

Cr (III)

1. ... (...) : 05.17.05. / ... , 1987. – 360 . 2. / ... , 1981. – . 446 – 452.
3. ... // – 1977. – . 42. – 6. – . 628 – 632. 4. / ... , 1975. – 272 . 5. Becke A.D. Density-functional exchange-energy approximation with correct asymptotic behavior // Phys. Rev. – 1988. – A. 38. – P. 3098 – 3100. 6. Lee C., Yang W., Parr R.G. Development of the Colle-Salvetti correlation-energy formula into a function of the electron density // Phys. Rev. – 1988. – B. 37. – P. 785 – 789. 7. Becke A. D. Density-functional thermochemistry. III. The role of exact exchange // J. Chem. Phys. – 1993. – Vol. 98. – . 5648 – 5652. 8. Hay P.J., Wadt W.R. Ab initio effective core potential for molecular calculations // J. Chem. Phys. – 1985. – Vol. 82. – P. 270 – 310. 9. Frisch M.J., Trucks G.W., Schlegel H.B. et al. Gaussian 92/DFT, Revision G.2 / Gaussian Inc. – Pittsburgh: PA, 1993. 10. “GAUSSIAN”: [...] /] . – : . . - . , 2003. – 88 .

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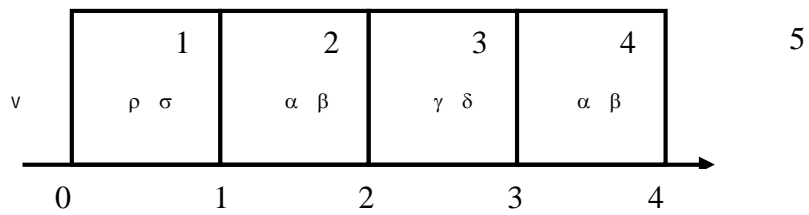
A generalised task on making multilayer diffusion silicide coatings is formulated. The equations to calculate parameters of phase formation and redistribution are given, e.g. co-ordinates of interphase boundaries and speed of these boundaries' dislocation. The boundary conditions for these equations are found.

[1 – 5].

[6 – 9].

($A -$), $X_x A_u$
 $($ $-$ $)$, v ($$
 $$, v
 $($ $. 1)$.

$r s$, $X_x A_u$, $ru - xs > 0$. $($ $1 - 4)$
 $(0 - 4)$. 1.



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[10].

1 – 5

$$(r + s - 1)X_r A_s \leftrightarrow rX_r^- A_s + X_r A_s^- \quad (5)$$

$$2, 3 \quad X_r A_s^- + X_x A_u \leftrightarrow X_r A_s + X_x A_u^- \quad (6)$$

$$X_r^- A_s + X_x A_u \leftrightarrow X_r A_s + X_x^- A_u \quad (7)$$

$$rX_x A_u + (ru - xs)X_r A_s^- \leftrightarrow (x + ru - xs)X_r A_s \quad (8)$$

$$sX_x A_u \leftrightarrow (xs - ru + u)X_r A_s + (ru - xs)X_r^- A_s \quad (9)$$

$$4 \quad X_r^- A_s + X \leftrightarrow X_r A_s + X^- \quad (10)$$

$$rX + (s - 1)X_r A_s \leftrightarrow sX_r A_s^- \quad (11)$$

$$X \leftrightarrow X - X^- \quad (12)$$

$$X_r A_s \leftrightarrow X_r A_s^- + A \quad (13)$$

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[10].

$$C_1^0 = P_{..v}^{\dagger} E^{KT} \left\{ \frac{1}{..v} X \frac{1}{...} \mathbb{E}_1 \right\}; \quad \sim_0 = \frac{1}{v} \left\{ \frac{1}{v} \mathbb{E} \right\};$$

$$\frac{1}{2} = \frac{1}{1} e^{\frac{1}{\{---\}_1}} = \frac{1}{1} f; \quad \left(\frac{1}{1} \right)^{\sim} (\tilde{1})^{\dagger} = \left(\frac{0}{1} \right)^{\sim} (\tilde{0}) = g;$$

$$\left(\begin{smallmatrix} *1 \\ 2 \end{smallmatrix} \right)^r \left(\frac{1}{2} \right)^{\sim} = e^{-\frac{1}{\{-+r\mathbb{E}^*+s\mathbb{E}\}}}; \quad \frac{2}{2} = \frac{3}{4} = = e^{\frac{1}{\left\{ \frac{x-r}{ru-xs} \mathbb{E} \right\}}}; \quad (14)$$

$$\frac{3}{3} = \frac{2}{3} = e^{-\frac{1}{\chi\Gamma - \chi S} \{ \chi - \Gamma - \mathbb{E}_3 \}}; \quad \frac{*2}{2} = \frac{*3}{4} = e^{-\frac{1}{\Gamma U - \chi S} \{ S - 3 - U - \mathbb{E}_3^* \}};$$

$$\frac{*3}{3} = \frac{*2}{3} = e^{-\frac{1}{\Gamma U - \chi S} \{ S - 3 - U - \mathbb{E}_3^* \}}; \quad \frac{4}{4} = e^{-\frac{1}{S} \{ \Gamma - \dots - \mathbb{E} \}};$$

$$\frac{*4}{4} = e^{-\frac{1}{\dots} \{ \dots + \mathbb{E}_5^* \}}; \quad \hat{C}^4 = e^{-\frac{1}{S} \{ \dots - \Gamma - 5 - \hat{\mathbb{E}} \}}; \quad \frac{*4}{5} = e^{-\frac{1}{\dots} \{ \dots + \mathbb{E}_5^* \}};$$

$$\frac{*}{5} / \dots = \frac{*}{0}; \quad \hat{C} / \dots = 0$$

$$\dot{G}^I(t) -$$

$$I_k^I(t) -$$

$$dt, \quad J_1^0 dt + C_1^0 |dG_1^0|.$$

(1)

$$\frac{\dots - 1}{\dots} [J_1^0 dt + C_1^0 N |dG_1^0|];$$

$$(1), \quad \dots V,$$

$$(\dots - I)V \ll \dots \gg,$$

$$|dG_1^0| = (1 - \frac{\dots - 1}{\dots}) [J_1^0 dt + C_1^0 N |dG_1^0|] \cdot \check{S}_1;$$

$$J_1^0 \check{S}_1 = -(\dots - C_1^0) \dot{G}_1^0;$$

$$D_1 \frac{\partial C_1}{\partial} = \dots G_1^0.$$

$$, \quad (2) \quad (\quad) \quad .$$

$$\dots \ddagger, \quad \tilde{j}, \quad (4)$$

$$r \ s \quad (5). \quad j^*, \quad :$$

$$\frac{\ddagger}{\dots + \ddagger - 1} \tilde{j} dt = \tilde{C}_1^1 N_1 dG_1^1 - \tilde{J}_1^1 dt ;$$

$$J_1^1 dt + \frac{\dots}{\dots + \ddagger - 1} \tilde{j} dt + \frac{S}{r + s - 1} j^* dt = J_2^1 dt + C_1^1 N_1 dG_1^1 + C_2^1 N |dG_2^1| ;$$

$$, \quad dt \quad (4)$$

$$\frac{\ddagger}{\dots + \ddagger - 1} \tilde{j} dt \quad , \quad (-\tilde{J}_1^1 dt),$$

$$\ll \quad \gg \quad ,$$

$$dG_1^1 (\tilde{C}_1^1 N_1 dG_1^1).$$

$$(J_1^1 dt) \quad (4) \quad (5),$$

$$\frac{\dots}{\dots + \ddagger - 1} \tilde{j} dt \quad \frac{S}{r + s - 1} j^* dt, \quad (J_2^1 dt)$$

$$(C_1^1 N_1 dG_1^1 + C_2^1 N |dG_1^1|).$$

$$dG_1^1 = \left(\frac{\ddagger}{\dots + \ddagger - 1} + \frac{\dots}{\dots + \ddagger - 1} - 1 \right) \tilde{j} dt \tilde{S}_1 = \frac{\tilde{j} dt \tilde{S}_1}{\dots + \ddagger - 1} \quad \left| dG_2^1 \right| = \frac{j^* dt \tilde{S}}{r + s - 1}.$$

$$, \quad dG_1^1 \quad (4), \quad dG_2^1 - \quad -$$

$$(5), \quad (3)$$

$$. \quad dG_1^1, \quad , \quad -$$

$$\dots \ddagger \quad dt$$

$$, \quad , \quad .$$

$$, \quad \dots \ddagger$$

$$(4) \left(\frac{\dots}{\dots + \dagger - 1} \tilde{j} dt + \frac{\dagger}{\dots + \dagger - 1} \tilde{j} dt \right)$$

« » $\tilde{j} dt$, .

$$= G_2^1(t) \quad :$$

$$D^* \frac{\partial C_2^*}{\partial} = r \dot{G}_2^1$$

$$N_1 \left\{ -D_1 \frac{\partial C_1}{\partial} + \frac{\dots}{\dagger} \tilde{D} \frac{\partial \tilde{C}}{\partial} \right\} = N \left\{ -D \frac{\partial C_2}{\partial} + s G_2^1 \right\} \quad (15)$$

$$V_{ik}(t) \quad \bar{i} \quad -$$

$$V_{1,2} = \dot{G}_2^0 - \dot{G}_1^0 = \dot{G}_2^1 - \dot{G}_1^1 = \dot{G}_2^1 - \frac{1}{\dagger} \tilde{D} \frac{\partial \tilde{C}}{\partial} \quad (16)$$

$$\frac{1}{\dots} D_1 \frac{\partial C_1}{\partial} - \dot{G}_2^0 \Big|_{=G_2^0(t)} = \frac{1}{\dots} \tilde{D} \frac{\partial \tilde{C}}{\partial} - \frac{1}{r} D^* \frac{\partial C_2^*}{\partial} \Big|_{=G_2^1(t)} \quad (17)$$

(8), \mathbf{j}^* - , (9). -

$$J_2^2 dt + C_3^2 N_3 dG_3^2 = j dt + J_3^2 dt + C_2^2 N dG_2^2$$

$$-J_3^{*2} dt + j^* dt + C_3^{*2} N_3 dG_3^2 = -J_2^{*2} dt + C_2^{*2} N dG_2^2$$

:

$$\frac{1}{ru - xs} (rj + sj^*) \check{S}_3 dt = dG_3^2$$

$$\left[\left(\frac{x + ru - xs}{ru - xs} - 1 \right) j + \left(\frac{xs - ru + u}{ru - xs} + 1 \right) j^* \right] \check{S} dt = dG_2^2$$

$$= G_2^2(t) \quad :$$

$$x \left(\frac{N_3}{N} D_3 \frac{\partial C_3}{\partial} - D \frac{\partial C_2}{\partial} \right) + u \left(D^* \frac{\partial C_2^*}{\partial} - \frac{N_3}{N} D_3^* \frac{\partial C_3^*}{\partial} \right) = (ru - xs) \dot{G}_2^2 \quad (18)$$

$$V_{1,2} = \dot{G}_2^2 - \dot{G}_3^2 = \dot{G}_2^2 + \frac{1}{ru - xs} \left\{ r \left(\frac{N}{N_3} D \frac{\partial C_2}{\partial} - D_3 \frac{\partial C_3}{\partial} \right) + s \left(D_3^* \frac{\partial C_3^*}{\partial} - \frac{N}{N_3} D^* \frac{\partial C_2^*}{\partial} \right) \right\} \quad (19)$$

:

$$- \quad x = G_4^3(t) :$$

$$x \left(\frac{N_3}{N} D_3 \frac{\partial C_3}{\partial} - D \frac{\partial C_4}{\partial} \right) + u \left(D^* \frac{\partial C_4^*}{\partial} - \frac{N_3}{N} D_3^* \frac{\partial C_3^*}{\partial} \right) = (ru - xs) \dot{G}_4^3 \quad (20)$$

$$V_{3,4} = \dot{G}_4^3 + \frac{1}{ru - xs} \left[r \left(\frac{N}{N_3} D \frac{\partial C_4}{\partial} - D_3 \frac{\partial C_3}{\partial} \right) + s \left(D_3^* \frac{\partial C_3^*}{\partial} - \frac{N}{N_3} D^* \frac{\partial C_4^*}{\partial} \right) \right] \quad (21)$$

$$- \quad = G_4^4(t) :$$

$$D \frac{\partial C_4}{\partial} + \frac{N_5}{N} \hat{D} \frac{\partial \hat{C}}{\partial} = s \dot{G}_4^4 \quad (22)$$

$$V_{5,4} = \dot{G}_4 \left(1 - r \frac{N}{N_5} \right) + D^* \frac{\partial C_4^*}{\partial} - D_5^* \frac{\partial C_5^*}{\partial} \quad (23)$$

(14) – (23).

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Al₂O₃ – SiC – C