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Electron theory analysis on Ti-6Al-4V and Au-8Pd-10Pt alloys ①

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Abstract: The valence electron structures and electron densities on some lattice planes of biomaterials Ti-6Al-4V and Au-Pd-Pt were calculated by using bond length difference method of the empirical electron theory of solids and molecules. The results show that there exist the planes with continuous densities in the three crystal cells involved, which verified to some extent the validity of "Atomic Boundary Condition" applying in biomaterials research. It was proposed that the sufficient understanding and reasonable modeling on microstructure of living body are necessary to evaluate directly the electron density continuity between biomaterial and living tissue.

Key words: alloy; electron theory; biology **Document code:** A

1 INTRODUCTION

Interface subject plays an important role in biomaterials field. The interface characteristic inside composite biomaterial and that between biomaterial and living tissue straightly influence the mechanical properties and biocompatibility. For instance, hydroxyapatite can induce bone formation[1,2] and combine smoothly with living tissue[3,4], but low strength and toughness limit their application[5,6]. Hydroxyapatite coating can be produced on titanium alloy surface and its performance can be modified, and thermal physical property difference is considered the main factor causing the peeling of coating[7,8]. To discover the intrinsic micro-mechanism of such problem, it is necessary to know the atoms state and their combining situation. The development of electron theory on atom bonds in alloy and phase stability will help to solve such subject. The empirical electron theory of solids and molecules (EET) has been successfully applied in study on alloy properties and interface[9,10], and the present work is to discuss the biological application of EET through the electron theory analysis on Ti-6Al-4V and Au-8Pd-10Pt alloys.

2 CALCULATIONS OF VALENCE ELECTRON STRUCTURE AND ELECTRON DENSITY

2.1 Ti-6Al-4V

The α and β phase stabilizing elements (Al and V) involved in the alloy formed the double phase microstructure. Here the valence electron structures and electron densities of HCP α unit cell containing Ti-Al and BCC β unit cell containing Ti-V were calculated.

The structural model of Ti-Al and Ti-V unit cells with lattice parameters being $a = 2.96$ Å, $c = 4.74$ Å and $a = 3.32$ Å are shown in Figs.1 and 2, respectively. The effect of alloying elements on lattice parameter can enter the final results through their effect on hybrid levels of atoms. From Fig.1, experimental bond lengths of Ti-Al cell can be got as follows:

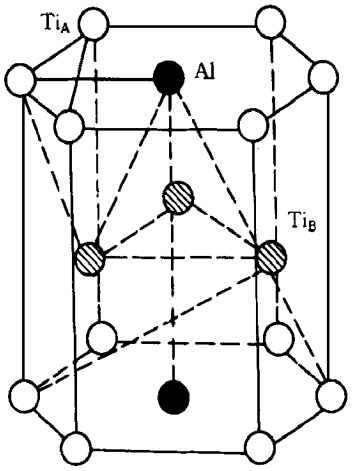

Fig.1 Structural model of Ti-Al cell

$D_a(\mathrm{Al\text{-}Ti_B}) = D_b(\mathrm{Ti_A\text{-}Ti_B}) = \sqrt{c^2/4 + a^2/3}$;
$D_c(\mathrm{Al\text{-}Ti_A}) = D_d(\mathrm{Ti_A\text{-}Ti_A}) = D_e(\mathrm{Ti_B\text{-}Ti_B}) = a$;
$D_f(\mathrm{Ti_A\text{-}Ti_B}) = \sqrt{c^2/4 + 4a^2/3}$;
$D_g(\mathrm{Al\text{-}Al}) = D_h(\mathrm{Ti_A\text{-}Ti_A}) = D_i(\mathrm{Ti_A\text{-}Ti_B}) = c$;
$D_k(\mathrm{Al\text{-}Ti_A}) = \sqrt{c^2 + a^2}$.

Identical bond numbers of the above bonds are: $I_a = 12$, $I_b = 24$, $I_c = 12$, $I_d = 6$, $I_e = 18$, $I_f = 12$, $I_g = 2$, $I_h = 4$, $I_i = 6$, $I_k = 24$。

Equations established according to the BLD

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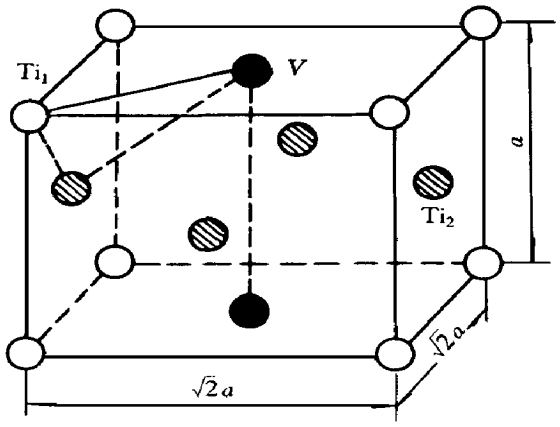

Fig .2 Structural model of Ti-V cell

method[11] in EET give the results, as listed in Table 1. Where σ is hybrid level of one atom, I_α is identical bond number of α bond, $\alpha = a, b, c, d \ldots k$; D_α is experimental bond length of α bond and D_α is theoretical bond length; n_α is covalent electron couple number on α bond; ΔD_α is the bond length difference between theoretical and experimental bond length, $\Delta D_\alpha < 0.05$ Å meets requirement.

Since some bonds with less valence electron are considered to be neglectable, the electron density calculations focus on the atomic planes with stronger bonds which are predominant in combinations with planes in other phase. For metallic bond, its lattice plane electron density $\rho_{(hkl)}$ calculated approximately in terms of covalent electron density[10].

$$\rho_{(hkl)} = n_c^{(hkl)} / S_{(hkl)} \quad (1)$$

where $n_c^{(hkl)} = \sum I_\alpha n_\alpha$; $S_{(hkl)}$, area of (hkl) plane in the unit cell, is calculated geometrically. The electron densities of some planes in Ti-Al cell and those of Ti-V cell obtained are listed in Table 2.

2.2 Au-8Pd-10Pt

Here "Average Atom Model" was employed to calculate the valence electron structure of the ternary substitutional solid solution. The atom on one lattice position was deem to be an "Average Atom" (Fig.3) with lattice parameters being $a = 4.078$ Å, its covalent electron number and single bond semi-length equal the values of mole fraction(%) average of involved atoms

$$n_c = \sum x(i)\, n_{ci} \quad (2)$$

$$R(1) = \sum x(i)\, R(1)_i \quad (3)$$

where $x(i)$ is the mole fraction(%) of element i, n_{ci} and $R(1)_i$ are covalent electron number and single bond semi-length, respectively. The calculated plane electron densities are listed in Table 3.

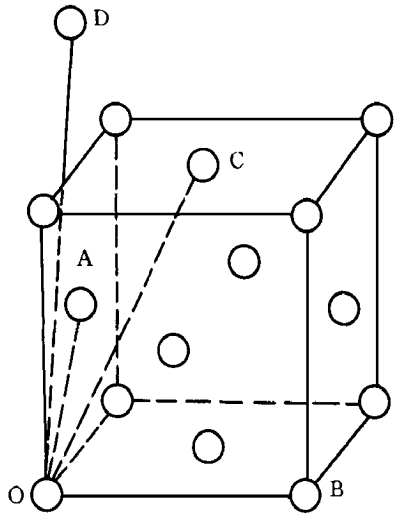

Fig .3 Structural model of Au-8Pd-10Pt cell

3 DISCUSSION

Interface theory is one of the focal point in the research on surface engineering and compound materials. The description about "Atomic Boundary Condition" gives the key to the problem. Cheng[12] pointed out that the interatomic boundary condition is just electron density to be continuous. More particularly, in terms of electron state, the boundary condition between unit cells is equal plane density of covalent electron number n_c on common lattice plane[10], namely,

$$[n_c^{(hkl)} / S^{(hkl)}]_1 = [n_c^{(hkl)} / S_{(hkl)}]_2 \quad (4)$$

that gives the requirement for two phases to form

Table 1 Principal data of valence electron structure of Ti-Al cell

Bond	I_α	D_α/Å	$\overline{D}_\alpha$/Å	n_α	ΔD_α/Å	Atom	σ
Ti_A-Ti_B	6	2.921 89	2.915 45	0.233 09	6.44×10^{-3}		
Ti_B-Ti_B	18	2.960 00	2.953 56	0.215 28	6.44×10^{-3}		
Ti_A-Ti_B	24	2.960 00	2.953 56	0.210 59	6.44×10^{-3}	Ti_A	12
Al-Ti_B	12	2.921 89	2.915 45	0.207 14	6.44×10^{-3}		
Al-Ti_A	12	2.960 00	2.953 56	0.179 06	6.44×10^{-3}		
Ti_A-Ti_B	12	4.159 21	4.152 77	0.004 31	6.44×10^{-3}	Ti_B	11
Ti_B-Ti_B	6	4.740 00	4.733 56	0.000 67	6.44×10^{-3}		
Ti_A-Ti_A	4	4.740 00	4.733 56	0.000 64	6.44×10^{-3}		
Al-Al	2	4.740 00	4.733 56	0.000 48	6.44×10^{-3}	Al	3
Ti_A-Ti_A	12	5.126 87	5.120 43	0.000 18	6.44×10^{-3}		
Al-Ti_A	24	5.588 31	5.581 87	0.000 04	6.44×10^{-3}		

Table 2 Plane electron densities in Ti-Al and Ti-V cells

Ti Al		Ti-V	
Plane	ρ/Å	Plane	ρ/Å
(0001)	112.387	(001)	163.798
(0002)	168.580	(002)	8.985
(0110)	30.480	(010)	14.434
(0220)	15.240	(020)	304.833
		(110)	113.113
		(101)	4.619

Table 3 Some plane electron densities in Au-8Pd-10Pt cell

Plane	ρ/Å
(001)	184.524
(111)	159.013
(110)	65.262

atomic boundary. It is known that phase transformation in solid processes commonly abiding by certain orientation relationship with the lower system energy, which is supported by the highly close electron densities on the common lattice plane of old and new phases[10]. Biomaterials research involves the interface inside compound materials and the interface between materials and living body. The former requires higher combining strength, the latter requires favorable biocompatibility. The excellent mechanical compatibility, interface adaptability and tissue associativity between biomaterials and living body imply that their unit cells should satisfy the "Atomic Boundary Condition" on common atomic plane. Presently EET and its BLD method have been mainly used in the known simple lattice structure and can't be applied to assess the electron density continuity between biomaterials and living body for the complex structure of living tissue. But it is reasonable to presume that there should exist atom plane with continuous electron densities amongst successfully employed biomaterials, because they all should have lattice planes with continuous electron densities with living tissues. Ti-6Al-4V and Au-8Pd-10Pt are frequently used as implant materials, and the three calculated unit cells have lattice planes with continuous electron densities (Table 4), which verifies the validity of "Atomic Boundary Condition" applying in biomaterials research. At present, to directly calculate the valence electron structure of living tissue is difficult. For instance, although most of the structural aspects of hydroxyapatite which is constituent of bone have been known, there is not enough foundation to carry out BLD calculation and to make certain some specific atom plane. Furthermore, the structure of organic tissue is more complex. But it is still possible to calculate the valence electron structures of living tissues and to directly evaluate the electron density continuity between biomaterials and living tissue after the sufficient understanding of structure information on living body and reasonable modeling for the structure. The significant progress will be achieved in micro-mechanism of biological performance and molecular design of materials.

Table 4 Some lattice planes with continuous electron density

Alloy	Lattice plane	ρ/Å
Ti-Al	(0002)	168.580
Ti-V	(001)	163.798
Au-8Pd-10Pt	(111)	159.013

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