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Structural and mechanical properties of Laves phases YCu_2 and YZn_2: First principles calculation analyzed with data mining approach

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ABSTRACT

Structural and mechanical properties of main YCu_2 and YZn_2 binary compounds with C14, C15 Laves phases and $CeCu_2$ structure in Cu–Y–Zn alloy are investigated by first-principles calculations. The related total energies versus occupations of nonequivalent lattice sites in all four structural forms were studied. Density functional theory is considered within framework of both pseudo-potentials and plane waves basis using VASP (Vienna ab initio Software Package). Formation heat has been computed and showed that the $CeCu_2$–YCu_2 and YZn_2 Laves phases have the strongest alloying ability and structural stability. Mechanical properties were calculated, discussed, and analyzed with data mining approach in terms of structure stability.

1. Introduction

This paper focuses on a particular class of intermetallic phases, the so-called Laves phases. These phases, forming the largest group of intermetallics with more than 1400 representatives, have the ideal AB_2 composition. The class of an intermetallic compound as a Laves phases is purely based on the geometry of the crystal structure. The Laves phases crystallize in three structure types: cubic $MgCu_2$ (C15), hexagonal $MgZn_2$ (C14) and hexagonal $MgNi_2$ (C36) [1–4]. An orthorhombic structure also exists where a number of AB_2 intermetallics are observed, namely the $CeCu_2$-type structure (Fig. 1).

Laves phases have attracted much interest in basic research. Furthermore, in the last decade, many metallurgists and engineers have studied phase transitions in these materials in order to improve mechanical and physical properties). This induced considerable efforts in the development of new structural materials based on Laves phases for extremely high temperatures. Current research on steel turbines is turned on using Laves phases precipitates in order to improve fatigue strength [5].

First-principles density functional theory calculations have been widely used to shed light on the electronic structural and mechanical properties of Laves phase compound. Linear muffin-tin orbital (LMTO-NFP) was used by two groups to study these compounds. Mayer et al. [6] studied the MAl_2 (M = Ca, Y, Sc and La) and MCr_2 (M = Ti, Zr, Nb and Ta), Kumar and Miracle [7], Kumar et al. [8] studied the MCr_2 (M = Ti, Zr, Ta, Nb, Sc, Y, and La). Other three groups have used the Vanderbilt-type ultrasoft pseudopotential (USPP) incorporated in the Vienna ab initio simulation package (VASP), Tao et al. [9] and studied MAl_2 (M = Sc, Y, La, and Ce–Lu), Ouyang et al. [10] studied the MMg_2 (M = La, Ce, Pr, Nd, Pm, Sm, and Gd), Kal et al. [11] studied the MZn_2 (M = Ca and Sr) and MAl_2 (M = Sr and Ba). Their results showed that density functional theory DFT calculations can give satisfactory results that would often not be easy to obtain directly from experiments.

The paper presents results of researches connected with the development of new approach based on data mining the bulk, shear and young modulus of polar intermetallic materials. Principal Component Analysis (PCA) and Partial Least Squares (PLS), numerical techniques, have been applied to study mechanical properties of polar intermetallics and to predict materials with high hardness and rigidity.

2. Calculation methods and crystal structures

Calculations were performed using the VASP [12–14] code based on the density functional theory (DFT) [15,16]. Ultrasoft Vanderbilt-type pseudopotentials [17] were used to describe the interactions between ions and electrons. The generalized gradient approximation (GGAPW91) of Perdew et al. [18] was applied to evaluate the exchange–correlation energies of all examined structures.

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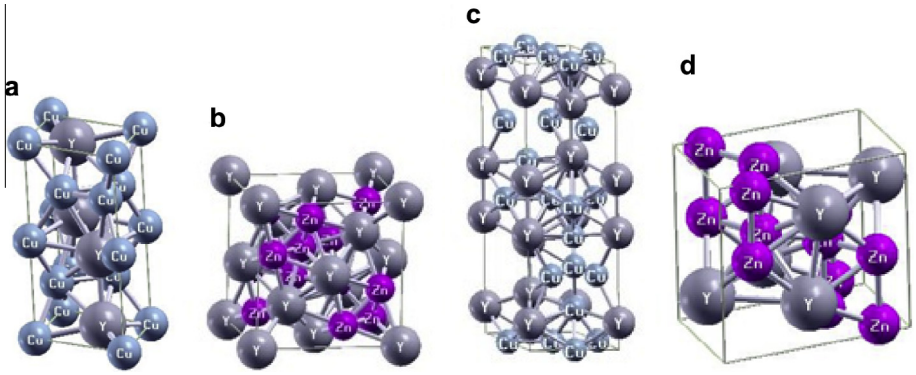

Fig. 1. Crystal structures of C14 (a), C15 (b) and C36 (c) AB_2 type Laves phases and $CeCu_2$ (d) type orthorhombic structure.

Sampling of the Brillouin zone was done via $13 \times 13 \times 13$ (cubic C15 structure), $13 \times 13 \times 11$ (C14 and C36 structure) and $11 \times 9 \times 9$ ($CeCu_2$ orthorhombic structure) k-points grid generated according to the Monkhorst–Pack scheme [19] for YCu_2 and YZn_2, respectively. The cut-off energy restricting the number of plane waves in the basis set was set to 310 eV for YCu_2 and YZn_2 compounds.

3. Enthalpy of formation

In order to obtain the most energetically stable structure amongst the four structures mentioned previously, the formation enthalpy for both tow compounds YM_2 (M: Cu, Zn) was evaluated by the following equation:

$$\Delta H_f = E_{\text{tot}}^{YM_2} - \left(E_{\text{solid}}^{Y} + 2E_{\text{solid}}^{M}\right) \quad (1)$$

E_{solid}^{A} and E_{solid}^{B} represent the energy per atom of A and B in solid states.

At zero Kelvin and under pressure zero Pa, the enthalpy equals to the energy, that is $\Delta E_f(AB_2) = \Delta H_f(AB_2)$ [20].

4. Data mining techniques

For materials design, not only the creation of data whether through calculation or experiment is important, but a way to analyze the data in an efficient and comprehensive manner is also necessary. Some of the challenges in the design of new materials include the difficulty of analyzing large amounts of data, understanding the correlations among various properties, and using these correlations to design a possessing the desired properties. Utilizing a multivariate analysis, the data can be examined so that trends and correlations become apparent.

The classification analysis is performed with Principal Component Analysis (PCA). PCA is an unsupervised learning approach for dimensionality reduction that uses correlation coefficients of the parameters to combine and transform them into a reduced dimensional space. PCA projects the spatial data onto a set of principal components (PC) and maps the data on a dimensionally reduced space [21]. PC1, the PC capturing the most information, is associated with the largest eigenvalue of the covariance matrix of the original dataset. All PCs are orthogonal to each other, and thus each captures unique information. The advantage of PCA is that typically a few PCs are sufficient for describing a system, and a dataset of n-dimensions can be reduced to a few dimensions with minimal loss of information. The PCs do not necessarily have an obvious physical meaning, but rather are a linear combination of variables which explain the largest variation in the data [22]. The reduction in dimensionality makes trends and correlations which are hidden in the data become more easily visualized and described in PC space.

Of interest from PCA are the scores and loadings plots. The scores plot classifies the samples, while the loadings plot shows the relationship among the descriptors in terms of their role in classifying the samples. The scores and loadings can be analyzed together so that the relationships between samples, properties, and samples-properties can be identified. A comparison of the loadings and scores will provide useful information on which properties are affecting the samples the most and which are irrelevant to certain samples.

Partial Least Squares regression (PLS) is a quick, efficient and optimal method based on covariance. It is recommended in cases where the number of variables is high, and where it is likely that the explanatory variables are correlated [22].

A great advantage of PLS regression over classic regression are the available graphs that describe the data structure. With the correlation and loading plots, it is easy to study the relationship among explanatory or dependent variables.

The score plot gives information about sample proximity and dataset structure. The biplot gather all these information in one map.

The biplots and the loading plots obtained by PCA and PLS were compared and various criterions were identified for YM_2 (M: Cu, Zn) materials crystallized in Laves phases and orthorhombic structures.

5. Results and discussion

5.1. Enthalpy of formation

Using Eq. (1), we calculated the enthalpies of formations of both compounds. Results are presented in Table 1. We can see that the enthalpy of formation for YCu_2 is −0.617, −0.546, −0.585, −0.884 eV/atom for C14, C15, C36 and $CeCu_2$ structures, respectively.

Table 1
Enthalpy of formation for YCu_2 and YZn_2.

	$\Delta H_f^{YCu_2}$ (eV/atom)	$\Delta H_f^{YZn_2}$ (eV/atom)
$CeCu_2$	−0.884	−1.188
C14	−0.617	−1.058
C15	−0.585	−1.137
C36	−0.546	−1.108