

t , t t t t t t

(-,)N

E, C, 80401, A
(26 3 2010; 3 12 2010; 15 2010)

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3 3 3 3 3 3 3 3 3 3 3

3 3 3 3 3 3 3 3 3 3 3 ()

- 3 3 ~50 3 3 3 3 () 3 -

3 3 27000 3 3 3 3 3 3 3 3

3 3 () 3 3 3 3 3 3 3

- 3 - 3 3 3 3

$\frac{1}{2} \left(\frac{1}{2} \right)^{n-1} = \frac{1}{2^n}$

$E(A|B_1, C) = E(AC, \cdot) + (1 - \frac{1}{2})E(BC, \cdot)$

$= 1870 \left(\frac{1}{2} \right)^{n-1} + 600 \left(\frac{1}{2} \right)^{n-1}$

$E(\cdot) = \sum_{k=0}^{\infty} \left(\frac{1}{2} \right)^k \left(\frac{1}{2} \right)^k = \sum_{k=0}^{\infty} \left(\frac{1}{4} \right)^k = \frac{1}{1 - \frac{1}{4}} = \frac{4}{3}$

\dots

1. Cluster expansion

$E(\cdot) = \sum_{k=0}^{\infty} \left(\frac{1}{2} \right)^k \left(\frac{1}{2} \right)^k = \sum_{k=0}^{\infty} \left(\frac{1}{4} \right)^k = \frac{4}{3}$

$$E(\cdot) = 0 + \frac{1}{2} \left[\sum_{k=1}^{\infty} \left(\frac{1}{2} \right)^k + \sum_{k=2}^{\infty} \left(\frac{1}{2} \right)^k + \sum_{k=3}^{\infty} \left(\frac{1}{2} \right)^k + \dots \right] + \sum_k$$

$\{ \dots \}$ $E ()$
 $\{ E () \}$.
 $() / ()$ $2()$
 $()$ $A B_1 C$ $() / ()$ $2()$
 $(. 30)$ 31.32
 $9 9 9$ 435
 E $1 /$ $()$ 33
 $(. , ())$ 24

2. Monte Carlo simulations of the atomic microstructures

$E/$ E
 27000
 0.0002
 $= 10000$ $()$ 0.06
 $= 0$
 $= 300$ 1000 50% $(. , = 0 20\%)$ 7.16

3. Relaxation of the atomic microstructures

$(. , ())$ $3 3$
 $3 3$

$$E^{(1)} = 1.1 \quad (45)$$

$$E^{(2)} = 0.62 \quad (46)$$

$$0.3 \quad 0.6 \quad 0.26$$

$$16.17$$

$$20\%$$

$$10^6$$

$$[A_{ij} B_{4j}] \quad (41)$$

$$16.17.22$$

$$[A_{ij} B_{4j}] \quad j=1 \dots 4$$

1. Empirical pseudopotential calculations

$$E^{(1)} \quad (42)$$

$$0.76 \quad (43)$$

$$E^{(1)} \quad (44)$$

$$18.44.45$$

$$0.06 \quad (18) \quad 0.62$$

[. 3(), 3 , 3
3 3 3 . 3 3 , 3
3 3 3 , 3
3) 3 3 3 (. , 3
) , 3 3 , 3

6() 6()
27000

16,17,33how-53ord536 041%,Tc

1. Random alloys

80% 75%
6() (3)
=20% [5()] =1% [4()]
6() (3) =10 20 %
5() 5() 3 20% 4() 4() 3 1%
3 3 3 3 3 3

2. Coherent alloys

()]

3 600) 3 3 1 ; () -

29 ... , 1687 (1999).

30 ... , 5048 (1981).

31 ... , 15 (1996).

32 ... A ... (... , 2007).

33 ...

34 ... , 521 (2002).

35 ... //

36 ... , 045208 (2002).

37 ... , 637 (1966).

38 ... , 4005 (1970).

39 ... , 16310 (1996).

40 ...

41 ... , 8240 (1990).

42 ... , 1642 (1997).

43 ... (...) .

44 ... , 2719 (1996).

45 ...

46 ... , 212109 (2009).

47 ... , 033308 (2008).

48 ... , 2394 (1994).

49 ... , 4725 (1998).

... , 061903 (2007).