CORRELATION IN DISTRIBUTION OF INTERSTITIAL ATOMS IN H.C.P. ALLOYS

Matysina Z.A.*, **Zaginaichenko S.Yu.[1]**, **Schur D.V.[1]**, **Vlasenko A. Yu.[1]**
Dnepropetrovsk National University,
72, Gagarin ave., Dnepropetrovsk, 49000 Ukraine
[1] Institute for Problems of Materials Science of NAS of Ukraine, lab. # 67,
3, Krzhizhanovsky str., Kiev, 03142 Ukraine

The physical properties of crystals are defined to a large extent by materials structure and character of atoms distribution in crystal lattice [1, 2]. The interstitial phases [3-23], as refractory, hard, high-temperature alloys, are of considerable current use in science and technology. The peculiarity of their physical properties is determined by the presence of structural defects induced by interstitial atoms.

In studies of correlation in distribution of atoms of different sort throughout the lattice sites and interstitial sites it can be established, the reality of short-range and local order forming, it can be ascertained the concentration and temperature ranges of phases homogeneity and chiefly it is possible to gain insight into the development of new materials based on old materials, to create new refractory metallic carbides, nitrides, borides without use of too costly alloying elements.

In the present paper the calculation of correlation parameters is carried out at first for h.c.p. alloys AB-C_{IN} with superstructure $B8_1$ and then with B19. The alloys of such type present in Ir-Si-C, Pd-Si-C, Pt-Si-C, Rh-Si-C, Nb-N systems and others.

The arrangement of interstitial atoms C in interstitial sites of two types: octahedral and tetrahedral is taken into account in calculation. It is suggested that C atoms (hydrogen, nitrogen, carbon, boron) are located in the centre of octahedron or tetrahedron.

In ordered state of alloys with $B8_1$ structure the one type of octahedral interstitial site O and two types of tetrahedral interstitial sites T_1, T_2 are distinguished in this lattice. The O interstitial site is surrounded by three sites of first type legal for A atoms and by three sites of second type legal for B atoms, the T_1 interstitial site has three nearest sites of first type and one site of second type and the T_2 interstitial site has one site of first type and three sites of second type.

The alloys with B19 structure have two types of octahedral O_1, O_2 and one type of tetrahedral T interstitial sites. The O_1 interstitial site is surrounded by four nearest sites of first type and by two sites of second type, the O_2 interstitial site has two nearest sites of first type and four – of second type. The T interstitial site has two sites of first type and two sites of second type from the four nearest sites.

For determination of correlation parameters the free energy is calculated. The method of configurations is used, i.e. all possible configurations of A and B atoms around interstitial sites are taken into account. The interaction of AC, BC atomic pairs is taken into consideration in the first coordination sphere.

For $B8_1$ structure the correlation parameters in substitution of sites i = 1, 2 and of interstitial sites O, T_1, T_2 respectively by atomic pairs AC, BC are found to be:

$$\varepsilon^{(10)} = \frac{cP_A^{(1)}P_B^{(1)}e}{K_1^4K_2^3}, \qquad \varepsilon^{(20)} = \frac{cP_A^{(2)}P_B^{(2)}e}{K_1^3K_2^4},$$

$$\varepsilon^{(1T_1)} = \frac{2cP_A^{(1)}P_B^{(1)}e'K_1'}{\left(K_1'^2 + K_2'^2\right)}, \quad \varepsilon^{(2T_1)} = \frac{2cP_A^{(2)}P_B^{(2)}e'K_1'^2}{K_2'\left(K_1'^2 + K_2'^2\right)},$$

$$\varepsilon^{(1T_2)} = \frac{2cP_A^{(1)}P_B^{(1)}e'K_2'^2}{K_1'\left(K_1'^2 + K_2'^2\right)}, \quad \varepsilon^{(2T_2)} = \frac{2cP_A^{(2)}P_B^{(2)}e'K_2'}{\left(K_1'^2 + K_2'^2\right)},$$

and for B19 structure and interstitial sites O_1, O_2, T they are equal to

$$\varepsilon^{(1O_1)} = \frac{2cP_A^{(1)}P_B^{(1)}eK_1}{\left(K_1^2 + K_2^2\right)}, \quad \varepsilon^{(2O_1)} = \frac{2cP_A^{(2)}P_B^{(2)}eK_1^2}{K_2\left(K_1^2 + K_2^2\right)},$$

$$\varepsilon^{(1O_2)} = \frac{2cP_A^{(1)}P_B^{(1)}eK_2^2}{K_1\left(K_1^2 + K_2^2\right)}, \quad \varepsilon^{(2O_2)} = \frac{2cP_A^{(2)}P_B^{(2)}eK_2}{\left(K_1^2 + K_2^2\right)},$$

$$\varepsilon^{(1T)} = \frac{cP_A^{(1)}P_B^{(1)}e'}{K_1'}, \qquad \varepsilon^{(2T)} = \frac{cP_A^{(2)}P_B^{(2)}e'}{K_2'},$$

where

* Fax: 38-044-424-0381; E-mail: shurzag@materials.kiev.ua

$$P_A^{(1)} = a + \frac{1}{2}\eta, \quad P_A^{(2)} = a - \frac{1}{2}\eta,$$

$$P_B^{(1)} = b - \frac{1}{2}\eta, \quad P_B^{(2)} = b + \frac{1}{2}\eta,$$

$$e = \exp\frac{\alpha}{kT} - \exp\frac{\beta}{kT},$$

$$K_1 = P_A^{(1)}\exp\frac{\alpha}{kT} + P_B^{(1)}\exp\frac{\beta}{kT},$$

$$K_2 = P_A^{(2)}\exp\frac{\alpha}{kT} + P_B^{(2)}\exp\frac{\beta}{kT},$$

the e', K_1', K_2' quantities are expressed by formulae as e, K_1, K_2 with α', β' in place of α, β; *a*, b, c are atomic concentrations of alloy components A, B, C; η is the atomic order degree, $\alpha = -\upsilon_{AC}, \beta = -\upsilon_{BC}$ are energies of AC, BC pairs interaction for octahedral interstitial sites, α', β' are identical energies for tetrahedral interstitial sites.

The derived formulae determine the dependence of correlation parameters on alloy composition, temperature and order parameters.

From the derived formulae it follows that correlation parameters are found to be equal to zero, firstly, in the case of completely ordered alloys of stoichiometric composition, secondly, at the equal energetic parameters $\alpha=\beta$, $\alpha'=\beta'$, thirdly, in uncombined metals A (or B), and fourthly, at very high temperatures ($T \rightarrow \infty$).

The derived analytical expressions for correlation parameters can be used in studies of many phenomena in alloys, as an example, at the investigation of intensity of diffuse scattering of X-rays, neutrons, electrons.

The regularity knowledge of functional dependences of correlation parameters can permit the prediction of atomic order and the correlation influence on physical characteristics of alloys and on occurred processes in them.

References

1. Schur DV, Zaginaichenko S Yu, Adejev VM, Voitovich VB, Lyashenko AA, Trefilov VI; Phase transformations in titanium hydrides, International journal of hydrogen energy, 21,11,1121-1124,1996, Pergamon
2. Schur DV, Tarasov BP, Zaginaichenko S Yu, Pishuk VK, Veziroglu TN, Shul'ga Yu M, Dubovoi AG, Anikina NS, Pomytkin AP, Zolotarenko AD; The prospects for using of carbon nanomaterials as hydrogen storage systems,International journal of hydrogen energy,27,10,1063-1069,2002,Pergamon
3. Tarasov BP, Shul'ga Yu M, Fokin VN, Vasilets VN, Shul'ga N Yu, Schur DV, Yartys VA; Deuterofullerene C 60 D 24 studied by XRD, IR and XPS,Journal of alloys and compounds, 314,1,296-300,2001,Elsevier
4. Tarasov BP, Fokin VN, Moravsky AP, Shul'ga Yu M, Yartys VA, Schur DV; Promotion of fullerene hydride synthesis by intermetallic compounds, Hydrogen energy progress, 2, 1221-1230,1998,
5. Schur DV, Zaginaichenko S Yu, Matysina ZA, Smityukh I, Pishuk VK; Hydrogen in lanthan–nickel storage alloys,Journal of alloys and compounds,330,70-75,2002,Elsevier
6. Matysina ZA, Schur DV; Hydrogen and solid phase transformations in metals, alloys and fullerites, Dnepropetrovsk: Nauka i obrazovanie, 420p (in Russian),2002,
7. Matysina ZA, Pogorelova OS, Zaginaichenko S Yu, Schur DV; The surface energy of crystalline CuZn and FeAl alloys,Journal of Physics and Chemistry of Solids,56,1,9-14, 1995,Elsevier
8. Schur DV, Lavrenko VA, Adejev VM, Kirjakova IE; Studies of the hydride formation mechanism in metals,International journal of hydrogen energy,19,3,265-268,1994,Elsevier
9. Schur DV, Matysina ZA, Zaginaichenko S Yu; Theoretical study of interstitial atoms distribution in the bulk and at the surface of crystal. Surface segregation,Journal of alloys and compounds,330,81-84,2002,Elsevier
10. Shul'ga Yu M, Martynenko VM, Tarasov BP, Fokin VN, Rubtsov VI, Shul'ga N Yu, Krasochka GA, Chapysheva NV, Shevchenko VV, Schur DV; On the thermal decomposition of the C60D19 deuterium fullerite,Physics of the Solid State,44,3,545-547,2002, Nauka/ Interperiodica
11. Schur DV, Matysina ZA, Zaginaichenko S Yu; Study of physico-chemical processes on catalyst in the course of synthesis of carbon nanomaterials,Hydrogen Materials Science and Chemistry of Metal Hydrides: Proceedings of the NATO Advanced Research Workshop on. Alushta Crimea, Ukraine, 16-22 September 2001,235,2002,Kluwer Academic Pub
12. Schur DV, Tarasov BP, Shul'ga Yu M, Zaginaichenko S Yu, Matysina ZA; Research of Fullerites Hydrogen Capacity,Hydrogen Materials Science and Chemistry of Metal Hydrides: Proceedings of the NATO Advanced Research Workshop on. Alushta Crimea, Ukraine, 16-22 September 2001,1,2002, Kluwer Academic Pub
13. Matysina ZA, Zaginaichenko S Yu, Schur DV, Pishuk VK; Theoretical investigation of isopleths of hydrogen solubility in transition metals,Journal of alloys and compounds, 330,85-88,2002,Elsevier
14. Trefilov VI, Schur DV, Pishuk VK, Zaginaichenko S Yu, Choba AV, Nagornaya NR; The solar furnaces for scientific and technological investigation, Renewable energy, 16,1,757-760, 1999, Elsevier
15. Трефилов ВИ, Щур ДВ, Загинайченко СЮ; Фуллерены-основа материалов будущего, 2001, Laboratory 67

16. Schur Dmitry V, Zaginaichenko Svetlana Yu, Veziroğlu T Nejat, Javadov NF; The Peculiarities of Hydrogenation of Fullerene Molecules C60 and Their Transformation, Black Sea Energy Resource Development and Hydrogen Energy Problems,191-204,2013, Springer Netherlands
17. Schur DV, Dubovoi AG, Anikina NS, Zaginaichenko S Yu, Dobrovol'skij VD, Pishuk VK, Tarasov BP, Shul'ga Yu M, Meleshevich KA, Pomytkin AP; The production of utrafine powders of fullerites by the salting out method,Proceedings of VII International Conference "Hydrogen Material Science and Chemistry of Metal Hydrides", Alushta-Cremia-Ukraine, September, 16-22, 2001,
18. Kharlamov AI, Loytchenko SV, Kirillova NV, Kaverina SN, Vasilev AD, Fomenko VV, Zolotarenko AD, Kazimirov VP; Tubular and filamentous nanostructures of hexagonal silicon carbide, Proceedings of VII International Conference "Hydrogen Material Science and Chemistry of Metal Hydrides", Ukraine, 572-574,2001,
19. Slys IG, Berezanskaya VI, Schur DV, Zaginaychenko SYu, Rogozinskaya AA, Adejev VM, Zolotarenko AD; Making the point metal coatings on the particles of hydride-forming intermetallides, Proceedings of VII International Conference "Hydrogen Material Science and Chemistry of Metal Hydrides", Ukraine,404-405,2001,
20. Muratov VB, Meleshevich KA, Bolgar AS, Zolotarenko AD; Application of dynamic c-calorimetry method for investigation of enthalpy at hydride dissociation,Proceedings of VII International Conference "Hydrogen Material Science and Chemistry of Metal Hydrides", Ukraine,342-343,2001,
21. Anikina NS, Schur DV, Simanovskiy AP, Zolotarenko AD, Dubovoy AG, Ivanchenko NV; Problem on fullerene production by electric arc method, Proceedings of VII International Conference "Hydrogen Material Science and Chemistry of Metal Hydrides", Ukraine,590-591, 2001,
22. Pishuk VK, Schur DV, Bogolepov VA, Savenko AF, Zaginaichenko SYu, Zolotarenko AD, Mar'yanchuk IV, Prikhod'ko AB; Problem on production of highly dispersed extra pure powders, Proceedings of VII International Conference "Hydrogen Material Science and Chemistry of Metal Hydrides", Ukraine,586-587,2001,
23. Lavriv LV, Anikina NS, Simanovskij AP, Zolotarenko AD, Schur DV; Features of fullerene extraction wth toluene, Proceedings of VII International Conference "Hydrogen Material Science and Chemistry of Metal Hydrides", Ukraine,596,2001