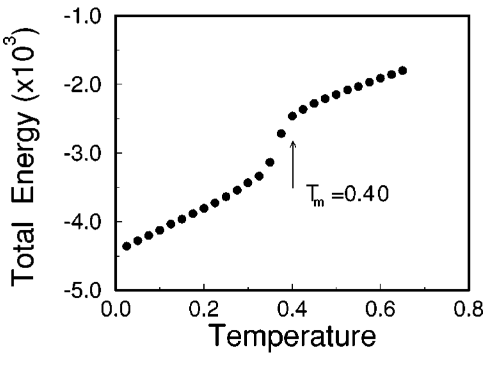
$\Delta t=0.02\sigma_{aa}(m_a/\epsilon_{aa})^{1/2}$. - B .

.[10]

$r_v=3\sigma_{aa}$. A , , .

. $c_x\times c_z=(3.5\sigma_{aa})^2$, .

$N=n_x\times n_z=27\times 270$ - $L_x\times Ł_z=27\times 2^{1/6}\times 451\sigma_{aa}^2$. x . z - , . 27 $\times 30$. ρ



. 6. .

$=0.5\sigma_{aa}^{-2}$, 27×240 , - .

.[10] z : $-210\sigma_{aa}\leqslant z\leqslant -231\sigma_{aa}$, $T_0=0$, $80\sigma_{aa}\leqslant z \leqslant 220\sigma_{aa}$, T_h, T_m . 1.2×10^5 Δt, . - $-z$, $v_p=4\times 10^{-3}(\epsilon_{aa}/m_{aa})^{1/2}$. z_{min} , . z_{min} z_{max} - . T_m - 1.5×10^3 $0.5\sigma_{aa}^{-2}$, - . . 6. T_m $=0.40\times\epsilon_{aa}/k_B$.

A. Units

: (a) (b). , - (b-b), - (a-a), - (b-a). $c_0=5\%$.

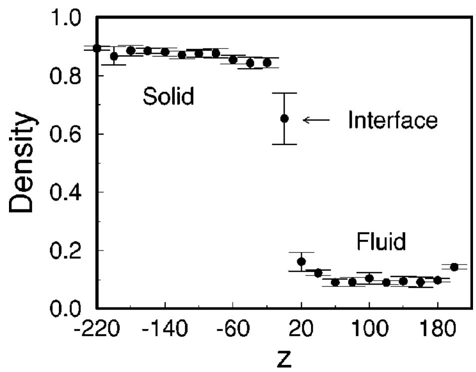
.

$\Delta z=20\sigma_{aa}$ ( ). A - ,

ϵ_{aa}, σ_{aa} m_a, $\epsilon_{ab}=0.5$, $\epsilon_{bb}=0.1$, $\sigma_{ab}=\sigma_{bb}=\sigma_{aa}=1$, $m_b=m_a=1$. A , - ϵ_{aa}/k_B $(m_a\sigma_{aa}^2/\epsilon_{aa})^{1/2}$, .

IV. RESULTS

. - 5.7 , . 7. V_p , , $\sim D/V_f^2=D/V_p^2(\rho_s/\rho_f)^2$. D ρ_f/ρ_s, $(\rho_f/\rho_s)^2$,



. 7. . -
5.7 .

δt .
$\rho_{f1}=0.7$ ( ) $\rho_{f2}=0.15$ ( ) ,
, $D_1\approx 0.1$ $D_2\approx 1.2$. $\delta t_2/\delta t$
$\sim D_2(\rho_{f2})^2/D_1(\rho_{f1})^2\sim 0.55$, ρ_s V_p ,
2
6. A
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, . B. -
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. (3).

A. Interface structure for pure material

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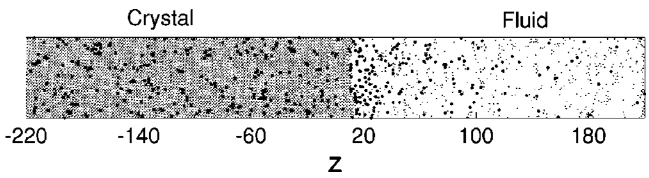
A -
. A. .[2] -



. 8.
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. A
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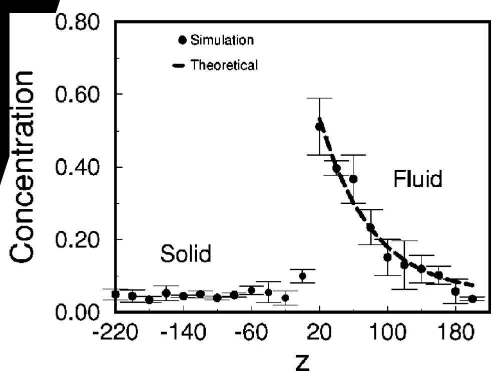

. 9. .
$z\approx 0$.
.

, α $\alpha=\xi L/k_b T_m$,
L ,
T_m , k_B
B , ξ
. $\alpha>2$, α
<2 . -
- -
. $\alpha<1$
. -
.
- α 1.

. 6
$L=0.59$
$T_m=0.40$. - -
(0,1), $\xi=2/3$. $k_B=1$
$\alpha=0.98$, . , -
-
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B. Solute concentration proÞle

-
$c_0=5\%$,
$V_p=0.004$. A
- . 8.
A
- -
. 9 (
. 2).
A .
(3) .
$K=0.094\pm 0.005$ $l_D=60$
± 5. . (3), $\rho_s/\rho_f=5.7$ $V_p=0.004$, -
$D=1.4\pm 0.1$.
D $\langle r^2\rangle=4Dt$, r
b t .
$D=1.3\pm 0.1$. B D
- -
. ,
- -
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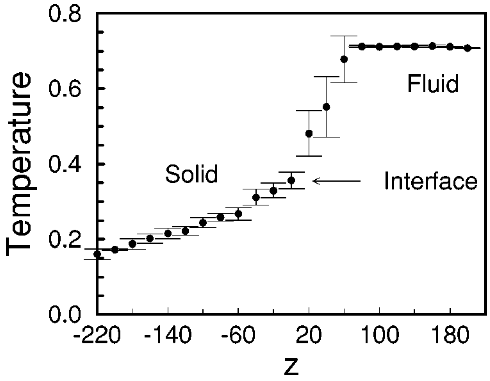


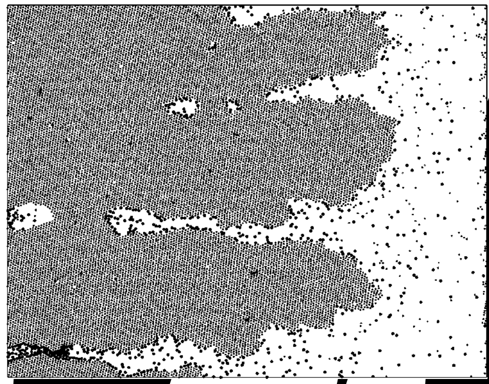
. 10. . A $z<-220$ $T=0$ $80\leqslant z\leqslant 220$ $T=0.70$.

C. Thermal length and cellular instability

. 10. ~ 0.35. 0.40. $mC_0\sim 0.40-0.35=0.05$. $l_T=mc_0(1-K)/KG$,[7] $K\approx 0.1$, $G\approx 0.005$ - $l_T\sim 20$. B $l_D\gg l_T$, . ., . B K V_p l_T $>l_D$. 11. A - .

V. CONCLUSIONS

B - . -



. 1 a,b . - . . . . .

ACKNOWLEDGMENTS

A , , A . A A , , , .

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