

Development of embedded atom potentials and prediction of properties for binary Ti-V^①

SHANG Shun-li(商顺利), LIU Yu-qin(刘玉芹),

BAI Ke-wu(白克武), SHEN Jian-yun(沈剑韵), WANG Xi-zhe(王希哲)

(General Research Institute for Nonferrous Metals, Beijing 100088, P. R. China)

[Abstract] The embedded atom potentials for binary Ti-V were developed and used to predict the mechanical properties of binary Ti-V solid solutions with hcp and bcc structures including lattice parameters, elastic constants and fracture toughness for Mode I fracture under plane strain. The calculation results show that with the increment of V-content, the lattice parameters and elastic constants decrease but the fracture toughness increases for hcp solid solutions, the lattice parameters decrease but the elastic constants and fracture toughness increase for bcc solid solutions. The calculation results agree well with the available experiment values.

[Key words] embedded atom potentials; Ti-V system; lattice parameters; elastic constants; fracture toughness

[CLC number] TG111

[Document code] A

1 INTRODUCTION

As an important β stabilizer element, vanadium can improve the ductility and the hot deformability of Ti-alloys. However, the limitation of the knowledge about the properties of Ti-V binary alloy hinders the development of V-contained titanium alloys.

Recent development of many-body potentials embedded atom method (EAM)^[1] has been used quite successfully in predicting numerous properties of intermetallic compounds and solid solutions^[2]. The purpose of the present work is to develop an embedded atom potential for the Ti-V binary solid solutions with hcp and bcc structures in order to perform atomistic simulation for obtaining the basic physical and mechanical properties including lattice parameters, elastic constants and the fracture toughness for Mode I fracture under plane strain. The predicted results agree well with the available experiment values.

2 EMBEDDED ATOM POTENTIAL OF Ti-V SYSTEM

Within the framework of the EAM theory^[1], the total internal energy E_{tot} of any atomic structure is described as the sum of two terms, an embedded atom term F which depends on the local electron density ρ , and a pair-potential term ϕ which depends purely on interatomic distances r :

$$E_{\text{tot}} = \sum_i F(\rho) + \frac{1}{2} \sum_{i,j} \phi(r_{ij}) \quad (\text{for } i \neq j) \quad (1)$$

By combining the density functional with the traditional pair potentials, the EAM potential makes the atomic simulation more reliable since it eliminates

two well-known problems associated with pair potentials^[3]: the Cauchy discrepancy and the cohesive energy-vacancy formation energy dilemma.

2.1 EAM potentials for pure components

The EAM potential for a system is generally set up on the basis of that for its constituent elements. Different functions of ρ , ϕ and F have been proposed for various elements according to their structures and properties. The function proposed by Pasianot and Savino^[4] is selected to describe EAM potential of Ti with the hcp structure, since it takes the contribution of internal relaxation to the elastic constants, which are termed inner elastic constants, into account, and there is the possibility of internal relaxation due to the existence of two kinds atom per primitive lattice cell in the hcp structure^[5]. The potential function proposed by Johnson and Oh^[6] is selected for V with the bcc structure because of the explicit functions for ρ , ϕ and F which can simplify the calculation.

The electronic density for the perfect lattice of vanadium was normalized to the same value as that of titanium, as was done for the binary Ti-Al by Farkas^[7].

2.2 EAM potentials for binary Ti-V

The mixed-pair potential calculation method proposed by Johnson^[8], which takes weighted averages of the individual $\phi^{\text{Ti}}(r)$ and $\phi^{\text{V}}(r)$ functions, is used to describe the Ti-V interactions. It is in the following form:

$$\phi^m(r) = \frac{1}{2} \left[\frac{f^{\text{V}}(r)}{f^{\text{Ti}}(r)} \phi^{\text{Ti}}(r) + \frac{f^{\text{Ti}}(r)}{f^{\text{V}}(r)} \phi^{\text{V}}(r) \right] \quad (2)$$

① [Foundation item] Project (59881002) supported by the National Natural Science Foundation of China

[Received date] 1999 - 10 - 17; [Accepted date] 2000 - 04 - 03

where $f^{\text{Ti}}(r)$ and $f^{\text{V}}(r)$ are the electronic functions of pure Ti and V, $\phi^{\text{Ti}}(r)$ and $\phi^{\text{V}}(r)$ are the pair potentials of pure Ti and V respectively, r is the distance between two atoms.

The EAM potentials for the Ti-V binary disorder solid solutions can be approximated by the equivalent atom method^[9]. It can simplify the calculation based on a linear combination of the corresponding functions for the constitute elements. This simplification is valid since Ti and V differ very slightly in atom mass (47.90 for Ti and 50.94 for V)^[10], electronegativity (1.4 for Ti and 1.9 for V)^[10] and atomic radius (0.145 nm for Ti and 0.131 nm for V)^[11]. Thus the EAM functions for every equivalent atom of Ti-V solid solutions are written as

$$\bar{E}_i = x_{\text{Ti}} F^{\text{Ti}}(\bar{\rho}) + x_{\text{V}} F^{\text{V}}(\bar{\rho}) + \frac{1}{2} \sum_{j, j \neq i} \phi(r_{ij}) \quad (3)$$

$$\bar{\rho} = \sum_{j, j \neq i} [x_{\text{Ti}} f^{\text{Ti}}(r_{ij}) + x_{\text{V}} f^{\text{V}}(r_{ij})] \quad (4)$$

$$\phi(r_{ij}) = x_{\text{Ti}}^2 \phi^{\text{Ti}}(r_{ij}) + 2 x_{\text{Ti}} x_{\text{V}} \phi^{\text{m}}(r_{ij}) + x_{\text{V}}^2 \phi^{\text{V}}(r_{ij}) \quad (5)$$

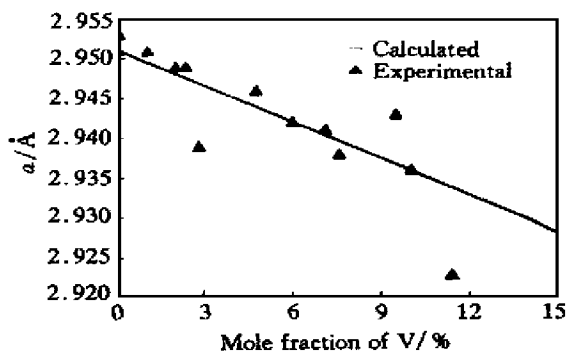
where “-” denotes the properties of an equivalent atom of the alloy, x_{Ti} and x_{V} are the mole fraction of atoms of Ti and V, $\bar{\rho}$ is the average electron density at the location of the equivalent atom, $F^{\text{Ti}}(\bar{\rho})$ and $F^{\text{V}}(\bar{\rho})$ are the energy to embed atoms Ti and V separately into the electron density $\bar{\rho}$, $\phi(r_{ij})$ is the pair potential between equivalent atoms i and j with the distance r_{ij} .

3 PREDICTION OF PROPERTIES FOR BINARY Ti-V

3.1 Prediction of lattice parameters

The lattice parameters can be obtained by searching for the minimum of the total energy E_{tot} using the simplex method^[12].

The predicted lattice parameters of Ti-V hcp solid solution and Ti-V bcc solid solution are presented and compared with the experimental data^[13] in Fig.1 and Fig.2.



From Fig.1 and Fig.2, it can be seen that the lattice parameters of Ti-V hcp and bcc solid solutions decrease with the mole fraction of vanadium increasing. The calculation results agree well with the experimental values.

3.2 Prediction of elastic constants

According to the elasticity theory, the elastic constants C_{ij} and bulk modulus B can be obtained by applying second derivative of the total energy to the displacement.

The calculated results of elastic constants C_{ij} and bulk modulus B of the Ti-V binary hcp and bcc solid solutions are presented in Fig.3 and Fig.4 respectively and compared with the available experimental data^[14,15]. The calculated results agree well with the available experimental values^[14,15] measured by pulse-superposition and pulse-echo overlap methods. It can be seen that all the elastic constants C_{ij} and bulk modulus K decrease with the raise of V-content in the hcp solid solution, whereas the elastic constants C_{11} , C_{12} and bulk modulus K increase evidently and C_{44} keeps unchanged with the addition of V in the bcc solid solution.

From Fig.4, it also can be seen that the elastic constant C_{11} increase more sharply than that of others with the addition of V in the bcc solid solution, which agree well with Fisher's conclusion^[16]. Fisher has shown that transition metal additions to single crystal bcc Ti alloys raise the modulus in [100] direction faster than that of others, and that this effect is due to increasing the number of electrons in the d-band. So the elastic constant C_{11} increases faster than that of others with the addition of V in the bcc Ti-V solid solution.

3.3 Prediction of fracture toughness

Fracture toughness K_{IC}^{G} represents the resistance to crack tip propagation of a material. According to Griffith criterion and linear elasticity theory^[17,18], the critical stress intensity factor, i.e. fracture toughness K_{IC}^{G} for Mode-I fracture under plane strain can be expressed as

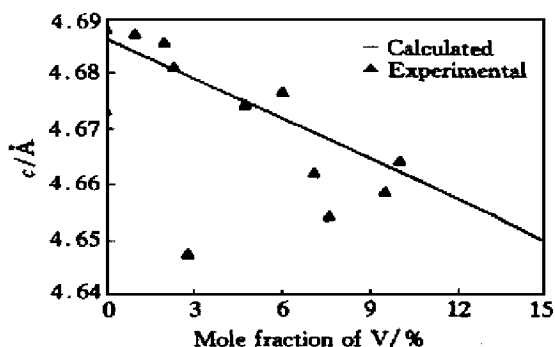


Fig.1 Lattice parameters a and c of hcp solid solution vs mole fraction of vanadium in binary Ti-V

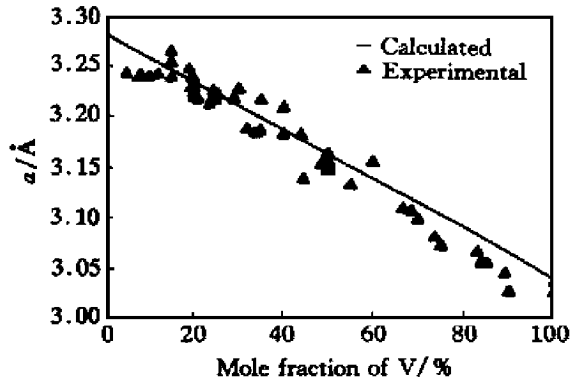


Fig. 2 Lattice parameter a of bcc solid solution vs mole fraction of vanadium in binary Ti-V

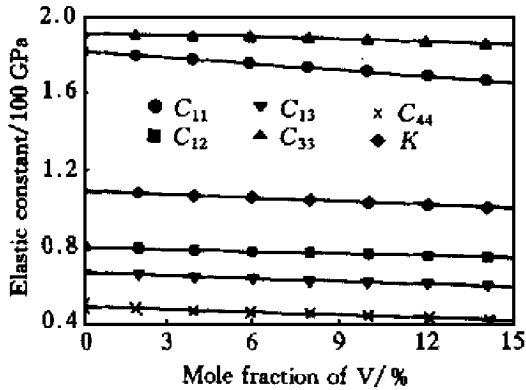


Fig. 3 Elastic constant of hcp solid solution vs mole fraction of vanadium in binary Ti-V

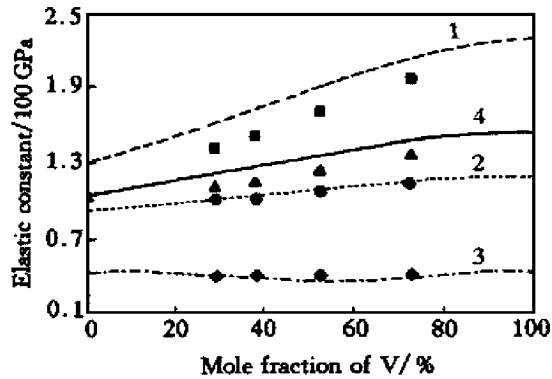


Fig. 4 Elastic constants of bcc solid solution vs mole fraction of vanadium in binary Ti-V

1 — C_{11} ; 2 — C_{12} ; 3 — C_{44} ; 4 — K ;

■ — Experimental data of C_{11} ; ● — Experimental data of C_{12} ;
◆ — Experimental data of C_{44} ; ▲ — Experimental data of K

$$K_{IC}^G = \sqrt{2 \gamma / A} \quad (6)$$

where γ is the surface energy, which is the energy difference of the system before and after surface formation and can be obtained by EAM calculation^[19]. For an orthotropic crack system^[17,18],

$$A = \left\{ \left[\frac{b_{22} b_{33}}{2} \right] \left[\left(\frac{b_{33}}{b_{22}} \right)^{1/2} + \frac{2 b_{23} + b_{44}}{2 b_{22}} \right] \right\}^{1/2} \quad (7)$$

where b_{ij} are functions of compliance constants s_{ij} , the indices 2, 3, and 4 refer to the directions of crack propagation, normal to the crack plane and parallel to the crack front respectively. The crack system is illustrated in Fig. 5, where direction 1 is equivalent to direction 4. This figure also presents the $[100](001)$ crack tip in orthotropic system or the $[2\bar{1}10](0001)$ crack tip in hexagonal system.

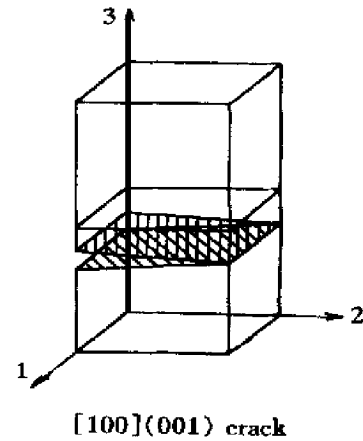


Fig. 5 Sketch drawing of crack-tip of Mode-I

For cubic structure

$$\left. \begin{aligned} b_{22} &= b_{33} = s_{11} - s_{12}^2 / s_{11} \\ b_{23} &= s_{12} - s_{12}^2 / s_{11} \\ b_{44} &= s_{44} \end{aligned} \right\} \quad (8)$$

For hexagonal close-packed structure:

$$\left. \begin{aligned} b_{22} &= s_{11} - s_{12}^2 / s_{11} \\ b_{23} &= s_{13} - s_{12} s_{13} / s_{11} \\ b_{33} &= s_{33} - s_{13}^2 / s_{11} \\ b_{44} &= s_{44} \end{aligned} \right\} \quad (9)$$

where, the compliance constants s_{ij} can be obtained from the elastic constants C_{ij} since the matrix of s_{ij} and that of C_{ij} are mutually inverted.

The K_{IC}^G of the $[100](001)$ crack tip for bcc structure and $[2\bar{1}10](0001)$ crack tip for hcp structure of the Ti-V system are studied with EAM calculation. The influences of V-content on K_{IC}^G for the hcp and bcc solid solutions of Ti-V system are presented in Fig. 6 and Fig. 7.

From Fig. 6 and Fig. 7, it can be seen that for the same composition the K_{IC}^G of bcc solution is greater than that of hcp solution and the K_{IC}^G of both hcp and bcc solid solutions increases with the raise of V-content. Thus the improvement of the ductility and hot deformability of Ti-alloys with the addition of V can be explained by two reasons: 1) V can stabilize bcc phase, of which the K_{IC}^G is higher than that of hcp phase; 2) the increments of V-content in both bcc and hcp phases of Ti-alloys are favorable for increasing K_{IC}^G .

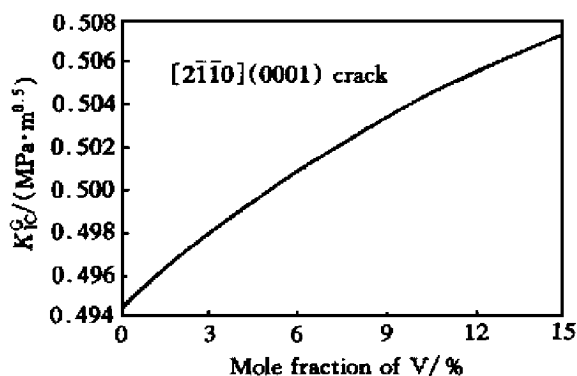


Fig. 6 K_{IC}^G in hcp solid solution of Ti-V binary system

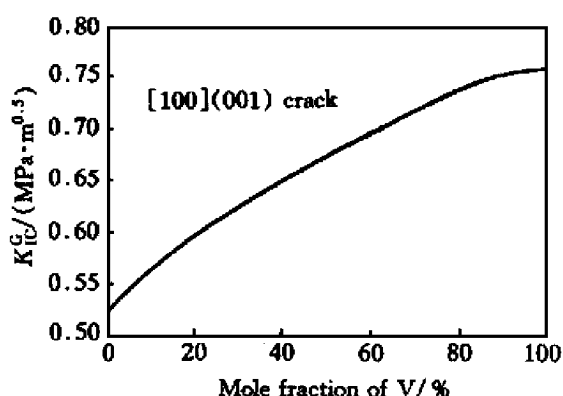


Fig. 7 K_{IC}^G in bcc solid solution of Ti-V binary system

4 CONCLUSIONS

The EAM potentials for Ti-V system are set up for studying the impact of V-content on lattice parameters, elastic constants and fracture toughness K_{IC}^G for Mode I crack tip under plain strain of the hcp and bcc solid solutions. The predicted properties of the binary system including lattice parameters and elastic constants agree well with the experimental data available.

The results of this work show that: 1) lattice parameters a and c , elastic constants C_{ij} and bulk modulus K decrease but fracture toughness K_{IC}^G increases with the increment of V-content for Ti-V hcp solid solution; 2) lattice parameters a decrease, however, elastic constants C_{ij} , bulk modulus K and fracture toughness K_{IC}^G increase with the increment of V-content for Ti-V bcc solid solution.

[REFERENCES]

[1] Daw M S and Baskes M I. Embedded-atom method:

Derivation and application to impurities, surface, and other defects in metals [J]. *Phy Rev B*, 1984, 29: 6443 - 6453.

[2] Baskes M I, Nelson J S and Wright A F. Semiempirical modified embedded-atom potentials for silicon and germanium [J]. *Phy Rev B*, 1989, 40: 6085 - 6100.

[3] Oh D J and Johnson R A. Simple embedded atom method model for fcc and hcp metals [J]. *J Mater Res*, 1988, 3: 471 - 478.

[4] Pasianot R and Savino E J. Embedded-atom method interatomic potentials for hcp metals [J]. *Phy Rev B*, 1992, 45: 12704 - 12710.

[5] Van Midden H J P and Sasse A G B M. Derivation of elastic constants from the embedded-atom potential in a lattice model [J]. *Phy Rev B*, 1992, 46: 6020 - 6030.

[6] Johnson R A and Oh D J. Analytic embedded atom method model for bcc metals [J]. *J Mater Res*, 1989, 4: 1195 - 1201.

[7] Farkas D. Interatomic potentials for Ti-Al with and without angular force [J]. *Modelling Simul Mater Sci Eng*, 1994, 2: 975 - 984.

[8] Johnson R A. Phase stability of fcc alloy with the embedded atom method [J]. *Phy Rev B*, 1990, 41: 9717 - 9720.

[9] Ackland G V and Vitek V. Application of many-body-potentials to noble metal alloys [A]. Vitek V, Srolovitz D J eds. *Atomistic Simulation of Materials Beyond Pair Potential* [C]. New York: Plenum, 1989. 193 - 201.

[10] Grujicic M and Dang P. Atomic-scale analysis of martensitic transformation in titanium alloyed with vanadium, Part I: verification of the embedded-atom method model [J]. *Mater Sci Eng A*, 1996, A205: 139 - 152.

[11] Kittel C. *Introduction to Solid State Physics* [M]. New York: Wiley Interscience, 1971. 39.

[12] Nelder J A and Mead R. A simplex method for function minimization [J]. *The Computer Journal*, 1965, 7: 308 - 313.

[13] Murray J L. The Ti-V system [A]. Murray J L ed. *Phase Diagrams of Binary Titanium Alloys* [M]. Metals Park, OH: ASM International, 1987. 319 - 335.

[14] Hadjicantis V, Varotsos C and Eftaxias K. Elastic moduli of V-Ti, Mo-Nb and W-Ta alloys [J]. *J Phys F*, 1988, 18: 1133 - 1136.

[15] Boyer R, Welsch G and Collings E W. *Materials Properties Handbook: Titanium Alloys* [M]. Metals Park, OH: ASM International, 1994. 99.

[16] Fisher E S. *Physics of Solid Solution Strengthening* [M]. New York: Plenum Press, 1975. 199.

[17] Sih G C and Liebowitz H. Mathematical theories of brittle fracture (Chapter 2) [A]. Liebowitz H ed. *Fracture: an Advanced Treatise (Vol II)* [M]. New York: Academic Press, 1968: 126 - 128.

[18] Cheung K S and Yip S. A molecular dynamics simulation of crack-tip extension: the brittle-to-ductile transition [J]. *Modelling Simul Mater Sci Eng*, 1994, 2: 865 - 892.

[19] Cai J and Ye Y Y. Simple analytical embedded-atom-potential model including a long-range force for fcc metals and their alloys [J]. *Phys Rev B*, 1996, 54: 8398 - 8410.

(Edited by YUAN Sai qian)