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First-Principles Study of Segregation Behavior of Cr/Ti/Y at Grain Boundary in Vanadium

Shujuan Lee, Yong Yi, and Peng Bee

***Abstract*—The atomic arrangement and segregation behavior of Ti, Cr, and Y in Σ3 (111) grain boundary of vanadium was performed to illustrate by first-principle calculation. The analyses on the binding energies and geometric positions show that Cr atom is more stable than Ti or Y atom both in the bulk and grain boundary, and Y atom would push away the surrounding V atoms. The computations of segregation energies show that Cr/Y atom segregates at the grain boundary, while Ti atom prefers to stay in bulk V rather than in grain boundary. Furthermore, it is found that Ti/Y atom has a strong driving force to surface segregation. The grain boundary energies calculations and the work of separation and the electron properties show that the segregated Cr can strengthen the grain boundary, whereas segregated Y has the strong tendency to decrease crystallite size.**

***Index Terms*—Grain boundary segregation, surface segregation, first-principles, vanadium alloys, alloying elements.**

I. INTRODUCTION

A combination of low induced radioactivity, good resistance to neutron radiation damage and good elevated-temperature strength makes vanadium-based alloys be very important structural materials in the nuclear industry. Vanadium alloys are candidate materials for fusion reactors. Many studies have reported that vanadium-based alloys containing *4-5%* Cr and *4-5%* Ti exhibit more excellent performance. In vanadium alloys, the addition of Cr would improve the high temperature mechanical performance of the vanadium alloys and the addition of Ti would suppress void swelling under neutron irradiation [1]-[6]. However, it is known that the interstitial impurities of carbon, oxygen, and nitrogen (C, O, N) of a V-4Cr-4Ti alloy also play an important role in radiation effects such as microstructural changes, irradiation hardening, and embitterment [7]-[10]. Recently, there are a large number of reports about how to change Ti(C, O, N) precipitates to improve properties of vanadium-based alloys. Many researchers found that Y-addition could improve the mechanical properties by dispersion strengthening [10]-[15]. It is worth noting that alloying elements would occurs segregation in the vanadium-based alloys during process and neutron irradiation. So it is very important to understand the segregation behaviors of alloying elements in the grain boundary or surface of vanadium-based alloy.

Since it is difficult to get accurate data of the thermo-dynamic quantities of interface with experimental methods, theory provides the applicable implements to obtain reliable information on grain boundary structural properties and energetic properties at an atomic level [16]-[18]. In this paper, we gave an investigation on the segregation behavior of low concentration of solute atom Cr, Ti, Y on the Σ3 (111) grain boundary of V. We have investigated the grain boundary structure of V with/without segregated alloying elements by DFT calculations, and studied their corresponding energy and electronic properties in the same way. The rest of the paper has been divided into three parts. In Section II, we introduces the grain boundary models, the free surface models and computational method in detail. The discussion of the calculations of the segregation behavior of single solute Cr, Ti or Y atom to validate the driving force of segregated Cr, Ti or Y are presented in Section III. At last, we have drawn a conclusion through the analysis above in Section IV.

II. MODELS AND COMPUTATIONAL METHODS

Density functional theory (DFT) [19], [20] calculations within the generalized gradient approximation (GGA) [21], [22], as implemented in the Vienna Ab Initio Simulation Package (VASP) [23] and integrated in the MedeA computational environment, are utilized in this study. The electron-electron exchange and correlation effects are described by Perdew-Burke-Emzerhof (PBE) [24]. The cutoff energy for the plane waves in the basis set was 500 eV. The Monkhorst-Pack [25] K-point mesh with a density of 0.5 $Å^{-1}$, which is forced to be centered on the gamma point, was employed. Partial occupancies was set using first order Methfessel-Paxton smearing with a width of 0.05 eV. Structural optimizations were performed until calculated energies on each atom converged to within about 1×10^{-5} eV and forces on each atom were less than 0.2 eV/Å, which can put the computational time and needed accuracy into a reasonable balance. The conjugate gradient technique is used to optimize and determine the equilibrium structure, which related to the relaxation of all the atoms in the system.

A. Bulk Vanadium Model

Firstly, Computations were performed on pure vanadium. Calculations on pure vanadium were used to assess accuracy of calculations, and the relaxed crystal lattices were later used to build grain boundary models of vanadium.

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Shujuan Lee is with School of Materials Science and Engineering, Southwest University of Science and Technology, Mianyang 621010,PR China

Yong Yi and Peng Bee are with School of Materials Science and Engineering, Southwest University of Science and Technology and Joint Laboratory for Extreme Conditions Matter Properties, Mianyang 621010, PR China (e-mail: yiyong@swust.edu.cn).

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According to the experimental structure, crystalline type of pure vanadium was the body-centered cubic (BCC) crystal structure with symmetry Im-3m. The calculation parameters used to optimize the lattice parameter of pure V will be more rigorous compared with the grain boundary geometric relaxation. The result of optimized lattice parameter was a=3.01 Å. This compares well with experimental results of a=3.03 Å.

B. Vanadium Grain Boundary Model

Based on the coincidence site lattice (CSL) theory, we constructed a V $\Sigma3$ (111) grain boundary with MedeA by rotating a grain around the $[1\bar{1}0]$ axis. The grain boundary model consists of two grains and has seven atomic (111) layer of V in each grain, a cross-sectional area of about 72.12 Å^2, and a total of 96 atoms. The optimized structure is inllustrated in Fig. 1. Due to similar atomic sizes of Ti, Cr, Y with V (The atom radii of Cr is 1.85 Å, Ti 2.00 Å, Y 2.27 Å and V 1.92 Å), the alloying atoms would occupy the substitutional positions along the grain boundary. To facilitate the expression, each atoms in the model are numbered (as shown in Fig. 1(a)). Considering the symmetry type, we only labeled the one part of the supercell, and other parts is the same with the labeled part. The atoms have same number occupy the equivalent positions. *X1* and *X2* indicate the positions of the additive atoms.

C. Vanadium Free Surface Model

The (111) free surface model was created by replacing the second grain system of grain boundary with a vacuum, which making the surface model have the same scales as the grain boundary model have other than containing 48 atoms (Fig. 2).

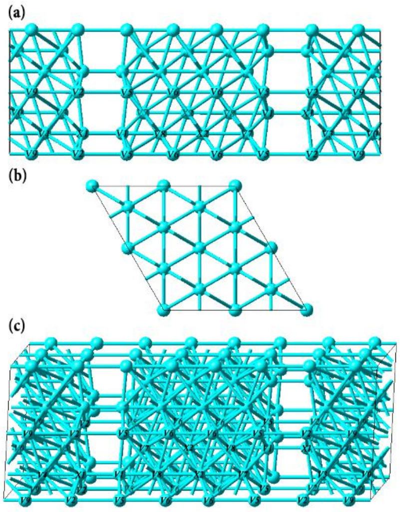

Fig. 1. (a) Side view, (b) top view and (c) 3D view of the computational model structure of the V Σ3 (111) grain boundary.

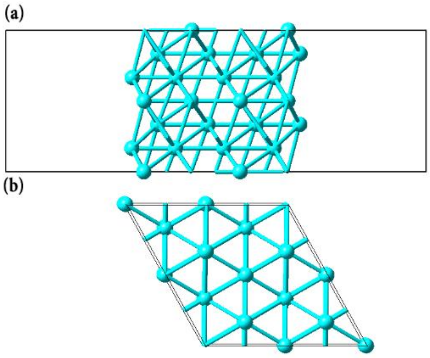

Fig. 2. (a) Side view and (b) top view of the computational model structure of the V (111) free surface.

TABLE I: THE DISTANCES BETWEEN THE ADDITIVE ATOM AND NEIGHBORING V ATOMS(V REPRESENTS THE GRAIN BOUNDARY OF PURE V, X/X1 MEANS THE CASE OF THE ADDITIVE X ATOM IS LOCATED ON X1 POSITION, X/X2 MEANS THE CASE OF THE ADDITIVE X ATOM IS LOCATED ON X2 POSITION)

	Volume (Å^3)	The distances between atoms (Å)									
		X1-V1	X1-V2	X1-V3	X1-V4	X2-V6	X2-V7	X2-V8	V2-V5	V6-V6	V7-V8
V	1373.66	2.35	2.47	2.74	2.26	2.59	2.64	2.51	2.90	2.58	2.66
Ti/X1	1406.83	2.45	2.52	2.87	2.52	2.58	2.67	2.93	3.22	2.62	2.66
Cr/X1	1355.33	2.28	2.46	2.69	2.17	2.59	2.67	2.51	2.79	2.60	2.66
Y/X1	1571.31	2.97	3.03	3.41	3.17	2.58	2.69	2.55	5.26	2.57	2.63
Ti/X2	1401.31	2.35	2.48	2.75	2.24	2.60	2.69	2.72	2.87	2.72	2.69
Cr/X2	1357.65	2.36	2.44	2.73	2.27	2.58	2.63	2.45	2.97	2.54	2.62
Y/X2	1532.50	2.29	2.69	2.88	2.34	3.36	3.06	2.94	2.21	6.92	2.96

III. RESULT AND DISCUSSION

A. Geometry Relaxations and Binding Energy

In order to acquire more accurate results, the configuration optimizations of various grain boundaries were performed. The value of volume for grain boundaries and bulk with or without Ti, Cr and Y are listed in Table I. For Ti-doped and Y-doped grain boundaries, the volume are larger than pure V grain boundary. However, the volume of Cr-doped grain boundary is smaller than pure V grain boundary. In addition, the changes caused by Ti, Cr, Y occupying the X1 position are more obvious than that resulted from Ti, Cr, Y in X2 position. The atomic distances of alloying atoms and neighboring V atoms are also listed in Table I. Compared with pure V grain boundary, the atomic distances of Ti-V1 and Y-V1 increased, while the distances of Cr-V1 decreased. Because the atomic radius of Ti/Y is larger than V. And the changes of Y-doped grain boundary are more significant than Ti-doped because the atomic radius of Y is also larger than Ti. Therefore, addition of Ti and Y causes the lattice expansion, while Cr makes the lattice contraction. While Ti/Cr placed X2 position, the distances between Ti/Cr and neighboring V atoms are very close to V-V in pure bulk V model. It is remarkable that when Y substitute for V atoms in the grain boundary or bulk, the volume increases rapidly. Whether Y is replaced the atom at X1 or X2, the distances between Y and neighboring V atoms increase greatly. Beyond that, the distances between V atoms around the additive Y are larger than other cases, such as V2-V5 in Y/X1 case and V6-V6 in Y/X2 case. In the configuration with Y after relaxation, the addition of Y makes that the distance between two V atoms which are adjacent and equivalent increase sharply so that the V-V bond is broken and the V grain divided into two grains.

In order to determine the stabilities of alloying atoms, the binding energies of various alloying atoms in V bulk, grain boundary, and free surface were calculated. The formula for calculation of the binding energy per alloying atom is shown as the following [25]

$$E_b^{X-doped} = E_{tot}^{X-doped} - E_{tot}^0 - E_{iso}^X + nE_{iso}^V \quad (1)$$

Here, $E_{tot}^{X-doped}$ and E_{tot}^0 represent the total energies of the X-doped and undoped system (including bulk V, grain boundary, surface), respectively; E_{iso}^X and E_{iso}^V are the energies of the isolated Ti, Cr, Y, or V atom, respectively. The n is the number of V atom substituted by Ti, Cr or Y atom in bulk V, grain boundary and surface system. As the symmetry of the grain boundary model, there are two effective V atoms are substituted by alloying atoms. The n equals to 2 when two V atom is substituted by the two alloying atom at various configurations. For the binding energy, the more negative value suggests that the additive alloying element is more favorable to occupy the corresponding position in energy. The binding energies of alloying atoms in various sites of grain boundary are listed in Table II. It is clearly shown that wherever in the bulk or on the grain boundary, the additive Cr atom has more negative binding energy than that of additive Ti and Y atoms. That is to say additive Cr atom is more stable than Ti/Y both in the bulk and grain boundary. The binding energy of the additive Ti/Cr/Y atom in the grain boundary is similar to that in the bulk that the stability of Ti/Cr/Y in grain boundary is close to that in the bulk. It is noticeable that Ti/Y atom has more negative value on the surface than in the grain boundary or bulk, while Cr atom is less stable than in the grain boundary or bulk. It is because the atomic radius of Ti/Y is larger than V, and the space on the surface is larger than in the grain boundary or bulk.

TABLE II: THE BINDING ENERGY OF THE ADDITIVE ALLOYING ATOMS IN THE GRAIN BOUNDARY, BULK, AND FREE SURFACE OF V

The additive atom	The binding energy (eV)		
	Grain boundary	Bulk	Free surface
Ti	-3.63	-3.64	-4.36
Cr	-4.84	-4.70	-4.54
Y	-3.67	-3.50	-4.41

B. *Single Element Segregation Behavior*

Single element segregation behavior can be characterized by segregation energy of single element. The segregation tendency of the additive alloying atoms can be described by segregation energy directly. The segregation energy is defined as the binding energy difference between the alloying atoms in the grain boundary or free surface zone and in the bulk, as the following expression [26]:

$$E_{seg} = E_b^{X-doped} - E_b^{X-doped}\,(bulk) \quad (2)$$

where, E_{seg} is the segregation energy to describe the tendency of the additive X (Ti, Cr and Y) segregates in grain boundary or free surface, $E_b^{X-doped}$ and $E_b^{X-doped}\,(bulk)$ are the binding energy of the additive X when it locates in grain boundary or free surface zone and in V bulk, respectively. In Table III, the segregation tendency of the additive X in various configurations is clearly listed. It can be seen from the positive segregation energy that the additive Ti does not have tendency to grain boundary segregation, instead, it has a slender tendency to remain in the bulk. Some researchers found that Ti is more likely to segregate at the crystal of V-based alloy because there is a good coherent relationship between titanium precipitates in the enriched-Ti zone and the matrix of V-based alloy, but the precipitates will be formed at the grain boundaries by iron ion implantation [27], [28]. The negative segregation energy suggests that the additive Y prefer to segregate at the grain boundary when it comes to Y. In grain boundary, the additive Y is more prone to segregation than Ti and Cr because of the more negative value. This result is entirely correspondent with the experimental observation. It is reported that the addition of Y, which is more likely to exist at the grain boundary, can refine the grain size of the V-based alloys to dispersion strengthened the alloy because of the pinning effects of fine Y dispersoids [10]-[15], [27]-[29]. Furthermore, we found that Ti/Y shows a strong driving force for free surface segregation. On the contrary, there is a larger propensity to grain boundary segregation than surface segregation for Cr, that is, the Cr atoms tend to segregate to the grain boundary rather than to the surface.

TABLE III: THE SEGREGATION ENERGY OF THE ADDITIVE ALLOYING ATOMS IN THE GRAIN BOUNDARY AND FREE SURFACE OF V

The additive atom	The segregation energy (eV)	
	Grain boundary	Free surface
Ti-doped	0.12	-0.71
Cr-doped	-0.14	0.15
Y-doped	-0.18	-0.92

C. *Grain Boundary Energy Calculations*

The effect of Ti, Cr, and Y atoms on V grain boundary strength can be confirmed by calculating the grain boundary energy, and the equation below can be used to calculate the ideal grain boundary strength of grain boundary with alloying element x:

$$W^x = \left(E_{s1}^x + E_{s2} - E_{grain\ boundary}^x\right)/2A \quad (3)$$

Here, E_{s1}^x and E_{s2} are total energies for surface models corresponding to two grains, $E_{grain\ boundary}^x$ is the total energy of a grain boundary model, A is a grain surface area, and the factor 2 accounts for presence of two grain boundaries in the model. Table IV lists the grain boundary energies of various configurations. Compared with the energy of pure V grain boundary, we found that the segregated Ti and Y make the grain boundary energies decreased, while the segregated Cr makes the grain boundary energies increased. That means that segregated Cr can enhance the strength of grain boundary in energy. While the segregated Ti and Y weaken the strength of grain boundary.

TABLE IV: THE GRAIN BOUNDARY ENERGIES (J/M^2) OF VARIOUS CONFIGURATIONS

Models	Pure V	Ti-doped	Cr-doped	Y-doped
Energies (J/m^2)	1.48	0.84	1.71	0.78

D. The Work of Separation

Rice and Wang have described the thermodynamic process of fracture with the work of separation on the basis of Griffith fracture theory [30]-[32]. The separation work can be calculated as below when the grain boundary doped with alloying atoms is cleaved into two free surfaces quickly, that is:

$$W_{sep} = W_{sep}^{0} + 1/S\,[E_{seg}(surface) - E_{seg}(grain\ boundary)] \tag{4}$$

Here, W_{sep}^{0} represents the work required to cleave a clean grain boundary into two free surfaces and S denotes the cross-sectional area. We can evaluated the contribution of the segregated Ti/Cr/Y in grain boundary with the segregated energy of grain boundary and surface,

$$\eta = E_{seg}(\text{surface}) - E_{seg}(\text{grain boundary}) \tag{5}$$

The more positive value of η indicates that more energy is required to cleave the grain boundary into two free surfaces when the additive Ti/Cr/V segregates in grain boundary, while the negative value is opposite. The value of η for the additive Ti, Cr, Y are -0.72, 0.30 and -0.73 eV, respectively. This result confirms that Cr can be regarded as a strengthening element in enhancing the cohesion of grain boundaries, while Ti and Y cannot achieve it.

E. Electronic Properties

The above discussions examine that the segregation behavior of Ti/Cr/Y atoms at grain boundary and surface. To understand the bonding characteristics between Ti, Cr, or Y and V better, the electronic characteristics were selected to describe the bonding more visually. In essence, the formation of chemical bonding is the consequence of the redistribution of the charge. Therefore, we present the charge density map of each grain boundary configuration in Fig. 3. Because of symmetry type, other parts are the same with the labeled part, Fig. 3 only shows the charge density of labeled part. In Fig. 3(a), we illustrate the charge density of pure V grain boundary. It is seen that the free charge between the neighboring V atoms, wherever in the grain boundary or in the grain, results in the formation of V-V metallic bond. With Ti-doped, the charge densities between the Ti atoms and V atoms are reduced (see Fig. 3 (b) and (c)). The charge densities between the Cr atoms and V atoms are quite raised, as shown in Fig. 3 (d) and (e). Compared with the charge density of pure V, the changes of charge densities due to the addition of Ti and Cr are not obvious. However, more significantly, the variability of charge density with Y is much explicitly. The charge densities with Y are shown in Fig. 3 (f) and (g). It is seen that the charge densities between the additive Y atoms and surrounding V atoms are too sparse, and the color between some V atoms around the Y atoms almost turns to blue. That means the bonds between partial surrounding V atoms are broken leading to the grain or grain boundary cleaved due to the addition of Y atom.

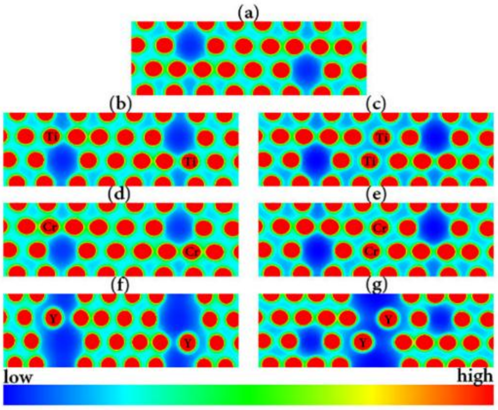

Fig. 3. The charge densities of (a) pure V, (b) (c) the additive Ti, (d) (e) the additive Cr, (f) (g) the additive Y.

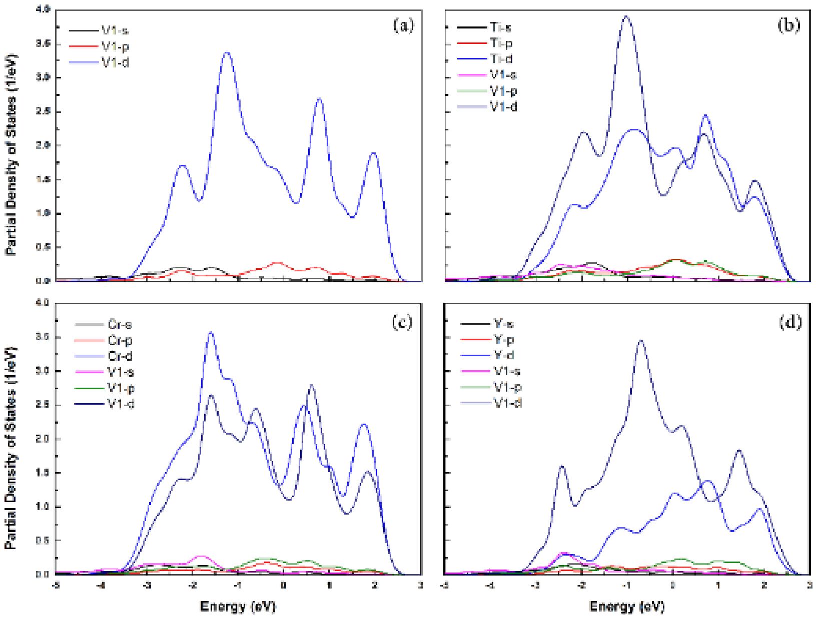

Fig. 4. The partial density of states (PDOS) of X1-V1 in various grain boundary.
(a) pure V, (b) Ti-doped, (c) Cr-doped, (d) Y-doped.

From the analysis of partial density of state (PDOS), we can find that the Cr-V1 chemical bond predominantly stems from the strong interactions between Cr-d and V1-d states at the region from -3.5 eV to -0.5 eV below the Fermi level (see Fig. 4(c)). The chemical bonding formed by charge accumulation between the additive Cr and its neighboring V atom indeed improve the cohesion of V grain boundary. The Ti-V1 chemical bond predominantly stems from the strong interactions between Ti-d and V1-d states, weaker than Cr-V1, at the region from -3 eV to -0.5 eV below the Fermi level, as shown in Fig. 4(b). Furthermore the little contribution of the Y-d and V1-d states at the region from -3 eV to 0 eV below the Fermi level to the Y-V1 chemical bond, shown in Fig. 4(d), can also be noticed. Thus the chemical bonding between the additive Ti or Y and their neighboring V atom cannot enough to enhance the cohesion of V grain boundary. The additive Y even may separate V grain boundary.

IV. SUMMARY

The segregation behavior of Ti/Cr/Y atom on V (111) grain boundary was studied using first principles DFT calculations. The calculations show that the additive Cr atom prefer to substitute V atom in the bulk instead of staying on the grain boundary, and are not easy to segregation, but the additive Ti and Y atom is more likely to segregate at the free surface. In comparison with pure V grain boundary, the grain boundary energy calculations indicate that the grain boundary energies have increased when Cr atom segregates at the grain boundary, while segregated Ti and Y atom make the grain boundary energy decreased. What’s more, our work also shows that there need more separation work to separate the grain boundary into two free surfaces when the additive Cr segregation in the grain boundary, which indicates that the segregation of Cr does enhance the V grain boundary cohesion. However, when the additive Ti or Y segregates in grain boundary, it is easier to cleave the grain boundary into two free surfaces. That suggests that the segregated Ti and Y are not the strengthening element to enhance the cohesion of V grain boundary. The segregated Y may even assist in segregating the grain boundary. The rearrangement of charge shows that the increased cohesion is achieved by stronger metallic binding between Cr and its surrounding V atoms, and the interaction between Cr-d and V1-d plays an important role in the formation of metal bonds. While the segregated Y not only forms the faint bond between Y and its neighboring V atoms, but also weakens the metallic binding between the V atoms surrounding Y atom. Our calculations demonstrate that no significant effect on the boundary strength of alloying element Ti, while Cr can serve as the strengthening element to enhance the cohesion of grain boundary, and Y has a negative impact on the cohesion of grain boundary.

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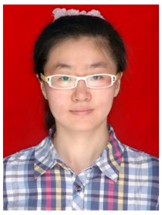
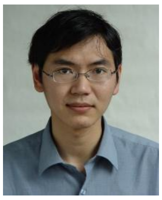


Shujuan Lee was born in Inner Mongolia, P. R. China in 1992. She is a postgraduate student at the School of Materials Science and Engineering, Southwest University of Science and Technology.



Yong Yi was born in Hubei, P. R. China in 1977. He is an associate professor at the School of Materials Science and Engineering, Southwest University of Science and Technology. His currently research include calculations and simulations of metal materials.

Peng Bee was born in Henan in 1985. He is a lecturer at the School of Materials Science and Engineering, Southwest University of Science and Technology. His currently research include calculations and simulations of metal materials.