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Structural and Mechanical Properties of CeN Using Interionic Potential Theory

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Abstract— Using the theory of interonic potential corrections for ionic charge, we investigate the cohesive energies, equilibrium lattice constant, pressure-volume relationship, phase transition and elastic constant of CeN, as well as the Coulomb scanning effect induced by d electrons. The compound undergoes a structural transition from NaCl (B1) to CsCl (B2) at 80 GPa. We also calculated the mass, Young's modulus and shear modulus, Poisson's ratio and anisotropy ratio of the NaCl(B1) sample and compared them with other results that gave good results.

Keywords— B1-B2 Phase transition; Elastic properties of solids

I. INTRODUCTION

In the past few years, many properties of materials such as structure, elasticity, optics and magnetism has been investigated using different experimental and theoretical methods. Due to problems in the synthesis and characterization of data, theoretical investigations through computer modeling have become an important tool for determining and predicting surface properties. Theoretical studies such as ab initio theory and computational models can not only explain known properties of certain objects but also predict properties of hypothetical data. The high pressurebehavior of binary rare earth compounds with the NaCl model has been widely investigated in the field of condensed matter physics. The properties of these solids depend on the properties and interactions of the 4f shell, 6s and 5d electrons [1]. The balance of the 4f shell, 6s and 5d electrons varies with different concentrations and can be affected by external applications. Various pressure dependent valence and structural phase transitions have been tested in rare earth nitrides [2,3]. These compounds have partial f-electron orbitals. The f electrons on Earth are not very localized and interact with the conduction band and p state of neighboring anions under pressure. Many theoretical [4] and experimental [5] studies have been carried out to understand the role of F electrons, especially in pressure. Due to the behavior of the f electrons of rare earth ions, the ion charge changes. In general, however, rare earth nitrides have been studied less frequently than chalcogenides and more intensively than pnictides because these compounds have been found to be difficult to prepare and generally unstable [6]. Due to the interaction of the incomplete 4f shell with the energy band around the material, the rare earth metal cerium and its compounds exhibit interesting physical and chemical properties [7]. CeN exhibits mixed behavior among Ce-based compounds. The compounds of the present invention crystallize in the sodium chloride structure and exhibit unusual properties compared to other rare earth nitrides. Denan et al. studied the temperature dependence of the lattice constant, magnetic susceptibility, and mixed valence state of Ce in CeN. [8] . Svane et al. [9]has been calculated bulk modulus of CeN. The theory of ion potential in solids is important because it allows a deeper understanding of the ionic interaction process between compounds and the quality of many crystal products. In this paper, we propose an interionic potential that changes the ion charge and explore the properties of CeN, including the results of Coulomb analysis.

II. METHOD OF CALCULATION

The interionic potential for the CeN in the frame work of rigid ion model is expressed as:

$$U(r)=\sum\frac{Z_m^2e^2}{r_{ij}}+\sum_{ij}b\beta_{ij}\exp\left[\frac{\left(r_i+r_j-r_{ij}\right)}{\rho_{ij}}\right]+\sum_{ij}C_{ij}r_{ij}^{-6}+\sum_{ij}D_{ij}r_{ij}^{-8} \quad (1)$$

These include long-range Coulomb interactions (first expression), short-range Hafemesiter and Flygare materials (second), and van der Waals multipolar interactions (third and final expression). Zme is the transfer ion charge parameterized to include the Coulomb screening effect due to the mixing of d electrons. b and p are short distances that can be determined from the equation. Thermodynamically, a phase transition occurs when a change in free energy causes a change in the structural properties of the phase. CeN changes from the original NaCl (B1) to CsCl (B2) type under pressure. The stability of a sample is determined by the minimum value of the Gibbs energy:

$$G=U+PV-TS \quad (2)$$

Where U is the internal energy corresponding to the cohesive energy, S is the vibrational entropy at absolute T, pressure P and volume V.

III. RESULTS AND DISCUSSION

We proceed to the calculation of the lattice constant, cohesive energies, structural pressure and the difference in volume change between NaCl and CeN in the CsCl type samples. These parameters are determined by volume as shown in Table 1. Since the B1 phase has the least power compared to the B2 level, it is seen that the stable phase of CeN is the B1 phase under ambient conditions. Under high pressure, CeN undergoes a structural transformation from the original NaCl type structure to the CsCl type structure.

TABLE I: INPUT PARAMETERS AND GENERATED MODEL PARAMETERS FOR CEN.

Solid	Input parameters		Model parameters	
	r_0 (Å)	B_T(GPa)	Z_m^2b(x 10^{-19}J)	ρ(Å)
CeN	2.50	1.53	2.87	21.00	0.025

TABLE II: COHESIVE ENERGIES AND PHASE TRANSITION PROPERTIES FOR CeN

Solid	Equilibrium inter-ionic distance (Å)		Cohesive energy KJ/mol		P_T
	R1(B_1)	R2(B_2)	U1(B_1)	U2(B_2)	(GPa)
CeN Pre.	2.510	26.6	-2577.87	-2414.37	80

The high conversion process of the compounds of the present invention is listed in Table 2. More relevant first-order phase transitions occur in higher transition phases. This discontinuity is called volume collapse. Volume should decrease by 5.79%.

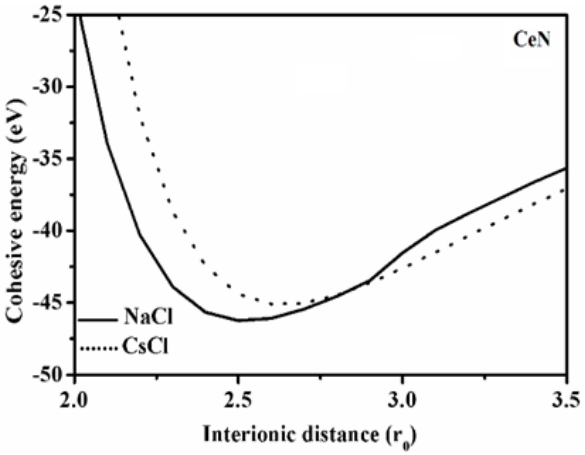

Figure 1: Energy Variation for CeN

The current model estimates the relative stability of the competition model as it satisfies the requirement that the change in cohesive energy (ΔU) be normal [10] (Table 2). Therefore, a positive value of ΔU indicates that the NaCl phase is the most stable phase at zero pressure. The measured phase transition pressure of CeN is 80 GPa. Due to the lack of experimental data for CeN, the transfer properties cannot be compared with our results. It is clear from Table 2 that the calculated values of the equilibrium lattice parameters in the NaCl-type and CsCl-type models are in good agreement with the present results [9]. We calculated Young's modulus (E), shear modulus (G), Poisson's ratio (ν), and anisotropy ratio (A) as 144 GPa, 67 GPa, 0.1536 and 0.119, respectively.We have also extended values of second-order elastic constant C11, C12 and C44 are 199, 33 and 33 GPa.

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