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Thermo-mechanical properties of V-5Cr-5Ti alloy: 3D molecular dynamics simulation

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This paper presents the results of the study of 3D molecular dynamics simulation to investigate the thermomechanical properties of the V-5Cr-5Ti ternary alloy. The main purpose of this work is to evaluate the quality of the Finnis-Sinclair potential for V-rich V-Cr-Ti random alloys with a body-centered-cubic (bcc) structure. The results demonstrated that the elastic constants of the V-5Cr-5Ti alloy are close to the corresponding value of pure metal vanadium. The two-phase method coexistence solid-liquid was applied to determine the melting point of this alloy at standard pressure. The equilibrium melting point was found at 2237 K, slightly higher than the melting point of Vanadium at the same pressure.

Key words: Thermomechanical, V-5Cr-5Ti, Finnis Sinclair potential, elastic constant, melting point, two-phase method.

INTRODUCTION

Considering the latest advances in production technology, Vanadium based alloys can be considered to be one of the most promising structural materials from the point of view of an application for a number of future thermonuclear systems, since they have high strength values at a temperature of 400 to 700°C, decent thermal creep behaviour, has good thermal conductivity and quite high radiation resistance under neutron irradiation, and much lighter than most metals, and long operating lifetime in the fusion environment. Vanadium-based alloys, which contain 4 to 5 wt.% chromium and 4 to 5 wt.% titanium (V-4Cr-4Ti, V-5Cr-5Ti), have been identified as the most viable materials for use in fusion reactors. Optimal V-based alloy compositions that can afford the extreme environments of fusion reactors have been intensively investigated in the past few years.

There has been much research, including theoretical end experiment, in an effort to search for high-performance V-based alloys which can afford the extreme environment of fusion reactors (Matsui et al., 1996; Kurtz et al., 2004). Among vanadium alloys, system alloys with the composition V-4Cr-4Ti, V-5Cr-5Ti have the best characteristics. Nevertheless, alternative alloys of other systems are also being developed, for example, V – Ga systems with small additions of silicon, which is introduced to increase the mechanical properties. According to calculations (Muroga et al., 2002), the decay rate of induced gallium radioactivity after irradiation in the neutron spectrum of the reactor is the highest of all hypothetically pure metal elements

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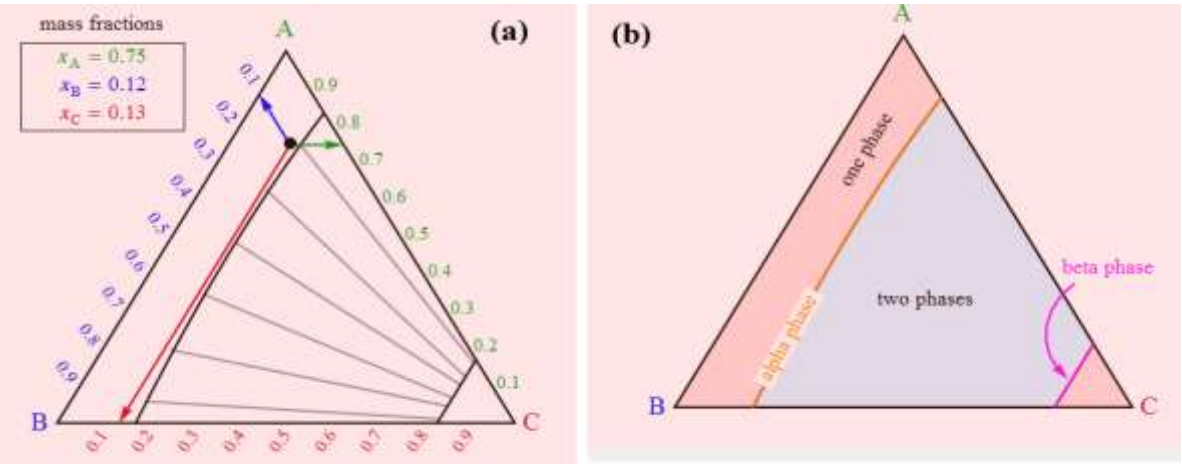

Figure 1. A ternary phase diagram with a phase envelope, the phase behavior of mixtures of V, Cr, and Ti components.

evaluated at present. This fact predetermines that alloys based on the V – Ga system will have a higher rate of decay of the induced radioactivity as compared to alloys of the V- Cr-Ti system, and silicon by its activation characteristics when irradiated with neutrons of different spectra is not inferior to chromium (Li et al., 2012; Smith et al., 1995; Chung et al., 1996).

The elastic properties of materials can be used to characterize the mechanical deformation and structural transformation under external loading (Starostenkov and Aish, 2014a, b; Aish and Starostenkov 2019, 2016; Starostenkov et al., 2013; Aish et al., 2015). For example, the Bulk modulus is used to detect the average bond strength, and the shear modulus is generally considered as an indicator of the mechanical characteristics for a large set of materials.

Figure 1 show a ternary phase diagram with a phase envelope, this diagram is used to represent the phase behavior of mixtures of three V, Cr, and Ti components that are only partially miscible over a range of compositions so that phase separation occurs. Figure 1b shows the two phases (α and β). The black dot is in the β phase as shown in Figure 1b.

A major concern about the use of vanadium-based alloys for fusion reactor first wall/blanket systems is their good mechanical properties and radiation resistance. Previous studies on Vanadium–Titanium–Chromium (V–Ti–Cr) alloys were mainly focused on swelling properties, the ductile-brittle transition temperature under irradiation, and impact toughness as a function of Cr and Ti contents. V–Ti–Cr alloys have attracted considerable interest and have been intensively investigated. Recently, the investigation of Ti1.26V0.63Cr1.08 and $Ti_{1.26}V_{0.63}Cr_{1.11}$ alloys, to which Zr_7Ni_{10} was added to enhance the activation process, was reported (Bibienne et al., 2015; Maisel et al., 2017). A simple example showing the structure and orientation of a 110 family of planes in the body-centred cubic crystal lattice is as shown in Figure 2.

In this paper, we employ Finnis Sinclair potential to investigate the thermo-mechanical properties of the bcc V-5Cr-5Ti based alloy by using molecular dynamics simulation. A supercell of 40 atoms (V-5Cr-5Ti, V36Cr2Ti2) with bcc structure, which have the highest cohesive energy was created, then studied by 3D molecular dynamics simulation.

THE INTERATOMIC POTENTIAL FOR V-5CR-5TI TERNARY ALLOY

The force calculation is the critical part of 3D molecular dynamic simulation, where the potentials are the main part of it. The precision of a 3D molecular dynamic is determined by how precise the interatomic potentials are. Several potentials have been developed for pure metal V, Cr, Ti and some of their alloys (Maisel et al., 2017; Mendelev et al., 2016; Farkas and Caro, 2018). Until recently there is only one empirical potential for V-Cr-Ti ternary alloys, which was developed by Fu et al. (2017) using a fitting method from experiment data (crystal structure, elastic constants and cohesive energy of pure metals V, Cr, Ti) and first-principles calculation (theoretical data of alloys ($V_{15}Ti$, $V_{15}Cr$ and Ti_8Cr_8)). This potential is an amended Finnis-Sinclair for vanadium V-Cr-Ti ternary alloys with bcc structure.

The original FS potential (Finnis and Sinclair, 1984) is an empirical many-body potential based on the idea of embedded atom method (EAM) (Daw and Baskes, 1984), where the total energy of atoms can be written as:

$$U_T = U_{pair} + U_N$$

where U_T is the total energy, U_{pair} is a conventional pair-wise potential term and U_N is an N-body term. N-body

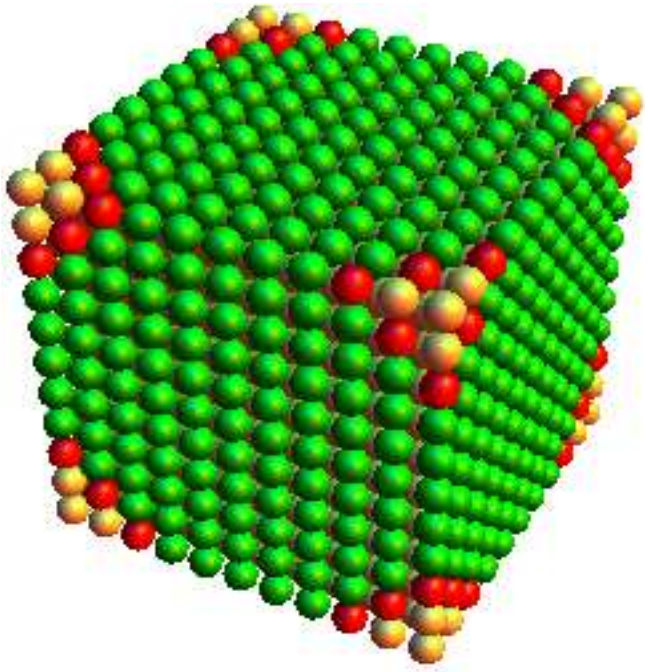

Figure 2. The bcc structure with (110) plane of orientation.

potential can be expressed as:

$$U_N = -A\sum_i \sqrt{\rho_i} = -A\sum_i (\sum_{j\neq i} \phi_r)^{\frac{1}{2}}$$

and

$$r = |r_{ij}| = |r_i - r_j|$$

where A is a positive constant, ρ_i is the embedding functional which represents the energy required to place atom i into the electron cloud. r_{ij} is the radial distance between atoms i and j. The cohesive term ϕ_r take over a parabolic form (Fu et al., 2017):

$$\phi_r = (r-d)^2 \xrightarrow{at} r \leq d \cdot or$$
$$\phi_r = 0.0 \xrightarrow{at} r \succ d$$

where d is a cut-off parameter which lies between the second and third neighbors. Furthermore, U_p is the pair-wise term which can be written as:

$$U_P = \frac{1}{2}\sum_{ij} V_r$$

The amended FS potential have a quadratic polynomial for the pair-potential function Vr (Fu et al., 2017):

$$V_r = (r-c)^2(c_0 + c_1 r + c_2 r^2) \xrightarrow{at} r \leq c \cdot or$$
$$V_r = 0.0 \xrightarrow{at} r \succ c$$

where c is the cut-off parameter which lie between the second and third neighbours, and c_0, c_1, and c_2 are the potential pair parameters. The pair-potential function for repulsive interaction can be expressed as:

$$V_r = D\exp(-\frac{r}{q})$$

where D and q are the pair potential parameters. Totally, there are eight parameters in the amended FS potential for V-Cr-Ti alloys, namely, d, c, c_0, c_1, c_2, A, D and q. Finally obtained amended FS potential parameters for V–Ti–Cr alloys are taken from Fu et al. (2017).

The amended Finnis Sinclair potential reported that this potential gave a good agreement of the predicted formation energies of mono-vacancy and self-interstitial of octahedral interstitial site with experimental and theoretical data confirms the validity of the amended Finnis Sinclair potential in pure V (Finnis and Sinclair, 1984). Furthermore, the agreement of defect properties and mechanical properties of this alloy (V-4Ti-4Cr) with experimental or other theoretical data also support the applicability of the amended Finnis Sinclair potential in V-rich ternary V-Ti-Cr alloys (Howells and Mishin, 2018; Daw and Baskes, 1984). In this work, the amended Finnis Sinclair potential was adopted as a reference potential to investigate thermo-mechanical properties of the V-5Cr-5Ti alloy.

THE CRYSTAL STRUCTURE PREDICTION OF V-5CR-5TI TERNARY ALLOY

As mentioned earlier, the amended Finnis Sinclair potential was developed for V-xCr-yTi ternary random alloys with bcc structure, where V atoms are replaced by Cr and Ti atoms. The physical properties of V-xCr-yTi not only depend on x, y but also the distribution of Cr, Ti atoms in bcc matrix lattice of Vanadium. In our case of research x = y = 5 wt.% or V-5Cr-5Ti, this stoichiometric ratio can be represented by chemical formula V_{18}CrTi which contains total 20 atoms.

Quenched 3DMD simulation, with periodic, constant-pressure boundary conditions, has been made for interstitials in all of the metals and Vanadium ternary alloys were studied in this paper. These degrees of freedom must be available in the calculation of interstitial formation. For atypical 203 block of pure Vanadium, they lower the energy by about 0.04 eV, compared with 163 blocks.

The smallest bcc supercell for k.(V_{18}CrTi) atoms, where

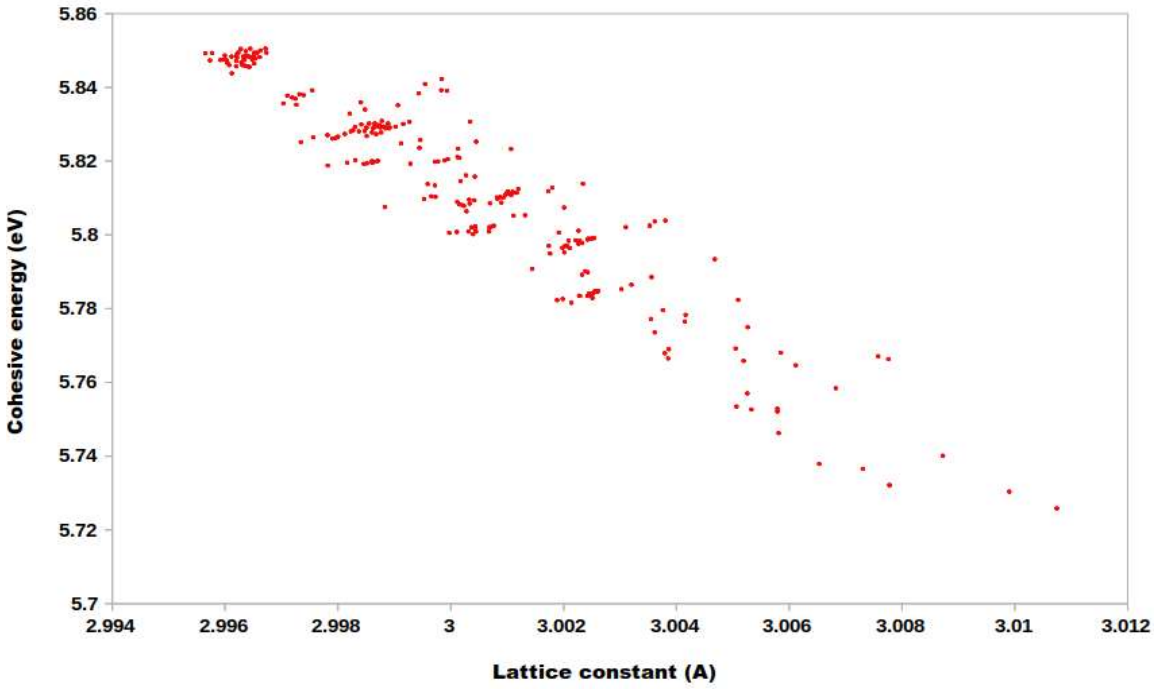

Figure 3. Distribution of cohesive energy-lattice constant from all possible combination of $V_{36}Cr_2Ti_2$ in a bcc supercell of 2×2×5 unit cell.

k is a positive integer, is a supercell of 2×2×5 unit cells with total 40 atoms (k=2). In this supercell 4 of 40 atoms, V are randomly replaced by 2 atoms Cr and 2 atoms Ti with total 2193360 possible combinations to construct the configuration of 2(V_{18}CrTi). In order to find the most stable structure configuration (the structure with lowest possible thermodynamic potential or Gibb free energy), we need to calculate the minimum global energy by global optimization methods (random sampling, simulated annealing, minima hopping, genetic and evolutionary algorithms). However, it is impossible to calculate Gibb free energy for all possible combination of the $V_{36}Cr_2Ti_2$ supercell due to the limitation of computer resource. Therefore in this paper, we just tried to find the equilibrium lattice constant and the corresponding cohesive energy from all possible combination of the $V_{36}Cr_2Ti_2$ supercell by energy minimization in 3DMD using the amended Finnis Sinclair potential. The results are depicted in Figure 3.

The data from Figure 3 shows that the highest cohesive energy structure (5.85 eV) corresponds to the equilibrium lattice constant of 2.995 A°. The V-5Cr-5Ti random ternary alloy $V_{36}Cr_2Ti_2$ can be created by random replaced 4 atom V in bcc supercell by 2 atoms Cr and 2 atoms Ti.

THERMOMECHANICAL PROPERTIES OF V-5CR-5TI ALLOY

Here, we conducted a series of molecular dynamics simulations using the amended Finnis Sinclair potential and 3DMD simulation to investigate some Thermomechanical properties of V-5Cr-5Ti alloy (Farraro and McLellan, 1979). All simulations except the melting annealing simulation were performed in a simulation box of 20×20×20 unit cells with total 16000 atoms (Figure 4). The periodic boundary condition is applied in all directions. We first calculated the volumetric density (g/cm^3) of the new alloy, its equilibrium lattice constant and cohesive energy.

For mechanical properties, we calculated the elastic constants at 0 K of 3 pure metal and the V-5Cr-5Ti ternary alloy. The 3DMD code can be modified for different lattice structure with different potential. The 3DMD created a simulation box 20×20×20 periodic unit cells with 16000 atoms at 0 K, by positive and negative deforming the simulation box in one of the six directions using the change box command and measuring the change in the stress tensor these constants can estimate. By using a dynamic technique, some mechanical properties have been measured for pure Vanadium at (Hoover, 1985). This work, using 3DMD technique, measured E = 125.6 GPa and G = 45.9 GPa at room temperature for V-5Cr-5Ti which are close to those for pure Vanadium. Young's modulus (GPa) values for V-5Cr-5Ti are about 5% higher than those for pure Vanadium. While equations give a Poisson's ratio equals 0.461 and 0.462 for V-5Cr-5Ti.

For understanding thermal properties the melting point, the specific heat (Cp), and thermal conductivity (k) have

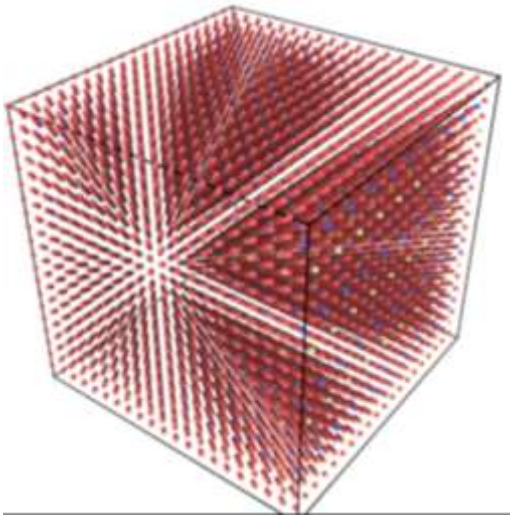

Figure 4. Simulation box of 20×20×20 unit cells which is extended from $V_{36}Cr_2Ti_2$ supercell (16000 atoms).

been measured for V-5Cr-5Ti alloy at standard pressure by using two-phase method which involves a heterogeneous melting of materials (solid and liquid coexistence). In this simulation, a simulation box of 10×10×20 unit cell was used. To control the temperature and pressure, the Nose-Hoover thermostat and barostat method was applied (Birzhevoy, 1997). To create the coexistence liquid-solid phase, the first half part of simulation box along the z-axis was frozen while the second part was heated to 3000 K, far beyond the estimated melting temperature (~vanadium melting point 1910°C). The radial distribution function was used to determine the liquid and solid state. At standard pressure when the temperature is below the melting point, the interface solid-liquid will move to liquid part. When temperature is above the melting point the interface will move to solid part.

From the solid-liquid coexistence when the free energies of solid and liquid state are equal, the melting point was determined. The results from our simulations are shown in Table 1. The thermal property values measured for V-5Cr-5Ti are within 5% of the literature values given for commercially pure Vanadium, which suggests that these properties are relatively insensitive to composition in the range considered. Significantly lower values of thermal conductivity are reported in Najmabadi et al. (1997).

As demonstrated in Table 1, the volumetric density of V-5Cr-5Ti alloy is equal to 6.17 g/cm^3, this result is in good agreement with experiment data from the reference (Starostenkov and Aish, 2014a, b). The elastic constants of this ternary alloy are very close to the corresponding values of pure vanadium (Starostenkov and Aish, 2014a, b; Najmabadi et al., 1997). The melting point of V-5Cr-5Ti Bulk alloy was found to be 2237 K, higher than the melting point of all pure metal in the alloy. The lattice constants and cohesive energies of 3 pure metals are also in good agreement with experiment data because they include the fitting data of amended Finnis Sinclair potential.

Conclusion

V-5Cr-5Ti has excellent thermomechanical properties for fusion reactor materials. On the basis of the present paper of the thermomechanical properties of V-5Cr-5Ti alloy, the major issues that have been adequately addressed in order to qualify a V-5Cr-5Ti alloy as the structural material for components infusion system can be summarized in:

(1) All the results obtained in this work including some physical properties which do not belong to fitting data of the potential are in good agreement with a report from experiment and theoretical work from other authors in literature. This work confirms the validity of the amended Finnis Sinclair potential in vanadium-rich V-5Cr-5Ti alloy. It suggested that we can employ this potential to investigate the radiation resistance property of this ternary alloy in future work.
(2) Cohesive energy has been obtained for V36Cr2Ti2, and compared with the theoretical work of other authors.
(3) The tensile properties, elastic constants, Young's modulus (GPa), Shear modulus (GPa), Bulk modulus (GPa), and Poisson ratio (%) of V-5Cr-5Ti alloy have been studied and compared with other experimental and theoretical papers (Starostenkov and Aish, 2014a, b,

Table 1. Mechanical and thermal properties of V-5Cr-Ti alloy from simulation.

Element		V	Cr	Ti	V-5Cr-5Ti (V18CrTi)
Structure configuration		bcc	bcc	hcp	bcc
Lattice constant (Å)		3.03	2.91	a,b:2.95 c:4.68	2.99
Density (g/cm3)		6	7.19	4.5	6.17
Cohesive energy (eV)		5.31	4.10	4.95	5.85
Young's modulus (GPa)		125.6	126	102	130.2
Shear modulus (GPa)		45.9	43.2	40.1	49.8
Bulk modulus (GPa)		160	160	110	159
Poisson ratio (%)		0.461	0.31	0.42	0.462
Elastic constant (GPa) Cij	C11	237	391	176	244
	C22	-	-	-	244
	C33	-	-	189	245
	C44	47	103	51	60
	C55	-	-	-	60
	C66	-	-	-	65
	C12	121	90	87	117
	C13	-	-	68	116
	C23	-	-	-	116
Melting point (K)		2183 [24]	2180 [24]	1941 [24]	2237
Specific heat (J/(g.K))		0.619	0.493	0.523	0.62
Thermal conductivity (W/(m.K))		23	19.2	22.1	26

2016; Starostenkov et al., 2013; Aish et al., 2015).
(4) The thermal property values measured for V-5Cr-5Ti are within 5% of the literature values given for commercially pure Vanadium, which suggests that these properties are relatively insensitive to composition in the range considered.

CONFLICT OF INTERESTS

The authors have not declared any conflict of interests.

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