SUMMARY OF DOCTORAL THESIS

The author's name: Le Hong Viet

Thesis title: Study on thermodynamic properties of defective ternary and binary interstitial alloys with face-centered cubic and body-centered cubic structures.

Scientific branch of the thesis: Physics

Major: Mathematical and theoretical physics **Code:** 9 44 01 03

The name of postgraduate training institution: Hanoi Pedagogical University 2

1. Thesis purpose and objectives

Applying statistical moment method (SMM) to study the thermodynamic, melting and structural phase transition properties of cubic defective interstitial alloy AC and substitutional and interstitial alloy ABC taking into account the influence of temperature, pressure, concentration of substitutional atoms, concentration of interstitial atoms and concentration of equilibrium vacancies.

The object of study is the thermodynamic properties of cubic defective interstitial alloy TaSi, WSi, FeC, AuSi, PtSi, FeCrSi, VWSi, AuCuSi và PtCuSi.

The research scope in the ranges of temperature, pressure, concentration of substitutional atoms, concentration of interstitial atoms and concentration of equilibrium vacancies corresponds to the experiment.

2. Research methods

The main research method is the SMM. In addition, in numerical calculations we use the Maple sofware and approximate methods such as approximate iteration.

3. Major results and conclusions

3.1. The major results

Build analytic expressions for thermodynamic quantities, melting temperature and structural phase transition temperature of cubic defective interstitial alloy AC and substitutional and interstitial alloy ABC using SMM.

Apply the obtained theory to calculate numerically for metals and alloys. The obtained numerical results are compared with the experimental data and the results calculated by other theoretical methods. Some numerical results can be predictive and guide future experiments. The thesis contributes to supplementing and perfecting the theory of the equilibrium vacancy and cubic interstitial alloy.

3.2. Conclusions

The thesis uses the SMM to build the theory of thermodunamics, melting and structural phase transition of cubic defective interstitial alloy AC and substitutional and interstitial alloy ABC at zero pressure and under pressure and apply the obtained theory to calculate numerically for some metals and alloys. The thesis has achieved the following main results:

1. On the basis of the model of cubic perfect interstitial alloy AC and substitutional and interstitial alloy ABC, the general analytic expressions of the displacement of the atom from the lattice node, the mean nearest neighbor distance between two atoms, the equilibrium vacancy concentration, the Helmholtz free energy, thermodynamic quantities, the absolute stability temperature of alloy state, the melting temperature and the structural phase transition temperature depending on temperature, pressure, concentration of substitutional atoms, concentration of interstitial atoms and equilibrium vacancy concentration are derived for cubic defective interstitial alloy AC and substitutional and interstitial alloy ABC. The theories of thermodynamics, melting and structural phase transitions of cubic defective metal, binary interstitial alloy, binary substitutional alloy are limit cases of the theory of thermodynamics, melting and structural phase transitions of cubic defective ternary substitutional and interstitial alloy corresponding for zero concentrations of substitutional atoms and interstitial atoms, zero concentration of substitutional atoms and zero concentrations of interstitial atoms.

2. Apply the obtained theoretical results to calculate numerically for some thermodynamic quantities of AuSi, PtSi, FeCrSi, VWSi, AuCuSi, PtCuSi, the melting temperature of TaSi, WSi, γ-FeC and the BCC-FCC structural phase transition temperature of Fe with the pair potential Mie-Lennard-Jones *n-m* depending on temperature, pressure, concentration of substitutional atoms, concentration of interstitial atoms and equilibrium vacancy concentration. The

results obtained by the SMM are in good agreement with other calculations using the *ab initio*, the Lindemann law, the MD, etc. and the experimental data. Other calculated results predict future experimental results.

Many numerical results obtained by the SMM have good agreement with experimetns and in many cases have better agreement than those calculated by other methods. The error compared with the experiment is only about 10%. That proves that the method that we have used for research in the thesis has high reliability.

The success of the thesis contributes to perfecting and developing the application of SMM to study the properties of interstitial alloy materials taking into account the influence of the anharmonicity effect of lattice vibrations.

On behalf of academic supervisors **PhD student**

Assoc. Prof. PhD Nguyen Quang Hoc **Le Hong Viet**