

Structural Analysis and Elastic Behaviour in CeN with NaCl-type Structure

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Abstract

We have expressed the Gibbs free energy for CeN compound as a function of pressure and charge transfer through improved interaction potential model (IIPM). The lattice energy in it has been represented by an IIPM consisting of the long range coulomb interaction, three body interaction, polarizability effect and overlap repulsive interaction effective up to the second neighbour ions. Using this approach high pressure phase transition phenomena in CeN have been explored. The phase transition pressure, volume collapse and elastic properties for CeN predicted from this approach are found to be the experimental data in future. This shows that the inclusion of three body interaction effects and polarizability effects makes the present model suitable for high pressure studies. Moreover, the elastic properties of CeN are also investigated.

Keywords: Rare earth compounds, Semiconductor, Phase transition, High pressure, Elastic properties

1. Introduction

Rare earth compounds attract much attention due to the intricate electronic properties related to the f-electrons. However rare earth nitrides in rock-salt structure remain almost totally unexplored [1]. These compounds are less studied and at the theoretical and experimental level. This is because rare earth nitrides (REN) are more difficult to prepare as they are less stable [2] due to the sensitivity to water vapour. The electronic configuration of rare earth nitride shows that 5d orbital are singly filled and 4f orbitals are progressively filled up with electrons. Among Ce-based compounds CeN exhibit mixed valence behaviour. The 4f electron makes the REs and their compounds attractive for applications [3], such as protective materials in reactor and fire sensitive materials.

The lack of theoretical and experimental of REN has motivated us to study the structural, elastic stability and phase transitional phenomena at high pressure for CeN using improved interaction potential model (IIPM). In the present paper, the results of the calculation on structural, elastic and phase transition pressure have been reported.

2. Improved interaction potential model

Hydrostatic pressure on materials causes a decrease in their volume, and consequently leads to a deformation of the overlapping electron shell (of a charge transfer). These transferred (or exchanged) charges appearing in the overlap region of adjacent ions interact with all other charges (or ions) of the lattice via Coulomb's law, and give rise to many body interactions [4]. Whose most significant contributions are the three body interactions (TBI). The effects of these TBI are incorporated in the Gibbs free energy ($G=U+PV$) at $T=0K$ through the lattice energy, U . Here, V is the unit cell volume at pressure P . Thus, the Gibbs free energy for NaCl (B1) and CsCl (B2) structures¹ can be written as:

$$G_{B1}(r) = U_{B1}(r) + PV_{B1}(r) \quad (1)$$

$$G_{B2}(r) = U_{B2}(r) + PV_{B2}(r) \quad (2)$$

$$U_{B1}(r) = \frac{-\alpha_M Z^2 e^2}{r} - \frac{12\alpha_M Z e^2 f(r)}{r} - \frac{e^2(\alpha_1 + \alpha_2)}{2r^4} + 6b\beta_p \exp\{(r_i + r_j - r)/\rho\} + 6b\beta_p \exp\{(2r_i - 1.414r)/\rho\} + 6b\beta_p \exp\{(2r_j - 1.414r)/\rho\} \quad (3)$$

$$U_{B2}(r) = \frac{-\alpha'_M Z^2 e^2}{r} - \frac{16\alpha'_M Z e^2 f(r)}{r} - \frac{e^2(\alpha_1 + \alpha_2)}{2r^4} + 8b\beta_p \exp\{(r_i + r_j - r)/\rho\} + 3b\beta_p \exp\{(2r_i - 1.154r)/\rho\} + 3b\beta_p \exp\{(2r_j - 1.154r)/\rho\} \quad (4)$$

With $U_{B1}(r)$ and $U_{B2}(r)$ as the lattice energies for NaCl and CsCl structures, α_M and α'_M as Madelung constants for NaCl and CsCl structure respectively, e as charge of electron and r and r' as inter-ionic separation for NaCl (CsCl). β_p is Pauling coefficients defined as $\beta_p = 1 + (Z_i/n_i) + (Z_j/n_j)$ with $Z_i(Z_j)$ and $n_i(n_j)$ as the valence and the number of electrons of the $i(j)$ th ion, b is hardness parameter while ρ is range parameter. Here, the first term is

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