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Ternary alloy material prediction using genetic algorithm and cluster expansion

by

Chong Chen

A thesis submitted to the graduate faculty

in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

Major: Condensed Matter Physics

Program of Study Committee:
Kai-ming Ho, Major Professor
Rana Biswas
Wenyu Huang
Soeren Prell

Iowa State University

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2015

This thesis is dedicated to those who supported and encouraged me during the study at Iowa State University.

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ABSTRACT

This thesis summarizes our study on the crystal structures prediction of Fe-V-Si system using genetic algorithm and cluster expansion. Our goal is to explore and look for new stable compounds. We started from the current ten known experimental phases, and calculated formation energies of those compounds using density functional theory (DFT) package, namely, VASP. The convex hull was generated based on the DFT calculations of the experimental known phases. Then we did random search on some metal rich (Fe and V) compositions and found that the lowest energy structures were body centered cube (bcc) underlying lattice, under which we did our computational systematic searches using genetic algorithm and cluster expansion.

Among hundreds of the searched compositions, thirteen were selected and DFT formation energies were obtained by VASP. The stability checking of those thirteen compounds was done in reference to the experimental convex hull.

We found that the composition, 24-8-16, i.e., Fe_3VSi_2 is a new stable phase and it can be very inspiring to the future experiments.

CHAPTER 1. INTRODUCTION

It is the materials which define the technologies accessible in a given era for human beings to utilize, from stone, bronze and iron in the far past, till semiconductors and nanomaterials today. The search and design for new materials have been continuously shaping the era and changing human lives. Thanks to the increasing scientific knowledge and tools, especially the dramatic increase of computational power for the past decades, the search and design of new materials in computer become possible, which helps create new materials much more efficiently and effectively than the traditional trial and error approach. The atomic structures of materials are the keys in understanding their physical and chemical properties. Given the composition of the elements and the arrangement of atoms, theoretically any property can be determined.

Chapter 1 gives a short description of the basics of atomic structure and crystal structure prediction.

Chapter 2 focuses on the Fe-V-Si system. We first looked into the current experimental data and then we did some random search on the sample compositions and made assumption of bcc underlying lattice for metal (Fe and V) rich compounds.

In chapter 3, we described our scheme in the computational search. And genetic algorithm, cluster expansion and convex hull analysis were briefly explained.

Chapter 4 shows our computational results, followed by some discussions.

The last chapter is the tentative conclusion and future work.

1.1 **Atomic structure of materials**

Study on structures of materials could be investigated on small scale as atomic, say, angstroms, to macro scale, say, meters. Structures on different scales explain different properties.

In this thesis, we are studying the structures at atomic scale, where the electrical, magnetic and chemical properties can be understood. Solid materials may be classified into two classes based on the arrangement of atoms: crystalline and non-crystalline, as illustrated in Figure 1.1.

The atoms in crystalline are highly ordered while non-crystalline lack any repetitive pattern of a crystalline. Our study focuses on atomic structures of crystal solids.

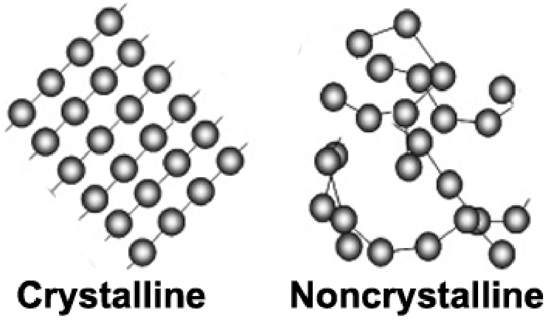


Figure 1.1 Crystalline (left) and non-crystalline (right)

A crystal structure is a certain arrangement of atoms or molecules in a crystalline solid and those particles are surrounded by like neighbors and exhibit repetitive geometry pattern. It describes a highly ordered structure, occurring due to the intrinsic nature of its constituents to form symmetric pattern. Systematic and detailed description on the crystallography may be found in a variety of textbooks [Ashcroft and Mermin, 1976; Kittel, 2005].

Only a few key concepts are briefly explained.

Symmetry is the periodic repetition of crystal structures. There are two general types of symmetry, translational and point symmetry. Translational symmetry describes the periodic repetition across all three spatial directions. While point symmetry explains the periodic repetition around one point, and the operators include reflection, rotation, inversion and improper rotation.

Both proper and improper rotation axes, reflection planes and centers of symmetry are called symmetry elements.

Point groups: It makes 32 possible crystal classes (point groups) by combining the point symmetry operations in different ways.

Space groups: Besides the point group operators, the space group also includes the translational symmetry operators, and there are 230 distinct space groups.

Bravais lattices: Lattice is an array of points periodically repetitive through the distance. By combining crystal classes with the various possible lattice centering, Bravais lattice describes the geometric arrangement of the lattice points, and thus the translational symmetry of crystals.

Unit cell: Unit cell is a small box containing one or more atoms arranged in three dimensions, as illustrated in Figure 1.2. The stacked unit cells in three dimensional spaces describe the bulk arrangement of atoms of the crystal. The unit cell itself can be represented in terms of its parameters, which are lengths of cell edges (a,b and c) and the three angles between (see Figure 1.2), while the positions of the atoms inside the cell can be described by sets of atomic positions (x,y and z).

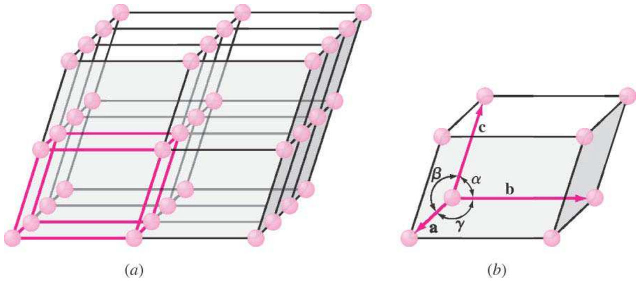


Figure 1.2 Unit cell (in solid line) and its parameters.

1.2 Crystal structure predictions

To predict the crystal structure solely based on the chemical composition is one of the most fundamental challenges condensed matter science [Woodley,2008]. The two main determinants of the crystal structure are its constituent chemical elements and the way it has been formed, governed by the laws of quantum mechanics, thermodynamics. The lower the energy structure are generally favored and viewed as more stable, which suggests that crystal structure prediction is searching for minimum energy among different arrangements of atoms. Two things are needed for solving the problem, an accurate method to calculate the energy and an efficient searching algorithm to reach the minimum energy quickly.

Based on quantum mechanics, theoretically, structure energy can be calculated by solving Schrodinger equation. While the equation for many-atom system is so complicated that it is analytically not feasible to solve. The problem was solved by density functional theory (DFT), which was developed in 1964 by Kohn et al [Hohenberg and Kohn, 1964; Kohn and Sham, 1965], along with various empirical potentials, as instruments to calculate the structure energies.

For search algorithms, several well-known candidates were invented and utilized to predicted the crystal structures, such as simulated annealing [Doll et al, 2007], genetic algorithm [Deaven and Ho, 1995; Wu et al., 2014] and ab initio random search [Pickard and Needs, 2011].

Each of the above algorithms has been successfully applied to the structure prediction for the formation of new compounds. Our study of Fe-V-Si system will be based on genetic algorithm to search for the lowest energy structures, and this algorithm will be shortly introduced in chapter 2.

1.2.1 Free energy

Generally, the Gibbs free energy of a structure was defined as:

$$G = E + PV - TS \qquad \text{(Equation 1.1)}$$

Where E is internal energy, P is pressure, V is volume, T is temperature and S is entropy.

1.2.2 Density functional theory

Stationary electronic states of an N-electron system can be described by many body time-independent Schrodinger equation with wave function Ψ :

$$\begin{aligned} &\hat{H}\Psi = E\Psi \\ &\hat{H} = \hat{T} + \hat{V} + \hat{U} = \sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m_i}\nabla_i^2\right) + \sum_{i=1}^{N} V(\vec{r}_i) + \sum_{i<j}^{N} U(\vec{r}_i, \vec{r}_j) \end{aligned} \qquad \text{(Equation 1.2)}$$

Where $\hat{T}$ is the kinetic energy , $\hat{V}$ electron-ion Coulomb attraction and $\hat{U}$ is electron-electron Coulomb repulsion.

Density functional theory (DFT) is a computational quantum mechanical modelling widely used in physics, chemistry and materials science to investigate the electronic structure (principally the ground state) of many-body systems, in particular atoms, molecules, and the condensed phases. Using this theory, the properties of a many-electron system can be determined by using functionals, i.e. functions of another function, which in this case is the spatially dependent electron density. It is among the most popular and versatile methods

available in condensed-matter physics, computational physics, and computational chemistry for calculations in solid-state physics since the 1970s. In many cases the results of DFT calculations for solid-state systems agreed quite satisfactorily with experimental data.
The Vienna Ab initio Simulation Package (VASP) is a computer program for atomic scale materials modelling, e.g. electronic structure calculations and quantum-mechanical molecular dynamics, from first principles. It computes an approximate solution to the many-body Schrödinger equation, either within density functional theory (DFT), solving the Kohn-Sham equations, or within the Hartree-Fock (HF) approximation, solving the Roothaan equations. Hybrid functionals that mix the Hartree-Fock approach with density functional theory are implemented as well. To determine the electronic ground state, VASP makes use of efficient iterative matrix diagonalisation techniques, like the residual minimization method with direct inversion of the iterative subspace (RMM-DIIS) or blocked Davidson algorithms.

1.2.3 Empirical potentials

Despite DFT give accurate calculation of the energy of many body problem (at T = 0K), it becomes computationally more expensive as the system size grows, say, up to 100 atoms. Besides the energy evaluation for larger system which takes longer, the exponentially increasing configuration spaces for larger system is the main reason. Empirical potentials have been developed as alternative ways for faster energy calculations for larger systems. Empirical potentials can be considered as pair potentials between pairs of atoms or many body potentials, including the interactions between three or more particles. Lennard-Jones potential is a simple example to calculate the van der Waals forces [Lennard-Jones, 1924]

$$U(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad \text{(Equation 1.3)}$$

Among the various empirical potentials, cluster expansion is one of the most widely used one and will be briefly described in the methodology part, chapter 3.

1.2.4 **Optimization algorithm**

As mentioned in 1.2.1, two things are needed to perform crystal structure prediction. One is an accurate method to evaluate the energy and it is usually different types of empirical potentials and the other one is an efficient search algorithm to get the optimal structure fast. Among a variety of algorithms developed in predicting crystal structures, genetic algorithm is applied in our study due to its accuracy of energy calculation and efficiency in structure exploration. It will be briefly discussed in chapter 3.

CHAPTER 2. Fe-V-SI

Fe-V-Si system had been studied due to its interesting magnetic and electronic properties [Endo,1995;Alam 2006;Watanabe,2005]. Report told that Fe_3VSi might be ferromagnetic, yet the structures was not known, though the structures of Fe_2VSi and FeVSi are experimentally known [Mochai,1967]. Experimentalists at Ames Lab are interested knowing the crystal structure of Fe_3VSi and hunting for other stable phases.

2.1 Experimental background and research interest

The first investigation of Fe-V-Si was performed back in 1940s [Vogel, R, et al 1940] and Vogel et al examined the liquid's surface in the region of Fe-FeSi-VSi2-V by thermal analysis, and a limited metallographic observation of the solid alloys system. Since then, Some 80 ternary alloys were examined, the compositions of which lay on composition lines from the silicon corner to the compositions 10, 20, 30, 40, 50 and 60 mass% V on the Fe-V axis [H.Xu et al 2008].

The current experimental findings was briefly summarized in Figure 2.1. and the known compounds were tabulated in table 2.1.

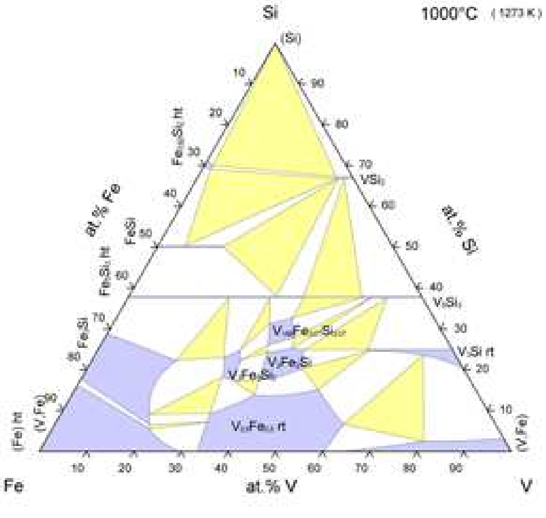


Figure 2.1 Experimental ternary plot on Fe-V-Si system [Raynor, et al, 1988]

Including pure Fe, V and Si, those experimentally known compounds works as reference to the computational predictions of new compositions. See table 2.1

Table 2.1 Crystallographic Data of Solid Phases

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
(V) <1910	cI2 Im-3m W	a = 302.4	pure V at 25°C
(αFe) < 912	cI2 Im-3m W	a = 286.65	pure Fe at 25°C
(αSi) < 1414	cF8 Fm-3m C (diamond)	a = 543.06	T = 25°C
α1, Fe3Si < 1235	cF16 Fm-3m BiF3	a = 565.0	D03 11.0 to 30.0 at.% Si
α2, Fe-Si < 1280	cP2 Pm-3m CsCl	a = 281	B2 10.0 to 22.0 at.% Si
β, Fe2Si 1212 - 1040	hP6 P-3m1 Fe2Si	a = 405.2 ± 0.2 c = 508.55 ± 0.03	19.93 to 21.31 at.% Si
η, Fe5Si3 1060 - 825	hP16 P63/mmc Mn5Si3	a = 675.9 ± 0.5 c = 472.0 ± 0.5	

Table 2.1 Continued

ε, FeSi < 1410	cP8 P213 FeSi	a = 451.7 ± 0.5	49.6 to 50.8 at.% Si
ζα, FeSi2(h) 1220 - 937	tP3 P4/mmm FeSi2	a = 269.01 c = 513.4	69.5 to 73.5 at.% Si
σ, FeV < 1252	tP30 P42/mnm σCrFe	a = 896.5 c = 463.3	39.9 to 70.4 at.% Fe
V3Si < 1925	cP8 Pm-3n Cr3Si	a = 472.72	19 to 25.5 at.% Si
V5Si3 < 2010	tI32 I4/mcm Si3W5	a = 943 c = 471	
VSi2 < 1677	hP9 P6222 CrSi2	a = 457.5 c = 638.5	
* τ1, Fe4V5Si4	tP56 P41212 Mn5Si2	a = 888 c = 867	30 to 40 at.% Fe
* τ2, Fe2V2Si	hR53 R-3 Co5Cr2Mo3	a = 1079.9 c = 1924.3	45.5 to 52 at.% Fe

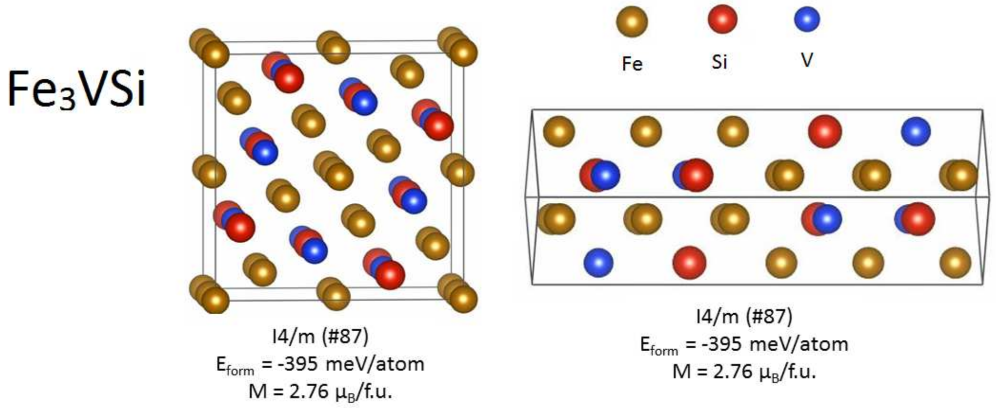
Table 2.1 Continued

* τ3, Fe5V3Si2	cI58 I-43m αMn	a = 884.3	32 to 44 at.% Fe
* τ4, Fe2VSi	cF16 Fm-3m AlCu2Mn	a = 567.4	L21 Heusler structure phase at 300 K

2.2 Theoretical assumption: bcc underlying lattice

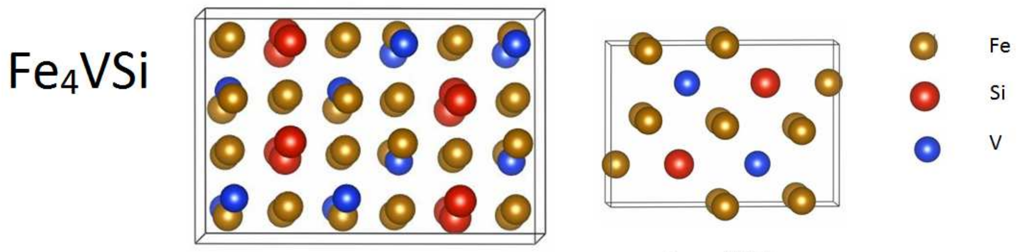
Cluster expansion method was applied as the empirical potentials to calculate the structure energies, and it requires the search on a given lattice, say, face centered cubic (fcc) or body centered cubic (bcc). Some initial random searches were done for three Fe-rich (or metal-rich, Fe and V) compounds, Fe_3VSi, Fe_2V_2Si and Fe_4VSi, with 2 and 4 formula units. We found that all the lowest energy structures of those compounds were bcc underlying lattice. Pure Fe and V are both bcc lattice. Therefore, structures searches using genetic algorithm and cluster expansion were based on the assumption of bcc underlying lattice for metal-rich compounds.

The two lowest energy structures from random searches were attached in Figure 2.2.



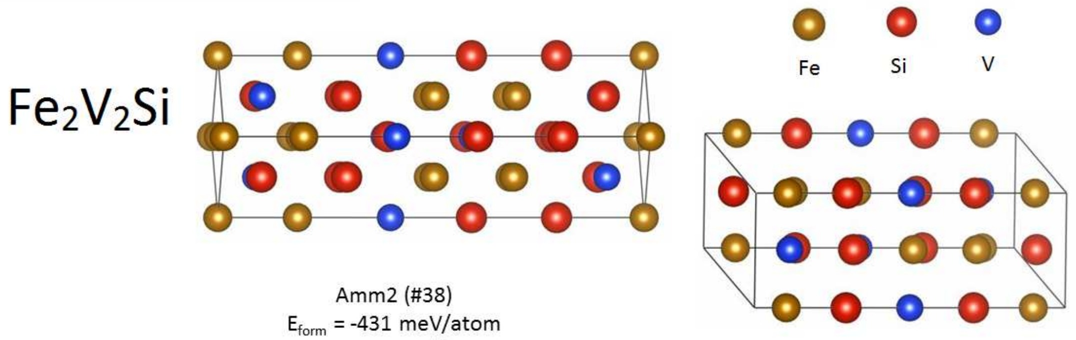
I4/m (#87)
E_{form} = -395 meV/atom
M = 2.76 μ_B/f.u.

I4/m (#87)
E_{form} = -395 meV/atom
M = 2.76 μ_B/f.u.



Cmcm (#63)
E_{form} = -226 meV/atom
M = …… μ_B/f.u.

Cmcm (#63)
E_{form} = -226 meV/atom
M = …… μ_B/f.u.



Amm2 (#38)
E_{form} = -431 meV/atom
M = 0.31 μ_B/f.u.

R-3m (#166)
E_{form} = -429 meV/atom
M = ~ 0.0 μ_B/f.u.

Figure 2.2 Lowest energy structures from random search are bcc underlying lattice.

CHAPTER 3. COMPUTATIONAL METHODS

3.1 Genetic algorithm

Genetic algorithm (GA), is a search heuristic that mimics the process of natural selection. It belongs to the larger class of evolutionary algorithms, which generate solutions to optimization problems using techniques inspired by natural evolution, such as inheritance, mutation, selection, and crossover. It was first developed to optimize atomic structures by Deaven and Ho, where the fullerene cluster structures up to C_{60} were efficiently found from random searches. Since then, it has been applied to various clusters [Ho et al., 1998], bulk crystal [Oganov et al., 2009] and interfaces and grain boundaries[Zhang et al., 2009, Zhao et al., 2014b].

The evolution usually starts from a population of randomly generated individuals (crystal structures, for instance), and is an iterative process, with the population in each iteration called a generation. In each generation, the fitness (structure energy) of every individual in the population is evaluated.

The more fit individuals (lower energy structures) are stochastically selected from the current population, and each individual is modified (recombined and possibly randomly mutated) to form a new generation. The new generation of candidate solutions is then used in the next iteration of the algorithm. The algorithm terminates when either a maximum number of generations has been produced, or a satisfactory fitness level has been reached for the population.

See Figure 3.1 for illustration.

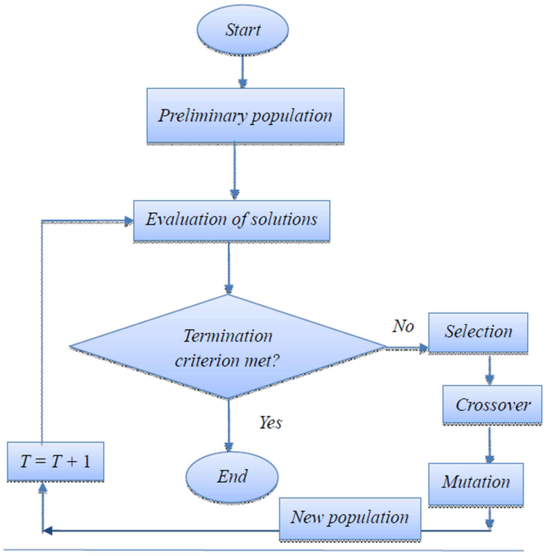


Figure 3.1 Flow Chart of Genetic Algorithm

3.2 Cluster expansion method

A classic example of a multiscale model is the cluster expansion method. In many materials, particularly (but not only) many metal alloys, there are distinct phases that differ only by the arrangement of individual elements on a lattice, but the underlying spatial lattice (bcc, fcc, etc.) remains in principle the same for several of these phases. If the underlying lattice is known, we know the actual positions ($R_1, \ldots, R_M$) in principle, we just don't know which kind of atom sits on each site and we don't know the configuration. E becomes a simple function of the occupation of these sites by the different elements (the configuration). One can always map the configurational energies $E(\sigma)$ of all possible configurations σ, if the model includes all types of cluster f that can be found among the lattice sites: all inequivalent pairs, triplets, quadruplets, etc., up to the N-body interactions.

By denoting $E(\sigma)$ the energy of a given configuration per lattice site, the equation of a cluster expansion on a lattice was given:

$$E(\sigma) = E^{CE}(\sigma) = \sum_f J_f \Pi_f(\sigma) \qquad \text{(Equation 3.1)}$$

Where J_f is the cluster expansion coefficients that denote effective interaction strength associated with a particular combination of lattice sites, f.

$\Pi_f(\sigma)$ is the spin-products averaged over the entire lattice and detailed description may be found in [IPAM, 2014].

In our study on the Fe-V-Si system under bcc underlying lattices, all the coefficients were obtained via the fitting of DFT calculations.

3.3 Convex hull analysis

The enthalpy of formation for any compound $A_xB_yC_z$ can be defined as:

$$\Delta H(A_xB_yC_z) = H(A_xB_yC_z) - xH(A) - yH(B) - zH(C) \qquad \text{(Equation 3.3)}$$

Where H is the total energy of the corresponding configuration and nature favors those compounds with a negative formation energy, which can be interpreted as being stable. In order to construct convex hull, the lowest energy of given compositions (or combinations of compositions that gives such composition). Simply put, the convex hull can be generated by linking the lowest energy structures. The linked line versus the composition curve, called convex hull, illustrated in Figure 3.2 for binary alloy A_xB_y.

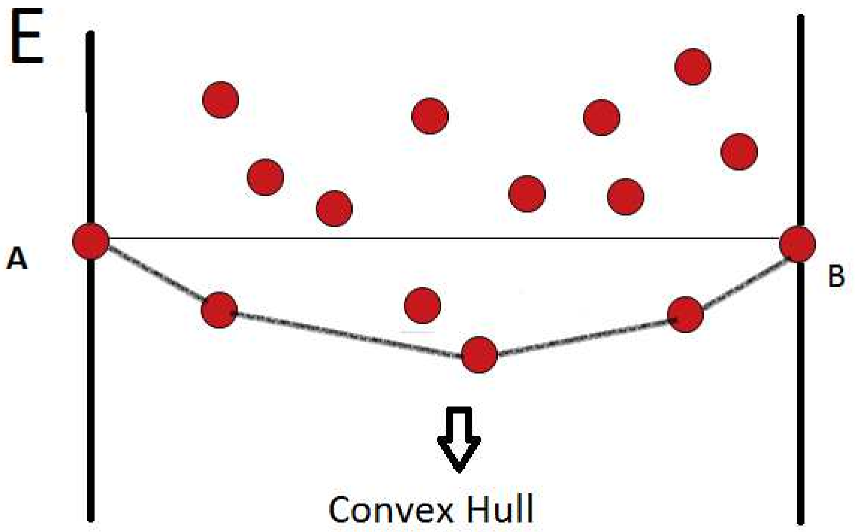


Figure 3.2 Convex hull of binary alloy A_xB_y, each red sphere denote a configuration And the two lying at the corners are pure A and B, respectively.

In the analysis, the vertical (energy) gap between the any configuration and the convex hull were calculated. For any configuration with the formation energy above the convex hull, the corresponding energy gap is great than zero, which suggests this configuration is not a new stable phase.

Compositions with formation energy below he convex hull may be perceived as stable since the energy gap is negative. When the new configuration lies on the hull, the energy gap is zero, and it may be stable.

3.4 The scheme and computational details

3.4.1 The scheme

On the theory side, our study on Fe-V-Si system started with random search of sample compositions as previously mentioned in chapter 2 and we found that all the three metal rich (Fe and V) compounds are bcc underlying lattice. Under bcc underlying lattice, we explored much broader configurational space across different system sizes, from 24 atoms up to 120 atoms with different supercells. Totally, we explored 1195 compositions across different system sizes and supercells. On the experimental side, we calculated the lowest DFT energies for those experimental known compounds, based on which we constructed the convex hull and it worked as the reference frame for stability prediction of new compositions. Our methodology can be clearly seen in Figure 3.4 and

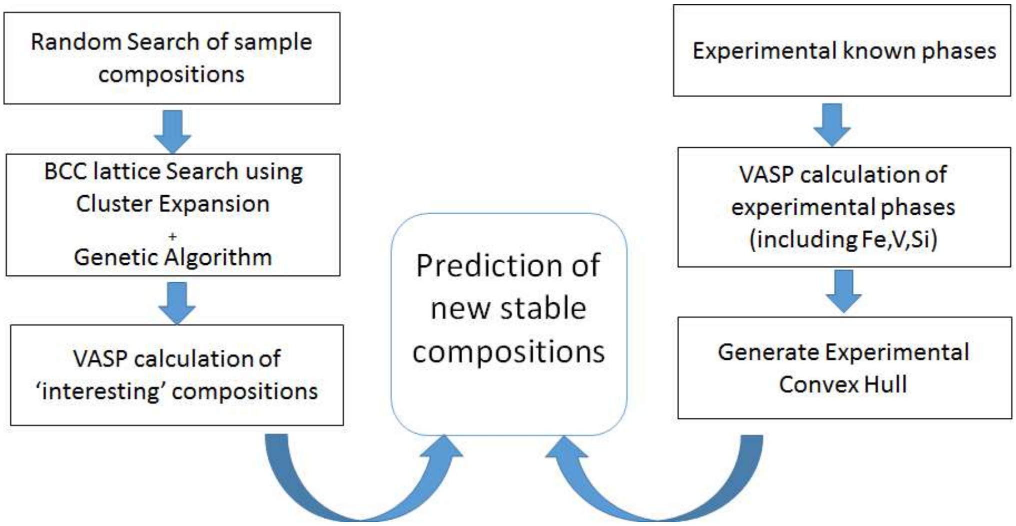


Figure 3.3 Computational procedure in predicting new compounds of Fe-V-Si

3.4.2 Computational details

The Fe-V-Si system we have explored are from 24, 30, 40, 48, 54, 60, and up to 120 atoms. After a careful comparisons among those searched energies, the 48 atoms system was adopted for a systematic searches with 720 compositions, which was illustrated in Figure 3.4. About the genetic algorithm, the pool size set as 800 and generation as 3000 for GA structure optimization. All GA searches converged at no more than 400 generations.

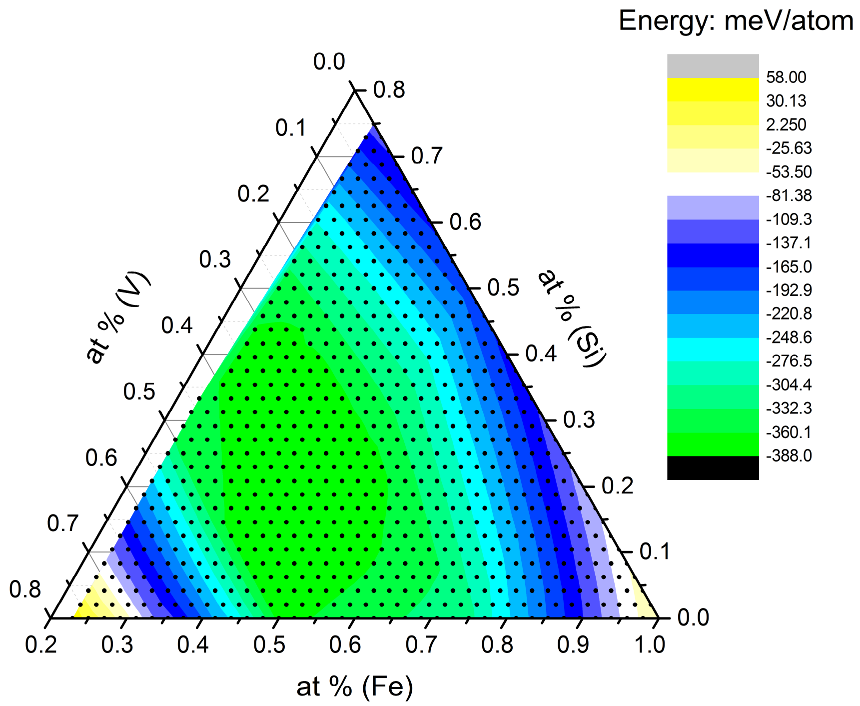


Figure 3.4 Ternary plot of systematic search for 48 atoms Fe-V-Si. 720 compositions (dots on the plot) are illustrated. The green area are those with lower formation energy.

DFT calculation (VASP) for both experimental compounds and new compositions were performed under the following setting, k-points 25, with spin polarization and the structures were fully relaxed.

CHAPTER 4 RESULTS

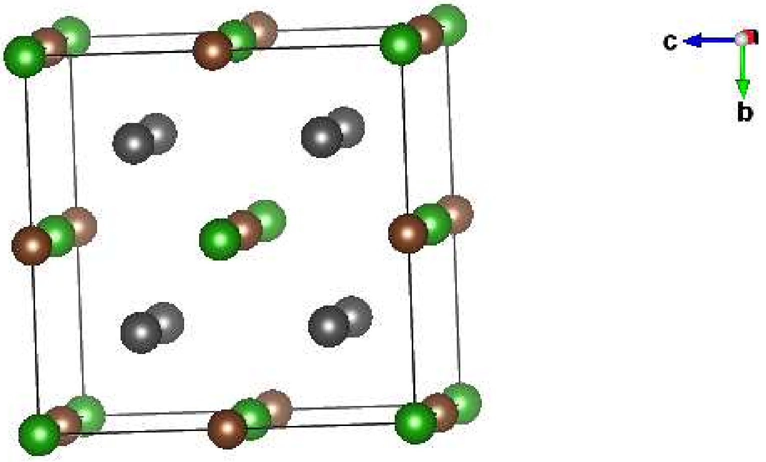
Our results will be briefly reported in two parts.

First, the experimental known phase, **Fe_2VSi**, under bcc lattice, was confirmed by our computational search by GA and Cluster expansion.

More importantly, one new stable compound, **Fe_3VSi_2** was discovered.

4..1 Confirmation of experimental phase Fe_2VSi

Our GA search first confirmed the experimental bcc phases, Fe_2VSi. See Figure 4.1.



a=5.785 angstrom(vs 5.67)
alpha = 90.00
Space group: Fm-3m
Symmetry Int No. 225

Figure 4.1 Lowest energy structure of Fe_2VSi from GA search**.**
Fe in grey, V in brown, and Si in green

This confirmation of experimental bcc phase suggests our search under bcc underlying lattice assumption is reliable and effective in its predictive power.

4.2 Discovery of new stable compound, Fe_3VSi_2

Among those 720 compositions from 48 atoms, one dozen were selected to be analyzed at first. The selection of those one dozen are based on lower formation energies. See Figure 4.1 for details.

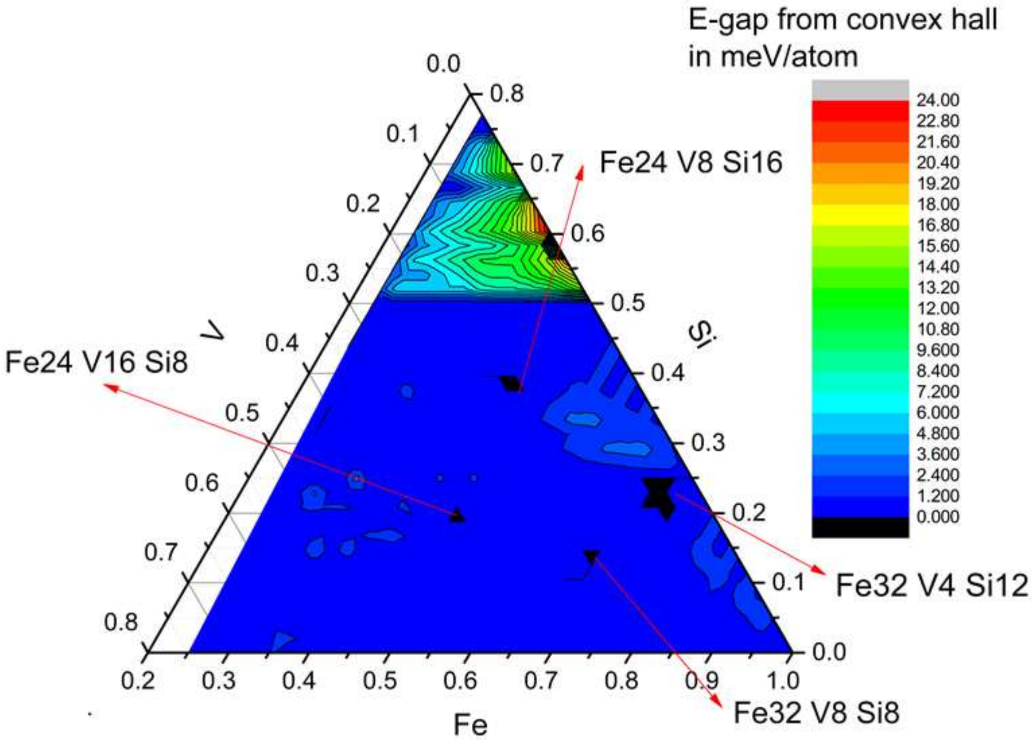


Figure 4.2 The ternary plot of 720 compositions from 48 atoms systematic search, 4 remarkable compositions were identified, as marked in the plot. The color tells the energy gap from convex hull constructed on the cluster expansion formation energies and it indicate the relative stability of each composition on the plot. Besides those four, 8 more were selected from the lowest energy among all.

One last compound the experimentalists were interested are 3:1:1, and the searches were done for different system size, 30, 40, 50 and 60 atoms, and the lowest formation energy (per atom) was from the 40 atoms system, i.e. 24-8-8, which was added to our pool of stability prediction and it makes 13 compositions, see Table 4.1.

DFT calculation was done for those compositions and formation energies obtained, and then put in the reference of experimental convex hull to check the possible stability. Interestingly, among those 13 compounds, the only one that lies below the experimental convex hull is 24-8-16, i.e. Fe_3VSi_2.

Table 4.1 Selected 13 compositions for stability prediction under convex hull. One new composition, 24-08-16, was found to be below convex hull. All energies in eV/atom. The ternary plot of the stability prediction can be seen in Figure 4.2.

Fe-V-Si	DFT energy	Energy gap (meV/atom)	Remarks
24-8-8	-506.82	32.83	3:1:1
24-8-16	-626.61	-5.9	3:1:2
24-16-8	-602.42	17.13	
32-08-8	-400.75	48.96	
18-12-18	-399.03	362.94	
20-10-18	-491.74	213.59	
21-9-18	-531.47	145.54	
22-9-17	-550.1	112.34	
23-6-19	-542.69	63.93	
23-8-17	-579.89	54.23	
24-5-19	-576.51	5.35	
24-7-17	-542.69	63.11	
32-4-12	-375.56	19.13	

The ternary plot of stability prediction on the new compounds can be clearly seen in Figure 4.3, where energy gap from experimental convex hull were classified as negative and positive and denoted by different colors.

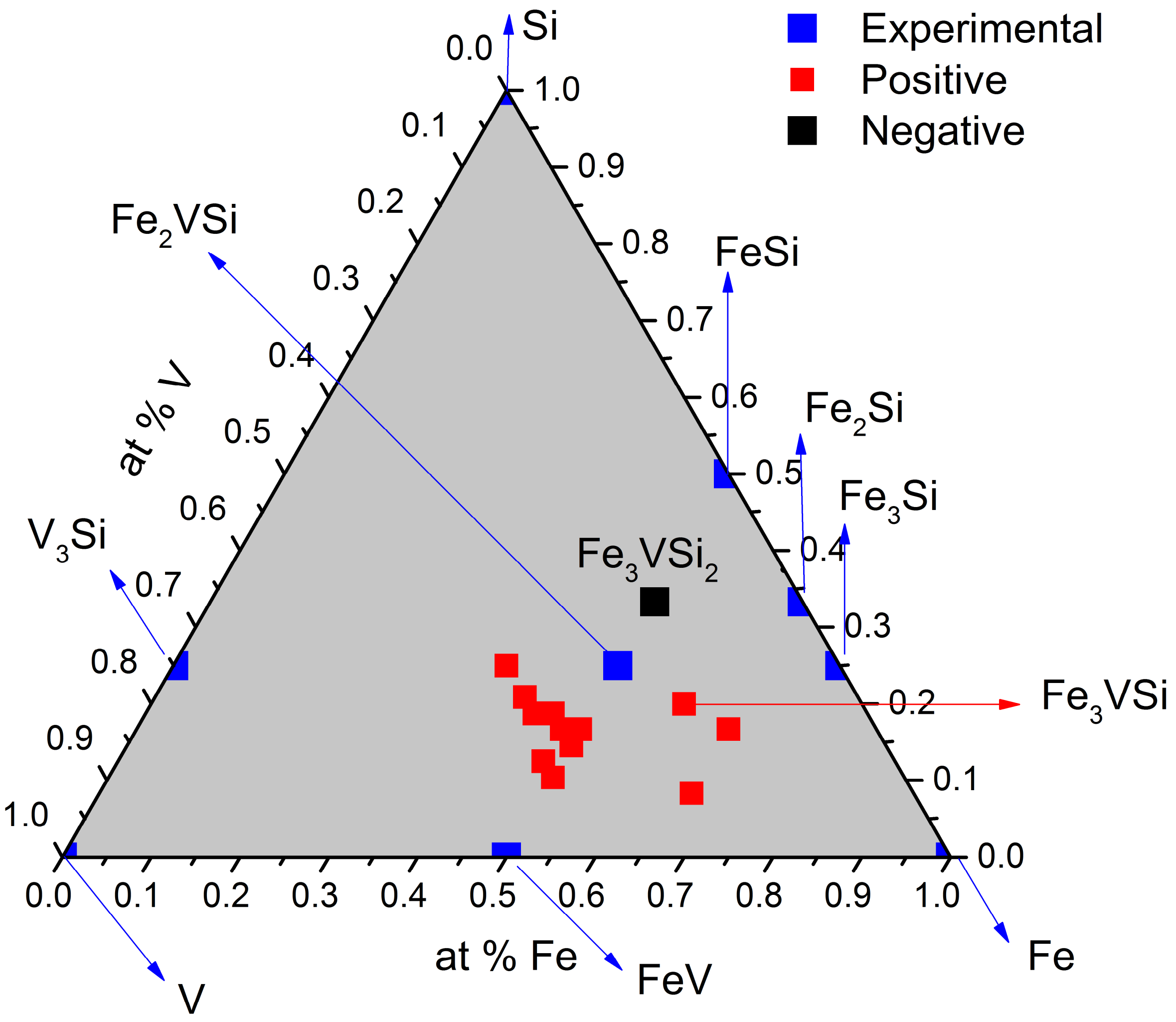
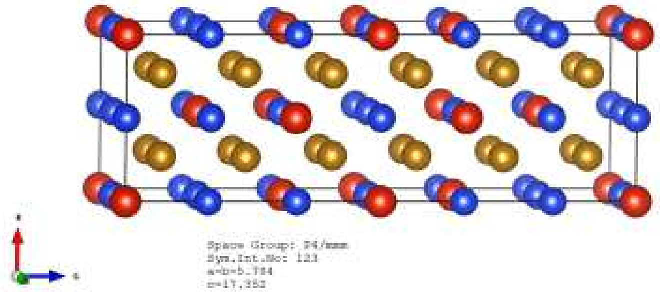


Figure 4.3 Ternary plot of stability prediction of 13 new compositions. The blue makers denote the ten experimental known phases. The energy gap of new compositions from experimental convex hull were classified as positive (above) and negative (below). Only one negative energy gap (6meV/atom below) were found, which is 24-8-16, i.e. Fe_3VSi_2, and can be seen as stable phase. While Fe_3VSi, denoted by a red arrow, is not stable since it lies above the convex hull by 33 meV/atom.

About the compound, Fe_3VSi, upon which the interest on Fe-V-Si was raised by the experimentalists, our study shows it is not stable due to the relatively high DFT energy. It is very interesting that we found new stable composition, 24-8-16, i.e., Fe_3VSi_2

The crystal structures, including its symmetric properties and magnetic moment of it's lowest energy structures can be found in Figure 4.4. And this is a B2 structures without any 2nd nearest neighbor of V-V.

New Stable Fe_3VSi_2 crystal structure



Fe in brown, Si in blue and V in red.

B2 ordering with Fe on α-site, V and Si on β-site
No V-V at 2nd NN

Magnetic moment

Fe1	**8r**	**0.41**
Fe2	**8r**	**0.39**
Fe3	**8r**	**0.19**
V1	4i	-0.06
V2	1a	-0.01
V3	2h	-0.03
V4	1b	0.01
Si1	2e	-0.01
Si2	1d	-0.02
Si3	4i	-0.01
Si4	2g	-0.01
Si5	2h	-0.01
Si6	1c	-0.01
Si7	2g	-0.01
Si8	2f	-0.01

tot moment 7.473

Figure 4.4. Crystal structures for the lowest energy composition, Fe_3VSi_2, the symmetry and lattice parameters were attach. Magnetic moment from each atom were listed on the right .

CHAPTER 5. CONCLUSION

Crystal structure prediction on Fe-V-Si was studied using genetic and cluster expansion. Hundreds of possible configurations were explored and 13 of them were selected for the stability prediction in reference to experimental convex hull, which was constructed based on the DFT energies of those 10 experimental phases.

Our finding suggests that Fe_3VSi_2 is a new stable compound and this sheds light on the future experiments.

While Fe_3VSi, as the experimentalists were interested, is not stable based on our study. About future work, more compositions from search are to be studied for stability prediction.

Other properties, like, magnetic and chemical property of compounds in Fe-V-Si system might be interesting for further study.

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