Superconductivity of superhydride CeH$_{10}$ under high pressure

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Keywords: superconductor, high pressure, cerium hydride

Abstract

A large class of metal superhydrides was found to be a conventional BCS superconductor under high pressures. In this work, we focused on cerium decahydride, CeH$_{10}$. Ce is a member of the so-called lability belt in the periodic table, where the physical properties can be largely affected by pressure. It was reported and we confirmed that CeH$_{10}$ can be formed with the Fm-3m structure, where a cerium atom is embedded in a H$_{13}$ cage. Our phonon calculations show that it is dynamically stable at around 300 GPa onwards. We examined the evolution under pressures of the phonons, the electronic states, the Fermi surface, and the electron localization function (ELF). There exists a small van Hove singularity (vHs), and it gradually moves to below the Fermi surface as pressure increases. This behaviour associating with the reducing value of the electron-phonon coupling strength ($\lambda$), causes the superconductivity transition temperature ($T_c$) to gradually reduce under pressures. The maximum $T_c$ is 45 K at 300 GPa.

Introduction

Metal polyhydrides have attracted large attention from condensed matter research community as they become a metal and possibly a conventional Bardeen–Cooper–Schrieffer (BCS) based superconductor with a high value of transition temperature ($T_c$) under pressure [1–13]. From the theoretical consideration, there were several theoretical surveys led by Peng et al [14] Semenok et al [15] Zurek and Bi [16], and Pinsook [17]. They gave a comprehensive overview of the current achievement on the structural prediction of polyhydrides and their superconducting properties at high pressures. Among large number of predicted structures, there is a noticeably large class of metal decahydrides, MH$_{10}$, where M = Sr, K, Y, La, Ac, Ce, Th, etc Most of these MH$_{10}$ share a common Fm-3m structure, which can be viewed as a clathrate structure. In this structure, hydrogen atoms form a H$_{13}$ cage which hosts a metal atom inside. Surprisingly, most of the metals that form MH$_{10}$ belong to the so-called lability belt, i.e. d$^0$ and d$^1$ belts in the periodic table. Furthermore, there are several members of this class that exhibit $T_c > 273$ K from theoretical calculations, i.e. LaH$_{10}$ ($T_c = 274–286$ K at 210 GPa) and YH$_{10}$ ($T_c = 305–326$ K at 250 GPa) [13]. The existence of LaH$_{10}$ has been confirmed by experiment at 180–200 GPa with $T_c$ around 260 K [18]. Another theoretical prediction on the Th–H system revealed the existence of ThH$_{10}$ with an Fm-3m structure [19], and it was predicted that $T_c = 220–241$ K at 100 GPa. The Fm-3m–ThH$_{10}$ was confirmed by experimental observation, and it was shown that $T_c = 159–161$ K at 170–175 GPa [20]. The YH$_x$ compounds have been synthesized [21]. The existence of YH$_6$ and YH$_9$ have been confirmed with $T_c = 227$ K at 237 GPa and $T_c = 243$ K at 201 GPa, respectively. However, YH$_{10}$ has not yet been found up to 237 GPa [21].

By comparison with LaH$_{10}$, we are particularly interested in CeH$_{10}$ because Ce shares some similarity with La. For example, they have similar $3^+$ ionic radii and similar atomic masses. However, Ce has two oxidation
states, i.e. $3^{+}$ and $4^{+}$. The $4^{+}$ ionic radius of the Ce atom is quite smaller as Ce has the [Xe] 4f$^{15}$d$^{6}$s$^{2}$ electronic configuration, whereas La has the [Xe] 5d$^{6}$s$^{2}$ electronic configuration. The discrepancy between trivalent and tetravalent metals would manifest in their different bondings under pressure. In addition, there will be some complication from the strong correlation of the f–electron. Recently, there has been a theoretical prediction on the existence of CeH$_{10}$ led by Peng et al. [14] and Li et al. [11]. By considering the structural convex hull, Peng et al predicted that the CeH$_{10}$ compound can be formed at 200 GPa with either Fm-3m or R-3m structure [14]. The R-3m structure can be viewed as a distorted Fm-3m structure as well. On the experimental side, the CeH$_{x}$ compounds have been synthesized by Salke et al. [22] using a laser–heated diamond anvil cell (DAC). Their compounds can be identified as CeH$_{2}$, CeH$_{3}$, and CeH$_{4}$ phases at different pressures by using synchrotron x–ray diffraction (XRD). The structure of CeH$_{9}$ was identified as a hexagonal clathrate structure with the P6$_{3}$/mmc space group at 80 GPa. We refer to this phase as Fm–CeH$_{9}$ from now on. Its $T_{c}$ has not been measured but it was estimated to be around 117 K at 200 GPa [22]. The existence of hcp–CeH$_{9}$ has been confirmed by another independent experiment by Li et al. [23] Salke et al. [22] also searched for CeH$_{10}$ up to 200 GPa, but they did not succeed.

In this work, we have followed the theoretical work of Peng et al. [14] and extended our investigation into CeH$_{10}$ and the evolution of its superconductivity under pressure in more detail. We have rechecked the structure searching for the possible structural deviation. Consequently, we used the DFT method to calculate the phonon dispersion, the electronic states, the Fermi surfaces, electron localization function (ELF), the electron-phonon coupling strength under pressure. The presence of the f-electron is properly taken into the account. We found that the Fm-3m phonons at 200 GPa contain some unstable modes. Thus, $T_{c}$ is calculated in the pressure range of 300–700 GPa only. Surprisingly, $T_{c}$ is quite low compared with that of LaH$_{10}$. We will discuss the cause that diminishes the electron–phonon coupling strength in CeH$_{10}$.

**Computational details**

All of the density functional calculations in this work used the generalized gradient approximation of the Perdew–Burke–Ernzerhof (GGA–PBE) functional [24] for the exchange-correlation functional. We employed the projector augmented wave (PAW) method [25], as implemented in the Vienna ab initio simulation package (VASP) [26]. The PAW potentials with 12 valence electrons (5s$^{2}$5p$^{6}$4d$^{4}$5s$^{3}$) for Ce and 1 valence electron (s$^{1}$) for H were applied with a plane wave basis set up to a cutoff energy of 700 eV and a 10 $\times$ 10 $\times$ 10 k-point mesh generated by the Monkhorst–Pack (MP) method [27]. The core radii of Ce and H are 2.57 Bohr and 0.80 Bohr, respectively, which are small enough that the overlap of spheres will not occur under applied pressure. All of the structural parameters are fully relaxed by using the Methfessel–Paxton smearing method [26] and the conjugate gradient scheme. All considered structures were relaxed at each pressure until the Hellman–Feynman forces became less than 10$^{-3}$ eV Å$^{-1}$. The phonon calculations were calculated by using the ab initio lattice dynamics with the finite displacement method, as implemented in the VASP code together with the PHONOPY package [28]. For the superconducting phase, we calculated the electron–phonon coupling (EPC) within the density functional perturbation theory [29] via Quantum Espresso (QE) package [30]. In order to compare the QE results with those of VASP, a compatible PAW potentials with 12 valence electrons (5s$^{2}$5p$^{6}$4d$^{4}$5s$^{3}$) for Ce [31] and 1 electron (s$^{1}$) for H have also been employed in QE. The plane-wave energy cutoff of 60 Ry was used. The Brillouin zone (BZ) integrations in the electronic and phonon calculations were performed using the MP meshes. The EPC matrix elements were computed in the first BZ on 4 $\times$ 4 $\times$ 4 q-meshes using individual EPC matrices obtained with a 24 $\times$ 24 $\times$ 24 k-points mesh. The Allen–Dynes equation [32] was used with the effective Coulomb pseudopotential parameter, $\mu$ = 0.10 and 0.13, as follows:

$$T_{c} = \frac{\omega_{log}}{1.2} \exp \left[- \frac{1.04(1 + \lambda)}{\lambda - \mu^{2}(1 + 0.62\lambda)} \right],$$

(1)

where $\omega_{log}$ is the logarithmic average of the spectral function, $\lambda$ is the total electron–phonon coupling strength. We found that $\lambda$ < 1.5 in most of our cases, thus this form of Allen-Dynes equation is quite sufficient.

**Results and discussion**

We have independently searched for the predicted phase of CeH$_{10}$ by using several structure searching methods [33, 34]. These methods give the same Fm-3m structure for CeH$_{10}$. Thus, we proceeded further to the calculation of its superconductivity and the associating Tc. Figure 1(a) illustrates the Fm-3m structure, where H atoms form an H$_{32}$ clathrate cage which hosts a Ce atom inside. The H$_{32}$ clathrate cage is shown in figure 1(b). The polygon faces of the H$_{32}$ clathrate cage contain six squares and twelve hexagons (the [46123] polyhedron). We shall refer to this phase as fcc-CeH$_{10}$ from now on. This phase is in good agreement with the structure of
CeH_{10} predicted by Li et al [11] and Peng et al [14]. We calculated the formation enthalpy of fcc-CeH_{10} compared with the H_{32} structure and fcc-Ce. We found that fcc-CeH_{10} can be formed at approximately 40 GPa. Peng et al [14] used convex hull calculation to show that fcc-CeH_{10} can be formed at 200 GPa.

As mentioned earlier, the R-3m structure can be considered as a distorted Fm-3m structure. Thus, we also compared the structural stability between the R-3m and Fm-3m structures. The convex hulls showed that the Fm-3m structure is more thermodynamically stable between 200–400 GPa. On the other hand, the convex hulls pointed out that the R-3m structure is likely to be a metastable structure, as shown in figure 1(left).

Next, we calculated the phonon dispersion in the pressure range of 200–700 GPa by using PHONOPY [28] associated with VASP [26]. At 200 GPa, we found that the phonon calculation produces some imaginary numbers, instead of finite frequencies, in some of the optical modes around the \( \Gamma \)-point, as shown in figure 2(a). These imaginary modes indicate that the fcc-CeH_{10} structure is dynamically unstable. At this pressure, the highest phonon frequencies are around 62 THz. At 300 GPa, the imaginary frequencies disappear. In fact, the previously unstable optical modes have finite frequencies of 7.39 and 9.17 THz at the \( \Gamma \)-point. Even though, the convex hull suggested that fcc-CeH_{10} can be formed from 200 GPa onward [14], we suggest here that it can only be dynamically stable from 300 GPa. This is in agreement with experimental finding that CeH_{10} has not been found up to 200 GPa [22]. It is worth noticing here that the vibrations of the Ce atom are dominated at the low frequency region, i.e. \(<10\) THz, whereas the vibrations of the H_{32} cage are dominated in the high frequency region, i.e. \(>20\) THz. There is a large frequency gap due to the large difference between the masses of Ce and H, and the coupling between the two constituent species. The highest phonon frequencies are around 76 THz at this pressure. At the pressure range of 300–700 GPa, the phonons are all stable. Generally, the phonon frequencies increase as pressure increases. The frequency gap between the low and high frequency regions still remains.

At this stage, we discuss the electronic states. The calculated electronic band structure and projected density of state (PDOS) of fcc-CeH_{10} at pressure 400 and 700 GPa are shown in figures 3(a)–(d). The electronic states have some variation under pressure, hence we chose 400 GPa as the center of our discussion. From figure 3, the PDOS exhibits significant contribution from the \( f \)-electrons at Fermi energy \( (E_F) \) under high pressure. The PDOS also indicates that fcc-CeH_{10} is a metal with quite low density of states at \( E_F \), i.e. 0.22 states/eV. This is because all of the energy bands cross the Fermi energy with steep slope. In the other words, there is no flat dispersion near the \( E_F \). In fcc-LaH_{10} [13, 36] and hcp-CeH_{6} [22], the density of states at \( E_F \) is quite large due to some flat bands in the former and shallow-slope bands in the latter. There is a small expression of the van Hove singularity (vHs) at the \( E_F \) at 400 GPa, marked by an arrow in figure 3(c), but it gradually moves down to lower energy as pressure increases. At 700 GPa, the position of the vHs is a little below \( E_F \), as marked by an arrow in figure 3(d). This makes the density of states at \( E_F \) even lower at higher pressure. Table 1 gives a summary on the number of states (\( N_f \)) at \( E_F \) of fcc-CeH_{10} comparing with the other related structures.

At around the \( \Gamma \)-point close to \( E_F \), the band dispersions are dominated by the weaving of the up-running bands from below \( E_F \) and down-running bands above \( E_F \). When up- and down-running bands cross each other with their steep slopes, there is a possibility that the dispersions around the crossing are likely to form the Dirac cones. For example, the crossing bands along the \( M \rightarrow \Gamma \) branch are likely to form the Dirac cones. Some of

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Figure 1. Left: the formation enthalpy per atom of CeH_{10} is presented in the form of convex hulls. Right: the crystal structure of fcc-CeH_{10}. (a) The Fm-3m structure. (b) The H_{32} clathrate cage with six square and twelve hexagonal \((4 \ 6 \ 7)\) faces and the Ce atom (draw by VESTA [35]).}
\end{figure}
these crossing bands along the $M \rightarrow \Gamma$ branch are broken at 700 GPa, as shown in the dashed circle in figure 3(b) comparing with that in figure 3(a).

As we explicitly brought the f-electron into the calculation, we would like to investigate the effect of strong correlation to the band structure as well. In order to verify this feature, we calculated the electronic band structure by including an effective Hubbard parameter, $U = 4$ eV, for the Ce atom (figure 4). We found that the ground states are mostly intact. The band structures around the Fermi level resemble those of the GGA calculation, except some low-lying excited states at $\Gamma$ point occur at lower energy, and some of the crossing bands along the $M \rightarrow \Gamma$ branch are broken, as shown in the dashed circle in figure 4. Nevertheless, the states near Fermi level are similar to those of the GGA. Thus, the strong correlation of the f-electron should have minimum impact on the superconductivity.

From the band structure, we can construct the Fermi surfaces of fcc-CeH$_{10}$. The associated Fermi surface (FS) at 400 GPa are shown in figure 5. The surface #1–#3 are from the down-running dispersion around the $\Gamma$-point with steep slopes. Thus, these surfaces are just small polyhedral objects in the larger Brillouin zone. They contribute almost nothing to the superconductivity. The most important contribution to the superconductivity of fcc-CeH$_{10}$ is from the surface #4–#5. In fact, the surface #4–#5 are very special. They come from the accidental crossing between the up- and down- running dispersions at exactly the Fermi energy along the $\Gamma \rightarrow X, \Gamma \rightarrow M$ and $\Gamma \rightarrow R$ branches for the surface #4, and along $\Gamma \rightarrow X \rightarrow M \rightarrow \Gamma$ branches for the surface #5. Consequently, there could be a large number of the Dirac cones at the band crossing. For example, there are 2 cones for each $\Gamma \rightarrow X \rightarrow M \rightarrow \Gamma$ branch, and there are 12 equivalent $\Gamma \rightarrow X \rightarrow M \rightarrow \Gamma$ branches in the Brillouin zone. Therefore, there are 24 Dirac cones associating with the surface #5. Furthermore, the shapes of the surface #4–#5 contain several parts that are parallel to each other, i.e. these parts can be connected by a common nesting vector. These are the so-called Fermi surface nesting, see [37] for example. Thus, the surface #4–#5 take an important role in the superconductivity of fcc-CeH$_{10}$. The surface #6 is in the form of small pockets which are barely connected to each other, and hence gives insignificant contribution to the superconductivity. The Fermi surfaces have a little variation under pressure.

In order to understand the nature of bonding of fcc-CeH$_{10}$, we analyze the electron localization function (ELF) [39] in the (001) plane, as shown in figure 6. The ELF was a useful tool to study the bonds in many
metals and compounds, such as Li [40], S [41] c and XeC [42]. At 0 GPa, the ELF shows no structured bonding, and most electrons are localized around the Ce atoms, as shown in figure 6(a). At 100 GPa, the H$_{32}$ cage is formed, but there is only weak interaction with the Ce atom, as shown in figure 6(b). There are several areas that have low electron population. Furthermore, the H$_1$–H$_2$ bonding seems to be weakly formed. At 100–200 GPa, there were reports on the so-called atomic-like states in hcp-CeH$_9$ [22, 23] and fcc-LaH$_{10}$ [13, 18]. This is not the case for fcc-CeH$_{10}$. At 400 GPa, the H$_{32}$ cage forms more structured bondings with the Ce atom, as shown in figure 6(c). The H$_1$–H$_2$ bonding seems to be more strongly established. However, the H$_1$–H$_2$ bond length is very short, i.e. 1.109 Å, only. This also approaches the atomic hydrogen limit. It is worth noting here that H–H cannot be too close as the quantum nucleus effect will be likely to keep them apart [43]. This would be a subject of future investigation.

Finally, we calculated the superconductivity of fcc-CeH$_{10}$, starting from calculating the central feature, i.e. the spectral function, $\alpha^2 F$ by using QE [29, 30]. The spectral function at 300 GPa is shown as a solid line in figure 7(a). The spectral function can be clearly divided into two parts, i.e. the heavier Ce atom and the lighter H$_{32}$ cage parts. From figure 7(a), the accumulated $\lambda$ is shown as a dashed line. It reflects the strength of the

Table 1. The calculated parameters and $T_c$ of fcc–CeH$_{10}$ compared with those of fcc–LaH$_{10}$ [13, 36] and hcp–CeH$_9$ [22].

| Metal hydrides | Pressure (GPa) | $N_f$ (states/eV) | $\lambda$ | $\omega_{\text{mp}}$ (K) | $T_c$ (K) |
|----------------|---------------|-------------------|------------|--------------------------|-----------|
| fcc–LaH$_{10}$ | 210           | 0.73              | 3.41       | 848                      | 238       |
| fcc–LaH$_{10}$ | 300           | 0.95              | 2.20       | —                        | 220       |
| hcp–CeH$_9$    | 200           | 0.73              | 2.30       | 740                      | 117       |
| fcc–CeH$_{10}$ | 300           | 0.22              | 0.64       | 1632                     | 45        |

$^a$ Reference [13].
$^b$ Reference [36].
$^c$ Reference [22].
$^d$ This work.
electron-phonon coupling (EPC) in each region of the phonon frequencies. The contribution of $\lambda$ in the lower frequency region from the heavier Ce atom is about 0.09, whereas the contribution of $\lambda$ in the higher frequency region from the H$_{12}$ cage is about 0.55. The total $\lambda$ is 0.64 at 300 GPa. In hcp-CeH$_9$ at 200 GPa, the contributions of $\lambda$ are about 0.6 and 1.7 from the Ce atom and the H cage, respectively [22]. In fcc-LaH$_{10}$ at 300 GPa, the contributions of $\lambda$ are about 0.4 and 1.8 from the La atom and the H cage, respectively [36]. By using Hopfield analysis [44, 45], the electron-phonon coupling strength parameter can be expressed as,

$$\lambda \approx \frac{N_f \Gamma^2}{M \omega_2^2},$$

where $\Gamma^2$ is the average strength of the electron-phonon interaction, $N_f$ is the density of states at the Fermi level, $M$ is the characteristic mass of the system, and $\omega_2$ is the characteristic frequency of the system. As discussed

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**Figure 4.** Electronic band structure of CeH$_{10}$ is calculated by using GGA + U ($U = 4$ eV) at 400 GPa.

**Figure 5.** Fermi surface of CeH$_{10}$ at 400 GPa (draw by XCrySDen [38]).
earlier, we found that there can be the Fermi surface nesting in the surface #4–#5, which could give rise to a significant value of $I^2$. Disappointedly, we also found from table 1 that $N_f$ is comparatively much lower in fcc-CeH$_{10}$ due to the steep slope of the energy dispersion close to $E_F$. This is in contrast with hcp-CeH$_9$ where the dispersion close to $E_F$ is quite shallow [22], and with fcc-LaH$_{10}$ where there exist several flat bands close to $E_F$ [36].

Figure 6. The electron localization function (ELF) in the (001) atomic plane of the CeH$_{10}$ framework under pressures of 0, 100, and 400 GPa (draw by VESTA [35]).

Figure 7. (a) The spectral function $\alpha^2F$ (solid line) and the accumulated $\lambda$ (dashed line) as a function of frequency of fcc-Ce$_{10}$ at 300 GPa. (b) Critical temperature as a function of pressure with $\mu^* = 0.10$ (black line) and 0.13 (red line), $\lambda$ (blue squares) and $\omega_{\log}$ (black squares) as a function of pressure are shown in the inset.
From the spectral function, the logarithmic average of the phonon frequency, $\omega_{\text{log}}$, can also be evaluated, and it is 1,632 K for fcc-CeH$_{10}$ at 300 GPa. In addition, we also calculated $\lambda$ and $\omega_{\text{log}}$ as a function of pressure, as shown in the inset of figure 7(b). Typically, $\lambda$ is a decreasing function of pressure, whereas $\omega_{\text{log}}$ is an increasing function of pressure. By using the Coulomb pseudopotential parameter $\mu^*$ = 0.10 and 0.13 and equation (1), we calculated the superconducting critical temperature $T_c$. We found that $T_c$ decreases monotonically between 300 and 700 GPa, as shown in figure 7(b). The maximum $T_c$ of fcc-CeH$_{10}$ is 45 K at 300 GPa with $\mu^*$ = 0.10. This $T_c$ is quite low compared with 117 K of hcp-CeH$_{9}$ at 200 GPa [22] and 220 K of fcc-LaH$_{10}$ at 300 GPa [36]. This behavior is solely because of the low value of $N_f$ and hence of $\lambda$, as they are approximately related by equation (2). All the parameters and $T_c$ are summarized in table 1.

**Conclusion**

In this work, we have calculated the superconductivity of CeH$_{10}$ under pressure by using DFT. We found that the ground state structure is the Fm-3m structure, which is a clathrate structure. The phonon calculation suggested that it is dynamically stable from 300 GPa onwards. Then, we calculated the electronic structure and reported the electronic dispersion around the Fermi level, the Fermi surface, and the electron localization function. We found that the f-electron states dominate the states at the Fermi level. However, the density of states at the Fermi level is quite low. In addition, the electronic structure suggested that CeH$_{10}$ could be an exotic material due to some special topology in the Fermi surface. Next, we calculated the spectral function and $T_c$ as a function of pressure. We found that CeH$_{10}$ have low lambda compared with those of CeH$_{9}$ and LaH$_{10}$ at similar pressures. This is due to low density of states at the Fermi level. The $T_c$ is maximum around 45 K at 300 GPa.

**Acknowledgments**

We are deeply grateful for the kindness of Dr. Lorenzo Paulatto for helping us generate the cerium PAW pseudopotential for using in the quantum espresso package. We gratefully acknowledge NSC (National Computer Center, Linköping, Sweden) for providing computing time. This research is supported by Ratchadapisek Somphot Fund for Postdoctoral Fellowship, Chulalongkorn University. This work has been partially supported by Sci Super-IV research grant, Faculty of Science, Chulalongkorn University. T B acknowledge Thailand Research Fund contract number RSA5880058. This research is funded by Chulalongkorn University; Grant for Research. R A and W L thank the Swedish Research Council and Swedish Research Links for financial support.

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