S a a (Ga,M

$$\Delta\hat{H}_{\gamma} / \Delta H_{\gamma} . E / J_0 + (2x. 1)J_1 + \sum J_{\cdot} D_{\cdot} \Pi_{\cdot}(\sigma)$$

$$+ \sum J D \Pi (\sigma). \qquad ( )$$

$$J \quad . D$$

$$\Delta H(x) \quad 0 \quad . \quad (3)$$

$$(111) \qquad (111)$$

$$(111) < (100) < (110) < (201). \qquad (3)$$

$$\Delta H(x)$$

$$\Delta H (x) / \Omega_1 x(1. x) + \Omega_2 x^2(1. x) + \Omega_3 x^3(1. x)\cdots \quad (4)$$

$\Omega_1 / 2 \cdot 3$ , $\Omega_2 / . 3 \cdot 0$ , $\Omega_3 / 23 \cdot$ .

( ) $E_{\cdot} . E$

$( )_1 / ( )$

(100) $x / 0. , 1$ $/ 1, 2, \ldots,$

$x / 1$ $x / 0.$ .

$\{J\}),$

## II. METHOD OF ESTABLISHING THE CLUSTER E PANSION

[1] $\Delta\hat{H}_{\cdot} / \Delta H_{\cdot} . E \quad \Delta\hat{H}_{\gamma}$ ,

$$\sum_{\sigma\in} |\Delta\hat{H}_{\cdot\cdot} \cdot \Delta\hat{H}_{\cdot\cdot}|^2 + \frac{\leftarrow}{\alpha}\sum J(\ )(\ \square^2)^{/2} J(\ )$$

$$/ \sum_{\sigma\in} |\Delta\hat{H}_{\cdot\cdot} \cdot \Delta\hat{H}_{\cdot\cdot}|^2 + \frac{}{2\alpha}\sum D_{\cdot\cdot} J^2_{\cdot\cdot},$$

( )

$J$ $\alpha$ [1]

$F$

$O(10^2)$

[24] ( ).

( )

( ).

( )

4

1.

( )

4×4×4

/ . 0 2 . $\Delta H_{\ }$ / 2•.04 , $\Delta H_{\ }$ / 2 .4 .

( ) [32]( ). -14,

( ) )$_2$ (301)

/ . 0 2 . H,

0. 0.2

$\Delta H_{\ }(\sigma)$,

$$\Delta H_{\ }(x) / \langle \Delta H_{\ }(\sigma) \rangle. \qquad (13)$$

$\Delta H_{\ }$ / 41.32 , $\Delta H_{\ }$ / 40.04 .

( )

x 0. ,

( )$_1$/( )$_3$ (100)

(110) (⁄3 3, ). ⁄3

$\Delta H_{\ }$ / 22.33 , $\Delta H_{\ }$ / 23.00

3 $\Delta H_{\ }$ / 30.00 , $\Delta H_{\ }$ / 32.04 .

( ) ( )

2

### C. T a a

. (13). ⁄

x/ 0.

. (4) $\Omega_1$/ 2•3 , $\Omega_2$/ . 3•0 , $\Omega_3$/ 23• . (4) [33]

$$\Delta G(x) / \Omega_1 x(1. x) + \Omega_2 x^2(1. x) + \Omega_3 x^3(1. x) + \cdot [x (x) + (1. x) (1. x)], \qquad (14)$$

.

where·

**D. $T=0$**

$\approx 3\times 10$

**E. S**

(3)

(100) (111)

2.

(110) (201)

11.

(100), (111), (201).

2

(100) (111)

11 (201)

**F. E**

10

)1/( ) , , ,
0. 0 )1/( ) , ,
, , , ,
, , , ,
, , , ,
, , , ,
, , , ,
, , , ,
11 ( )
4 B. , , (100), (110),
(111) ,
( )2( )1 ( )4( )1,
(201) ,
(201) , ,
0.3
0 2 0 2 0 2 0 2 -434. -434. .1 3-434. 3-434. 2
4 4 -33 - .1 2 -1.1 / 1 1.040 0 / 3 1 0.3 2 0
22 0 22 0.+04 123 - .3 - 10 2 / 1 * ,442 1 1.42 1 0 0 / 3 1

(