



# Atomistic simulation on the structure and lattice vibration of $\text{RCo}_2\text{Al}_8$ (R = La, Ce and Pr)

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## ABSTRACT

The structural properties of  $\text{RCo}_2\text{Al}_8$  (R = La, Ce and Pr) compounds are simulated by using pair potentials based on *ab initio* method and lattice-inversion technique. The calculated lattice constants and atomic coordinates are found in good agreement with the experimental values. Further, some simple mechanical properties such as the elastic constants and bulk modulus are investigated for these materials. In particular, the phonon densities of states for  $\text{RCo}_2\text{Al}_8$  are first evaluated. A qualitative analysis is carried out with the relevant potentials for the vibrational modes, which makes it possible to predict some properties related to lattice vibration.

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## 1. Introduction

The ternary compounds R–Co–Al, where R stands for a rare earth element or uranium have been widely studied for both fundamental and technological aspect of magnetism. The magnetic properties of these compounds were studied, revealing interesting behaviors. For examples, the  $\text{RCoAl}_4$  compounds with R = Ce and Pr order antiferromagnetically at low temperature [1,2], whereas the  $\text{R}_2\text{Co}_3\text{Al}_9$  with R = Gd and Tb order ferromagnetically with  $T_c$  above 100 K [3]. In theory, there are few works about rare-earth compounds with 4f electron. Chen et al. have performed an atomistic simulation on phase stability, site preference and lattice parameters for  $\text{RFe}_{12-x}\text{T}_x$  [4],  $\text{RM}_{13-x}\text{T}_x$  [5],  $\text{R}_2\text{M}_{17-x}\text{T}_x$  [6,7] and  $\text{R}_3\text{Fe}_{29-x}\text{T}_x$  [8,9] (R = rare earth metals; M = Fe, Co; T = transition metals), suggesting the validity of application of inverted pair potentials on structure simulation of such rare-earth compounds. In this work, the structural properties of  $\text{RCo}_2\text{Al}_8$  (R = La, Ce and Pr) compounds are simulated by inverted interatomic pair potentials. Particularly, some lattice vibrational properties for these kinds of materials are

evaluated, from which the Debye temperature are obtained. These are explorations for the structures of complex materials using the interatomic potentials.

## 2. Methodology

The atomistic simulation has been widely used in the investigation of the structures, defects and thermodynamic properties of various materials. One of the key problems in atomistic simulation method is the determination of the interatomic potentials. With the lattice inversion theorem developed by Chen [10,11], we can do without complicated fitting and parameter adjustment when obtaining the interatomic potentials.

### 2.1. Chen's lattice-inversion technique

The cohesive energy  $E(x)$  of a crystal can be expressed as a sum of interatomic pair potentials, i.e.

$$E(x) = \frac{1}{2} \sum_{R_i \neq 0} \phi(R_i) = \frac{1}{2} \sum_{n=1}^{\infty} r(n) \phi[b(n)x] \quad (1)$$

where  $x$  is the nearest-neighbor interatomic distance,  $r(n)$  the  $n$ th-neighbor coordination number,  $b(n)$  the relative distance between

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**Table 1**  
Part of Morse parameters of the converted pair potentials

	$R_0$ (Å)	$D_0$ (eV)	$\gamma$
La–La	4.7585	0.2938	6.4607
Pr–Pr	4.2278	0.3099	7.2894
Al–Al	3.0059	0.4232	8.9191
Co–Co	2.7087	0.6766	8.9030
La–Al	3.6488	0.4617	8.8925
Pr–Al	3.5175	0.4771	8.8287
Ce–Co	3.1778	0.7099	9.4369
Co–Al	2.6970	0.6477	9.1129

**Table 2**  
The atomic positions of  $\text{PrCo}_2\text{Al}_8$ 

Atom	Site	In this work	Literature [12]
Pr (1)	4g	(0.3410, 0.3178, 0)	(0.3405, 0.3184, 0)
Co (1)	4g	(0.0341, 0.4063, 0)	(0.0347, 0.4058, 0)
Co (2)	4g	(0.1565, 0.0938, 0)	(0.1518, 0.0964, 0)
Al (1)	4h	(0.0271, 0.1301, 0.5002)	(0.0252, 0.1318, 1/2)
Al (2)	4h	(0.1596, 0.3795, 0.5002)	(0.1602, 0.3790, 1/2)
Al (3)	4h	(0.2410, 0.1717, 0.5002)	(0.2364, 0.1729, 1/2)
Al (4)	4h	(0.3286, 0.4881, 0.5002)	(0.3317, 0.4911, 1/2)
Al (5)	4h	(0.4518, 0.1790, 0.5002)	(0.4525, 0.1800, 1/2)
Al (6)	4g	(0.0969, 0.2508, 0)	(0.0959, 0.2531, 0)
Al (7)	4g	(0.3418, 0.0429, 0)	(0.3402, 0.0445, 0)
Al (8)	2d	(0, 0.5002, 0.5002)	(0, 1/2, 1/2)
Al (9)	2a	(0, 0, 0)	(0, 0, 0)

the origin and the  $n$ th set of lattice points and  $\Phi(x)$  the pair-potential function. Then, the general equation for pair the potential  $\Phi(x)$  can be expressed as

$$\Phi(x) = 2 \sum_{n=1}^{\infty} I(n)E[b(n)x] \quad (2)$$

The coefficient  $I(n)$  can be obtained by

$$\sum_{b(n)|b(k)} I(n)r \left[ b^{-1} \left[ \frac{b(k)}{b(n)} \right] \right] = \delta_{kl} \quad (3)$$

$I(n)$  is uniquely determined by the geometry of the crystal structure and is not related to the concrete element category. Then the interatomic pair potentials can be obtained from the known cohesive energy function  $E(x)$ .

**Table 3**  
Lattice parameters and cohesive energy of  $\text{PrCo}_2\text{Al}_8$ 

Initial state			Final state		
$a, b, c$ (Å)	$\alpha, \beta, \gamma$ (deg)	Cohesive energy (eV/atom)	$a, b, c$ (Å)	$\alpha, \beta, \gamma$ (deg)	Cohesive energy (eV/atom)
6, 7, 8	90, 90, 90	126.2625	12.9036, 14.9140, 3.8786	90, 90, 90	−4.0627
9, 9, 9	85, 75, 90	17.2515	12.9036, 14.9140, 3.8786	90, 90, 90	−4.0627
10, 12, 9	80, 90, 85	1.8841	12.9036, 14.9140, 3.8786	90, 90, 90	−4.0627
12, 14, 3	90, 120, 90	6.9838	12.9036, 14.9140, 3.8786	90, 90, 90	−4.0627
16, 18, 20	90, 80, 90	−0.8049	12.9036, 14.9140, 3.8786	90, 90, 90	−4.0627
12.9, 14.9, 3.87	80, 90, 120	−1.2508	12.9036, 14.9140, 3.8786	90, 90, 90	−4.0627

**Table 4**  
Comparison of related lattice constants before and after atomic random motion of 0.6 Å for  $\text{RCo}_2\text{Al}_8$  (R = La, Ce and Pr)

	$\text{LaCo}_2\text{Al}_8$			$\text{CeCo}_2\text{Al}_8$			$\text{PrCo}_2\text{Al}_8$		
	$a$ (Å)	$b$ (Å)	$c$ (Å)	$a$ (Å)	$b$ (Å)	$c$ (Å)	$a$ (Å)	$b$ (Å)	$c$ (Å)
Before random motion	12.9811	14.6239	4.0122	12.8508	14.5674	3.9113	12.9036	14.9140	3.8786
After random motion of 0.6 Å	12.9811	14.6239	4.0122	12.8508	14.5674	3.9113	12.9036	14.9140	3.8786
Experimental [12]							12.4623	14.3700	4.0117

**Table 5**  
Elastic constants and bulk moduli for  $\text{RCo}_2\text{Al}_8$  (R = La, Ce and Pr)

Compounds	Elastic constants $C_{ij}$ (GPa)						Bulk modulus (GPa)
	$C_{11}$	$C_{12}$	$C_{13}$	$C_{33}$	$C_{44}$	$C_{66}$	
$\text{LaCo}_2\text{Al}_8$	148	57	70	114	85	37	92
$\text{CeCo}_2\text{Al}_8$	146	61	73	109	85	36	93
$\text{PrCo}_2\text{Al}_8$	137	56	76	100	87	34	90

## 2.2. Extraction and transferability of the pair potentials

In order to obtain the effective interatomic potentials with the lattice-inversion technique, a practical method of performing an *ab initio* calculation of the cohesion curve is needed. For this, the search and design of some simple structures which can be used to invert the necessary interatomic potentials are important for us. First, let us consider the structure of BCC Co in the B2 or CsCl structure with two simple cubic (SC) sublattices  $\text{Co}_1$  and  $\text{Co}_2$ . Thus,

$$E(x) = E_{\text{Co}}^{\text{BCC}}(x) - E_{\text{Co}_1}^{\text{SC}}(x) - E_{\text{Co}_2}^{\text{SC}}(x) \\ = \sum_{i,j,k \neq 0}^{\infty} \Phi_{\text{Co-Co}} \left( \sqrt{\frac{4}{3} \left[ \left(i - \frac{1}{2}\right)^2 + \left(j - \frac{1}{2}\right)^2 + \left(k - \frac{1}{2}\right)^2 \right]} \chi \right) \quad (4)$$

Here  $x$  is the nearest-neighbor distance in the bcc structure,  $E_{\text{Co}}(x)$  represents the total energy curve with the bcc structure,  $E_{\text{Co}_1}(x)$  or  $E_{\text{Co}_2}(x)$  is the total energy function for the simple-cubic structure. Now,  $E(x)$  automatically becomes the cohesive energy function of one  $\text{Co}_1$  atom with all the  $\text{Co}_2$  atoms. Here, the  $\text{Co}_2$  atoms constitute a simple-cubic structure, and only one  $\text{Co}_1$  atom is located at the center of any cube. Then the pair potentials  $\Phi_{\text{Co-Co}}(x)$  between identical atoms can be obtained directly by using Chen's lattice-inversion technique.

The *ab initio* calculation of the total energy curve related to  $\Phi_{\text{R-Co}}(x)$  is very hard to perform. We find that the calculation for  $\text{R}_3\text{Co}$  with the  $\text{L1}_2$  structure can be used to invert the pair potential  $\Phi_{\text{R-Co}}(x)$ . The total energy of  $\text{R}_3\text{Co}$  with the  $\text{L1}_2$  structure is given by

$$E(x) = E_{\text{R}_3\text{Co}}^{\text{L1}_2}(x) - E_{\text{Co}}^{\text{SC}}(x) - E_{\text{R}}'(x) \quad (5)$$

where  $E_{\text{Co}}^{\text{SC}}(x)$  is attributed to the simple-cubic structure, in which all the atoms occupy the corner sites and  $E_{\text{R}}'(x)$  is attributed to the atoms occupying the face-center sites. Thus, the pair poten-

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