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Prutthipong Tsuppayakorn-ae

Chulalongkorn University

Thipok Bovornratanaraks

Triam Udom Suksa School

Wei Luo

Uppsala University

Rajeev Ahuja

Indian Institute of Technology (IIT) Ropar

Thiti Bovornratanaraks (✉ thiti.b@chula.ac.th)

Chulalongkorn University

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Existence of yttrium allotrope with incommensurate host-guest structure at moderate pressure: First evidence from computational approach

Prutthipong Tsuppayakorn-aek^{1,2}, Thipok Bovornratanaraks^{3,4}, Wei Luo⁵, Rajeev Ahuja^{5,6}, and Thiti Bovornratanaraks^{1,2,**}

¹Extreme Conditions Physics Research Laboratory (ECPRL) and Physics of Energy Materials Research Unit, Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok, 10330, Thailand

²Thailand Centre of Excellence in Physics, Ministry of Higher Education, Science, Research and Innovation, 328 Si Ayutthaya Road, Bangkok 10400, Thailand

³Triam Udom Suksa School, 227 Phyathai Road, Patumwan, Bangkok, 10330, Thailand

⁴Development and Promotion of Science and Technology Talents Project (DPST), The Institute for the Promotion of Teaching Science and Technology (IPST), 924 Sukhumvit Rd, Phra Khanong, Khlong Toei, Bangkok 10110

⁵Condensed Matter Theory Group, Department of Physics and Materials Science, Uppsala University, Box 530, SE-751 21, Uppsala, Sweden

⁶Department of Physics, Indian Institute of Technology (IIT) Ropar, Rupnagar 140001, Punjab, India

**thiti.b@chula.ac.th

ABSTRACT

We predict an allotrope of yttrium with an incommensurate host-guest structure by using *ab initio* random structure searching technique, based on first-principles calculation. Along with, we propose a set analogous commensurate supercells, which is incommensurate ratio (c_H/c_G), by approximating the different the number of guest atoms in channels in along c axis of the host structure. Herein, our results show that $c_H/c_G = 5/4$ is energetically stable. Subsequently, an incommensurate host-guest structure is found to be thermodynamically and dynamically stable within harmonic level. The hybridization of spd explains the stability of the host-guest structure under high pressure conditions. The distributions of electrons between the host and guest atoms are indicated strong and weak electron localization of spd bonds. This findings suggest that the host-guest structure is more likely to be achieved experimentally in this metallic element at moderate pressure.

Introduction

The understanding of structural phase transitions is interested since several of simple elemental metals can be transformed into a highly complicated structure, such as an incommensurate host-guest (HG) structure at high pressures.^{1,2} The HG structure was first discovered in barium (Ba) above 12 GPa by Nelmes *et al.*³ To the best our knowledge, the crystal structure of Ba at ambient pressure has a simple structure with a body-centered cubic (bcc). With increasing pressure, the bcc structure transformed into a hexagonal structure at a pressure of 5.5 GPa, and then it transformed into the complex HG structure.⁴ This is, however, very unexpected in metallic element and it should mentioned that this HG structure was observed at high pressure. Additionally, the HG structure has been exhibited a built of two containing substructures with the superspace group (it is here referred to be the host structure) and the subspace group (it is here referred to be the guest structure). The HG structure explained as composite structure consist of body-centered tetragonal (bct) host and face-centered tetragonal (fct) guest structures, as can be seen in figure 1. This gives, however, rise to an unanswered question, regarding the existence of the incommensurate HG structure is discovered at high pressures, it should clearly deserve further investigation.

As aforementioned, one can see the solution in the alkali-earth metal (AEM) such as calcium (Ca), strontium (Sr), and Ba. These elements in the same column manifested the HG structure. For example, Ca has theoretically predicted to be the HG structure by using the *ab initio* calculation.⁵ Subsequently, the predicted HG structure in Ca has experimentally observed by the x-ray powder diffraction (XRD).⁶ As result of the experimental study, it demonstrated that the HG structure can be synthesized in an element at high pressure. It is interesting to note that the striking resemblance in AEM shown that they share a similar transition sequence under high pressure. Therefore, the perspective for looking of the existence of HG structure by considering the resemblance of structural behaviour is very attractive.

It is interesting to note that the HG structure was also experimentally observed in scandium (Sc) at moderate pressure.^{7,8}

Following crystallography of HG structure, Arapan and co-worker⁹ have been propose a set analogous commensurate supercells which has the incommensurate ratio (c_H/c_G) = 4/3. Apart from this, However, there is an unexpected result in the prediction of high pressure structural sequence. The enthalpy of sm-type structure is competing with those of hexagonal and HG structure at the transition point. As a result of this, it has been pointed out that all three structures appear to coexist in the vicinity of transition pressure, by approximately 17 GPa, This imply that one might think of a complex mechanism of the transition as well as it should clearly deserve further systematic investigation. Curiously, recent extensive studies of the HG structure in Sc were studied in the ideal incommensurate ratio at moderate and high pressure,¹⁰ indicating that the host and guest structures can interpenetrate to be the incommensurate HG structure.

Motivated by the similarity of having HG structure in the entire column of AEM and a competing with those other structures at moderate pressure in Sc. It is worth to noting that Y is another very probable candidate for this remarkable structure in addition to those elements already explored. As a possible cause of this, one might think that a complex mechanism of the coexistence in the vicinity of transition pressure similar to those of Sc. The challenging of finding the answer is not only intriguing but it is also encouraging to search for the HG structure in elemental metals. Therefore, in this work, we used the *ab initio* random structure searching (AIRSS) to predict the HG structure in Y. Moreover, our calculations demonstrate the HG structure is thermodynamically and dynamically stable at moderate pressure region. The further investigation of this HG structure is carried out by using the electron localization function (ELF) in order to explain nature of bonding of Y, leading to display a stability of the HG structure.

Methods

We used AIRSS technique^{11,12} to look through the HG structure under compression. In this structure searching, Y atoms were placed randomly in the cell without symmetry constrain. The setup containing 2, 4, 6, 8, 10 and 12 atoms of Y at 0, 20, 40, 80, and 100 GPa were explored. The ground state structure can be obtained from a relaxed shape of cell and atomic coordinates of Y atoms can also be identified. We used the on-the-fly (OTF) ultrasoft pseudopotentials¹³, as implemented in the CASTEP code.¹⁴ The OTF pseudopotentials with an 11-electron for Y was carried out with a cutoff energy of 340 eV and an initial Brillouin-zone (BZ) sampling grid of spacing $2\pi \times 0.05 \text{ \AA}^{-1}$ was found to be sufficient for the searching. The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE)¹⁵ was used. The AIRSS technique carried out by the simple linear approximation¹² and the enthalpies of the phases at any pressure can be obtained from equation (1)

$$H(p) \simeq H(p_s) + V_s(p - p_s), \quad (1)$$

where p is pressure and V_s is the volume of structure at p_s . The quantities $H(p_s)$, p_s and V_s were calculated for each relaxed structures.

We calculated the structural phase transitions by using the GGA-PBE.¹⁵ The projector augmented wave (PAW) method¹⁶ was performed, as implemented in the VASP code.¹⁷ The PAW potential with an 11-electron for Y was performed. A cutoff energy of 700 eV and the initial BZ sampling grid of spacing $2\pi \times 0.02 \text{ \AA}^{-1}$ were used. All of the structural parameters are fully relaxed by using the Methfessel-Paxton smearing method. All structures were calculated by conjugate gradient scheme until the Hellman-Feynman forces became less than $10^{-3} \text{ eV/\AA}$.

Results and discussion

It is true that nowadays structural predictions of metallic elements play an important role for the high-pressure research. As mentioned previously, the main issue for the current investigation is that if Y is likely to posses the HG structure at moderate pressure. For this reason, the present work carried out the AIRSS technique, based on density functional theory, to predict the HG structure. This because AIRSS technique is one of the most powerful tools for structure predictions, and it is suitable for this particular job in elemental metal.^{10,18-21} For example, the AIRSS technique has been performed to predict the HG structure of aluminum at extreme pressure.¹⁸ According to explanation of detail of the HG structure from introduction section, the similarity of structural behaviour in the same column elements as in AEM led to an accurate prediction of the HG structure in transition metal (figure 2). Especially for the AIRSS technique, we found particularly low-enthalpy structure which correspond to the space group $I4/mcm$. In order to demonstrate the existence of this HG structure in Y. The calculation is carried out by approximating the parameter of c_H/c_G , the so-called γ , which is defined by the different the number of guest atoms in channels in along c axis of the host structure, such as c_H/c_G : 4/3. Our calculations presented the key factor of structural relaxation. The optimized supercell containing crystal shape and atomic positions as well as the final total energy can be obtained. Our investigation used $\gamma = 5/4, 3/2, 6/5, 10/7$ and $4/3$.

Regrading structural behaviour, as a first step, the commensurate value c_H/c_G is demonstrated by considering the different the number of guest atoms in channels along c axis of the host structure. Following this, the commensurate value c_H/c_G is

calculated at a pressure of 20 GPa. As a result of this, structural relaxations manifested the commensurate value c_H/c_G of 5/4 and is energetically stable favored over those of the commensurate value c_H/c_G of 3/2, 6/5, 10/7 and 4/3, respectively. This is shown in figure 3. To further explore the stability of the commensurate value at a pressure of 40 GPa. The remarkable results displayed that the $\gamma = 5/4$ is favored under compression. Confirming that the c_H/c_G parameter is interpreted by examining the total energy as can be seen in Fig. 3. One may immediately imply that the 5/4 is energetically stable at 20 and 40 GPa. The HG structure is then optimized to obtain the relaxed HG structure having $a = 8.182$ Å and $c = 3.721$ Å with Y atoms located at (0.148, 0.648, 0) for the host structure and placed at (0, 0, 0) and (0.5, 0.5, 0) for the guest structure. This structural phase transition of Y is explained by the enthalpies-pressure relation. The high-pressure transformation sequence is hcp $\rightarrow$ sm-type $\rightarrow$ dhcp $\rightarrow$ HG $\rightarrow$ dfcc at 4, 6, 7, and 39 GPa, respectively. This high-pressure transformation sequence shown that the sm-type and dhcp structures are stable in a very narrow pressure range. While the HG and dfcc structures are stable in a wider pressure range. This scenario opened the possibility that it arrived a new transformation sequence of Y (Fig. 4). As mentioned in the introduction, it is interesting that this phenomenon is similar to those of Sc. Moreover, The most surprising result is that the sm-type is competing with dhcp structure and HG structure, indicating that these structures appear to be coexist in the vicinity of arrow pressure range. One might say that this reveals a complex nature of this transition mechanism.⁹

Nevertheless, the HG structure is found to be thermodynamically stable, favoring moderate pressure. For this reason, we concluded that by neglecting the entropy contributions, the structures were considered at 0 K, indicating that only the enthalpy can be used to confirm the phase stability under high pressure. This is, however, not enough to guarantee the exact thermodynamic stability. At this stage, we would like to extend our study to consider the vibration dynamically. We further our investigation to explore the dynamical stability by performing the phonon calculations. Our results demonstrate that, at the pressure of 20 GPa, the HG structure is dynamically stable because they do not exhibit imaginary frequencies, as shown in Fig. 5. This remarkable results confirm the existence of HG structure in Y. As discussed in the complex mechanism of the transition,⁹ considering the allotrope of Y, it seems to be still unclear whether this structure can be attained at such a high pressures alone. This is because both thermodynamic variables, pressure and temperature, are required in order to overcome the finite potential well, leading to the formation of the stable crystal structure.^{22,23} To further our understanding experimentally, which is beyond the scope of this present work, the effect of temperature can also be considered. We thus suggested a possible path way for achieving the HG structure in Y by using both pressure and temperature effect similar to the reported case of the β -tin structure in Ca.^{24,25}

We now extend our investigation to the electronic property of the HG structure. This is carried out by the analysis of electronic band structure and the partials density of states at a pressure of 40 GPa. Herein, the band structure displayed that their dispersions exhibited electronic state at the Fermi level (E_f), resulting in the metallic state. Following this, we further discuss the the stability of the HG structure by considering the partial band structures.^{26,27} First of all, their dispersions showed that there are crossing band around E_f . One can see the weaving of the up-running bands and down-running bands from below E_f and above E_f . As a result of this, their dispersions around E_f showed the hybridization due to interplay between the p -orbitals and the d orbitals, as shown in the figure 6. Moreover, the band dispersions are dominated by the d orbitals, leading to the stabilization of HG structure. As a possible cause of this, one might think of the s -to- d electron transfer. Basically, to the best of our knowledge, the s electron transfer into the d electron under compression. This has been described extensively by Duthie et al.,²⁸ which paves the way for achieving stable structure in Y.^{26,27} In addition, the calculated electronic density of states of HG structure is shown in figure 6. The partial densities of states (PDOS) of s , p , and d orbitals, respectively, near the Fermi level indicates that the electrons are much more localized at a pressure of 40 GPa. This exhibited electron hybridization, which was described by Häussermann and co-worker,²⁹ are in good agreement with the result from the electronic band structure. Remarkably, the PDOS calculation showed that the d -electron dominated at E_f . As a result of this, it is interesting to mention that the static stability of the HG structure might also be explainable by the domination of d -electron.

At this time, it is interesting to investigate the electron localization function (ELF).³⁰ By considering the ELF, we can further our understanding by adopting the uniform distribution of electron gas with the same density. The ELF calculations are used extensively in materials science under high pressure.^{10,31–36} We therefore used the ELF calculation to investigate the HG structure. The results were shown in figure 7. To begin with, the ELF calculations of the HG structure is carried out in the (100) plane. Overall, the ELF of HG structure is computed at a pressure of 0 GPa, 20 GPa, and 40 GPa, respectively. Firstly, we discuss the uniform distribution of electron gas with the same density at a pressure of 0 GPa. With this in mind, the ELF without the effect of pressure showed that the electron slightly accumulated between the host and guest atoms through the interplay between the accumulation of the host and host atoms, indicating that the nearest neighbors (NN) of the host-host NN is 4.950 Å. Secondly, the electrons accumulated between the host-host atoms decreased as the pressure increased up to 20 GPa. However, it is found that the electrons contribution increases around the interplay between the accumulation of the host and guest atoms at NN 3.123 Å. Finally, the electron significantly contributed around the interplay between the accumulation of the host and guest atoms at NN 2.888 Å at a pressure of 40 GPa within the positive value (range between 0 and 1) in the blue colour regime. Subsequently, the remarkable result of ELF demonstrated that the interplay between the host and host atoms (the host and guest

atoms) supported the stability of the HG structure by adopting the electron accumulation, similar to the case of the P6₂22 structure.²⁶ Without a doubt, we would like to suggest further that, by adopting electronic property, the *spd* hybridization state is definitely present and the bonding nature can be determined as covalent bonds.³⁷ Lastly and most importantly, it might be worth trying to study the superconducting properties of the HG structure because it possessed metallicity. Moreover, it is possible to become a superconductor at high temperature since the *d*-electron is dominated at E_f . This is, however, beyond the scope of this work, but the issue clearly deserves further investigation. We thus suggest that the HG structure is more likely to be attained experimentally and theoretically in metallic elements by considering the current capability of the electronic properties.

Conclusion

In summary, yttrium allotrope can be obtained from the *ab initio* random structure searching, based on the density functional theory under compressed conditions. Consequently, the current capability of AIRSS technique predict that the HG structure is thermodynamically stable at moderate pressure. Apart from this, we present a set of analogous commensurate supercells which are actually incommensurate ratios (c_H/c_G) but the different the number of guest atoms in channels in along a *c*-axis of the host structure were approximated. Herein, our results show that $c_H/c_G = 5/4$ is energetically stable. In the same way, the HG structure is dynamically stable. Additionally, the electronic structure pave the way for achieving stable structure. Positively, the findings suggest that the HG structure can possibly be achieved at moderate pressure and low temperature, similar to the β -tin structure in Ca.

Data Availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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Author contributions statement

Author contributions: P.T., and T.B. designed the research; P.T., T.B., W.L., and T.B. performed the research; P.T., T.B., R.A., and T.B. analysed the data; and P.T., T.B., and T.B. wrote the paper.

Competing interests

The authors declare that they have no competing interests.

Figure 1. (a) Structure of host–guest type, where the dark–green and light–green spheres represent host and guest atoms, respectively. (b) The host–guest structure analogue with $c_H/c_G=5/4$.

Figure 2. The illustration of host-guest structure, where the dark-green and light-green spheres represent host and guest atoms, respectively.

Figure 3. Total energies of the HG structures as a function of γ , where γ is commensurate value.

Figure 4. The enthalpies as a function of pressure of Y up to 80 GPa.

Figure 5. The phonon dispersion of the host-guest structure at pressures of 20 and 40 GPa, respectively.

Figure 6. Partial electronic band structure and partial density of states to s , p , and d orbitals of the of the host-guest structure of Y at a pressure of 40 GPa.

Figure 7. The electron localization function (ELF) of the host-guest structure as shown in the (001) atomic plane at 0, 20, and 40 GPa, respectively.

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