SUMMARY OF THE PHD THESIS

The author's name: Vu Quang Tho

Thesis title: Study of thermodynamic quantities of materials in anharmonic XAFS theory.

Scientific branch of the thesis: Theory of Solid.

Major: Theoretical and Mathematical Physics.
Code: 9 44 01 03.

The name of postgraduate training institution: Hanoi Pedagogical University No.2.

1. **Thesis purpose and objectives**

- Investigation and expansion of the anharmonic correlated Einstein model in the X-ray absorption fine structure (XAFS) spectrum. Determine of thermodynamic parameters, expand the cumulants to the fourth-order, consider anharmonic perturbation coefficients, anharmonic factor, and the mean square relative displacement of metals, and alloys.

- Study the dependence of thermodynamic parameters and cumulants on the doped ratio at a given temperature and pressure.

- Perform numerical calculations and compare them with experimental data collected to test the correctness of the theory.

2. Supervisor Information.

Full name: **Nguyen Ba Duc.**

Institution:. Tan Trao University

Academic Title: Assoc Prof: 2010, PhD: 2015

Major: Theoretical and Mathematical Physics.

Full name: **Ho Khac Hieu.**

Institution: Duy Tan University

Academic Title: Assoc Prof: 20, PhD: 2014

Major: Theoretical and Mathematical Physics .

3. Training institution: Ha Noi Pedagogical University 2.

4. Summary of the new results of the thesis.

The thesis has directly contributed to solving some important and topical problems of modern XAFS theory, namely:

- The dissertation has built up general analytical expressions of thermodynamic parameters through structural coefficients with anharmonic contributions.

+ The expressions obtained contain classical results at the high-temperature limit and contain the zero energy contribution, a quantum effect at low temperatures.

+ The coefficient of thermal expansion has the form of isothermal capacity heat, so it satisfies the basic theory of thermal expansion.

- The thesis has built up the effective interaction potential representing the relationship between the pair interaction potential and the effective interaction potential of the system with the contribution of neighboring atoms.

+ Present structural coefficients through which it is possible to simplify the memorization of thermodynamic expressions and cumulants, and to infer the structure of materials knowing these coefficients.

- The thesis has expanded the research to calculate the thermodynamic parameters and cumulants for systems with doped cubic structures. Describe the dependence of the thermodynamic parameters and the cumulants on the doping rate of the material. Discovering structural anomalies with CuAg50 alloy opens a new research direction for graduate students of this material.

- The thesis has studied the dependence of thermodynamic parameters on temperature and the influence of pressure according to the Anharmonic correlation Debye model in the non-conditioned XAFS spectrum.

On behalf of academic supervisors **PhD. Student**

Assoc.Prof. .Nguyen Ba Duc **Vu Quang Tho**

Assoc. Prof . Ho Khac Hieu