The intermediate pressure phases of cerium: a LDA+Gutzwiller method study

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Abstract

The ground state of cerium metal in the intermediate pressure regime (5Gpa<P<12Gpa) is studied in detail by the newly developed LDA+Gutzwiller method, which can include the strong correlation effect among the 4f electrons in cerium metal properly. Our numerical results show that the $\alpha''$ phase, which has the distorted body centered tetragonal structure, is more stable in the intermediate pressure regime and all the other phases include the $\alpha'$ phase($\alpha$-U structure), $\alpha$ phase (fcc structure) and bct phases are either meta stable or unstable. Our results are quite consistent with the most recent experimental data.

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I. INTRODUCTION

Due to the strong correlation effect, the 4f electrons in Lanthanide metal usually participate very weakly into the chemical bonding, which makes these materials to be approximately s-band metal with close packed crystal structure. An very important exception of this qualitative understanding is the cerium metal, where the 4f electrons do participate in chemical bonding in the α fcc phase under ambient pressure. While the α fcc phase is quite close to the instability, an isostructure phase transition happens by raising the temperature above 116K, after which the crystal structure remains unchanged while the volume expands by 16% and the 4f electrons become localized\[1\]. Further numerical studies by implementing the first principle methods with dynamical mean field theory\[2, 3\] show that the γ phase may be stabilized by the entropy\[4\].

Another mysterious phenomena in cerium is the intermediate pressure phase. At zero temperature, the cerium metal form the face centered cubic(fcc) structure for pressure below 5 GPa and body-centered tetragonal (bct) structure for pressure above 12 GPa. But the experimental results of stable phases in the intermediate pressure region between 5 to 12 GPa are still quite controversial\[5–10\], as will discussed below in detail.

Ellinger and Zachariasen applied X-ray diffraction studies on high pressure cerium with a diamond-anvil cell\[5\], and they reported that for pressure between 5 and 12 GPa, the orthorhombic α′-Ce phase with α-uranium type of structure, is the most stable phase. They also found another meta stable phase α′′ phase, which is monoclinic body centered with a deformed cubic face-centered structure. The conclusion that α′-Ce is the most stable phase between 5 and 12 GPa while α′′ phase is meta stable has been supported by some of the follow up experiments, i.e. \[6\] and \[7\]. While another group of experiments led to opposite conclusion, which indicated that the α′′ rather than the α′ phase is the most stable phase in the intermediate pressure regime. Using diamond anvil cell and synchrotron radiation Olsen et al. studied the high-pressure phase diagram of cerium up to 46 GPa\[8\]. They reported that α′′ phase is the stable intermediate pressure phase of Ce, and no evidence for α′ phase with α-uranium structure was found. This was the first experiment reporting the α′′ phase to be the stable intermediate pressure phase for cerium. After that several other groups also reported the similar experimental results supporting α′′ phase to be the most stable phase of cerium for pressure between 5 and 12 GPa \[9, 10\].
The first principle calculation is a powerful theoretical tool to predict the ground state phases of solid. During the past two decades, many efforts have been made to reveal the true ground state phase for cerium under intermediate pressure by first principle calculations. The early results of linear muffin-tin orbital (LMTO) method found the $\alpha'$ phase to be stable in the intermediate pressure regime between the low pressure fcc phase and high pressure bct phase\cite{11,12}, which was consistent with the early experiments. After that, P. Soderlind and Eriksson et al. applied the generalized-gradient approximation (GGA) based on full-potential linear muffin-tin orbital (FPLMTO) method to the same problem\cite{13} and found that $\alpha''$ phase was the most stable phase only in a small pressure interval. P. Ravindran et al. have made systematic electronic structure and total-energy studies on Ce and didn’t find any stable intermediate phases between the low pressure fcc phase to high pressure bct phase\cite{14}. According to their results, both the $\alpha'$ and $\alpha''$ phases are meta stable with $\alpha''$ phase being lower in energy. After that, LDA or GGA type calculations by other groups using plane wave method\cite{15} or exact muffin-tin orbitals (EMTO) method\cite{16} also got similar results, that both $\alpha'$ and $\alpha''$ phases are not stable and the true ground states in energy of cerium are $\alpha$ phase (low pressure) and bct phase (high pressure).

Although the 4$f$ electrons in the $\alpha$ phase are delocalized, the strong repulsive interaction among them still modifies its electronic structure significantly. Due to the insufficient treatment of the correlation effects, the bonding strength of the $\alpha$ cerium has been over estimated by the LDA type calculations, which leads to smaller volume and larger bulk modules comparing with the experimental data. In the present paper, we apply the newly developed LDA+Gutzwiller method, which can satisfactorily treat the strong correlation effects in the 4$f$ shell, to determine the ground states of cerium under pressure. We first apply the above method to study the ground state properties of $\alpha$ cerium under the ambient pressure. Our results show that both the volume and bulk modules are improved dramatically, which manifests the importance of the strongly correlation effect for the 4$f$ electrons in $\alpha$ cerium. Further we apply the same method to study the intermediate pressure phases of cerium, and the results show that in the intermediate pressure region the $\alpha''$ phase is the most stable phase and all other states are either meta stable or unstable, which is quite consistent with the recent experiments\cite{9,10}.

The rest of the paper is organized as following. A brief introduction of LDA+Gutzwiller method are given in Sec. II. In Sec. III we discuss the main results of our LDA+Gutzwiller
calculations with the comparison to the recent experimental results and LDA(GGA) results. The summary and conclusions are given in the last section.

II. LDA+GUTZWILLER METHOD

Gutzwiller first introduced Gutzwiller variational approach to study the itinerant ferromagnetism in systems with partially filled $d$ bands described by the Hubbard model\[17\]. Since then, the Gutzwiller variational approach has been widely applied to various of strongly correlated systems\[18–22\]. Recently, we developed a computational method to incorporate LDA with Gutzwiller variational approach named LDA+Gutzwiller method(simply called LDA+G hereafter)\[23–25\], by successfully applying to a number of typical correlated materials, the reliability and feasibility of this method have been demonstrated. In the following we present the method briefly, please refer to our previous paper\[25\] for more details.

Similar with LDA+U or LDA+DMFT methods, in the LDA+G method, the LDA Hamiltonian, which can be extracted from the first principle calculation, is implemented by a Hubbard-like local Coulomb interaction, which is not adequately treated within LDA. The effect of this local Coulomb interaction can thus be considered within the Gutzwiller variational approach. The Hamiltonian can be usually expressed as

$$H = H_{LDA} + H_{int} - H_{DC}, \tag{1}$$

with

$$H_{int} = \sum_{i,\alpha,\beta(\alpha \neq \beta)} U_i^{\alpha,\beta} \hat{n}_{i\alpha} \hat{n}_{i\beta}, \tag{2}$$

where $H_{LDA}$ is the LDA part Hamiltonian extracted from the standard LDA calculation, $H_{int}$ is the on-site interaction term, where $\alpha$ and $\beta$ are combined spin-orbit indices of localized basis $\{\phi_{i,\alpha}\}$ on site $i$, among which the local Hubbard interaction is implemented, $\alpha = 1, \ldots, 2N$ ($N$ is orbital number, e.g. $N = 7$ for $f$ electrons). $H_{DC}$ is the double counting term representing the average orbital independent interaction energy already included by LDA. Without the $H_{int}$ term, the ground state can be exactly given by the Kohn-Sham uncorrelated wave function(KSWF) $|\Psi_0\rangle$, which is a single Slater determinant made from the single particle wave functions. However, with the increment of the interaction strength, the KSWF is no longer a good approximation because it gives too much weighting factor for those energetically unfavorable configurations. In order to give a better description of the
ground state, the weighting factor of those unfavorable configurations should be suppressed, which is the main idea of Gutzwiller wave functions (GWF) $|\Psi_G\rangle$. GWF is constructed by acting a many-particle projection operator on the uncorrelated KSWF, which reads

$$|\Psi_G\rangle = \hat{P}\Psi_0 = \prod_i \hat{P}_i |\Psi_0\rangle,$$

(3)

with

$$\hat{P}_i = \sum_{\Gamma} \lambda_{i\Gamma} \hat{m}_{i\Gamma},$$

(4)

$$\hat{m}_{i\Gamma} = |i, \Gamma\rangle \langle i, \Gamma|,$$

(5)

where $\hat{m}_{i\Gamma}$ is the projector to the specified configuration $|\Gamma\rangle$ on site $i$. In equation (3), the role of projection operator $\hat{P}$ is to adjust the weight of each atomic configuration through variational parameters $\lambda_{i\Gamma}(0 \leq \lambda_{i\Gamma} \leq 1)$. The GWF falls back to KSWF if all $\lambda_{i\Gamma} = 1$. On the other hand, if $\lambda_{i\Gamma} = 0$, the configuration $|\Gamma\rangle$ on site $i$ will be totally removed. In this way, both the itinerant behavior of uncorrelated wave functions and the localized behavior of atomic configurations can be described consistently, and the GWF can give a more accurate description of the correlated metallic systems than KSWF.

The total energy of the above system can be expressed as the expectation value of the Hamiltonian equation (1) using GWF, which takes the form

$$E_{Total} = \langle \Psi_G | H | \Psi_G \rangle = \langle \Psi_G | H_{LDA} | \Psi_G \rangle + \langle \Psi_G | H_{int} | \Psi_G \rangle - E_{DC},$$

(6)

In equation (6), the interaction energy is given as

$$\langle \Psi_G | H_{int} | \Psi_G \rangle = \sum_{i,\Gamma} E_{i\Gamma} m_{i\Gamma},$$

(7)

where $m_{i\Gamma}$ is the weight of configuration $\Gamma$

$$m_{i\Gamma} = \langle \Psi_G | \hat{m}_{i\Gamma} | \Psi_G \rangle$$

(8)

According to equation (3), the LDA energy of equation (6) can be written as

$$\langle \Psi_G | H_{LDA} | \Psi_G \rangle = \langle \Psi_0 | \hat{P} H_{LDA} \hat{P} | \Psi_0 \rangle = \langle \Psi_0 | H_{LDA}^G | \Psi_0 \rangle.$$  

(9)

$H_{LDA}^G$ is called the effective Hamiltonian under Gutzwiller approximation.
The DFT calculations for realistic materials are always done in reciprocal space, so the formulas above should transform to the reciprocal space. We define the Bloch states of localized orbitals $|i\alpha\rangle$

$$|k\alpha\rangle = \frac{1}{N} \sum_i e^{ikR_i} |i\alpha\rangle$$

Then $H_{LDA}^G$ in $k$ space can be written as

$$H_{LDA}^G = \left( \sum_{k\alpha} z_\alpha |k\alpha\rangle \langle k\alpha| + 1 - \sum_{k\alpha} |k\alpha\rangle \langle k\alpha| \right) H_{LDA} \left( \sum_{k'\beta} z_\beta |k'\beta\rangle \langle k'\beta| + 1 - \sum_{k'\beta} |k'\beta\rangle \langle k'\beta| \right)$$

$$+ \sum_{kk'\alpha} (1 - z^2_\alpha) |k\alpha\rangle \langle k'\alpha| H_{LDA}^G |k\alpha\rangle \langle k\alpha|,$$

where $z_\alpha$ is renormalization factor for local orbital $\alpha$ which depends on those Gutzwiller variational parameters $\lambda_\Gamma$, for those non-interacting orbitals, the corresponding $z$ factor equals to 1.

According to equation (6, 7, 9, 11), the total energy reads

$$E_{Total} = \langle \Psi_0 | \left( \sum_{k\alpha} z_\alpha |k\alpha\rangle \langle k\alpha| + 1 - \sum_{k\alpha} |k\alpha\rangle \langle k\alpha| \right) H_{LDA} \left( \sum_{k'\beta} z_\beta |k'\beta\rangle \langle k'\beta| + 1 - \sum_{k'\beta} |k'\beta\rangle \langle k'\beta| \right) |\Psi_0\rangle$$

$$+ \sum_{\alpha} (1 - z^2_\alpha) n_\alpha \varepsilon^\alpha_{LDA} + \sum_{\Gamma} E_{\Gamma m_{\Gamma}} - E_{DC},$$

where $\varepsilon^\alpha_{LDA} = \sum_k \langle k\alpha| H_{LDA}^G |k\alpha\rangle$ and $n_\alpha = \sum_k \langle \Psi_0 | k\alpha\rangle \langle k\alpha| \Psi_0\rangle$.

The total energy expressed in equation (12) depends on both the uncorrelated ”starting” wave function $|\Psi_0\rangle$ and those Gutzwiller variational parameters $\lambda_\Gamma$, which can both be determined by minimizing the total energy. After we obtain the ground state wave function, we can calculate most of the ground state properties based on it, please refer to our paper [25] for more details.

III. RESULTS AND DISCUSSIONS

Like the LDA+U and LDA+DMFT methods, in LDA+G method the Hubbard-like local Coulomb interaction U will be chosen as the only empirical parameter. For $4f$ electrons in
cerium metal we set $U=4$eV, which is consistent with other LDA+U and DMFT calculation. First we calculate the equilibrium volume and bulk modulus for $\alpha$-Ce under ambient pressure to check the validity of the $U$ value. Our results are shown in Tab. I together with the results from the all-electron FPLMTO calculations\[26\], pseudopotential Plane-Waves calculations\[15\], and experiment\[5, 8\]. We can see from the table that the LDA calculation usually over estimate the bonding strength among cerium atoms, which makes the ground state volume obtained by LDA to be about 20% smaller and bulk modules to be 60% larger. After treating the correlation effect more carefully by Gutzwiller variational method, our results are in very good agreement with experiments. Thus we set $U=4$eV for all the calculations for cerium with different volume, and spin-orbital coupling effect is always fully included.

Early experiments have reported two intermediate-pressure phases of cerium, $\alpha'$ phase and $\alpha''$ phase, together with the low pressure $\alpha$ phase and high pressure bct phase. The instability of these four phases under pressure is the main interest of the present work. Neglecting the tiny distortion in the $\alpha''$ phase, all these three phases including $\alpha$, $\alpha''$ and the high pressure bct phase can all be treated within the same bct structure but with the different ratio of the lattice constants $c/a\[8, 9, 13\]$, which is illustrated in Fig. 1. The $c/a$ ratio is exactly $\sqrt{2}$ for $\alpha$ phase with the fcc structure and is found to be around 1.65 for the high pressure bct phase. The $c/a$ ratio of $\alpha''$ phase is reported experimentally to be around $1.5 \leq c/a \leq 1.56\[5, 8\]$. Therefore in the present paper, we first apply the LDA+G method to minimize the total energy of the cerium with bct structure respect to the $c/a$ ratio as the function of volume, which mimics the competition among the $\alpha$, $\alpha''$ and high pressure bct phases under pressure, and after that we will compare the total energy of these phases and the $\alpha'$ phase. Our main results have been plotted in Fig. 2 with the comparison to LDA and GGA. The results obtained by all the three methods agree quite well for volume smaller than 20Å$^3$ indicating that the bct phase with $c/a = 1.65$(denoted by the green arrow in Fig. 2) is the most stable phase, which is also quite consistent with the experiments\[5, 8\]. For volume between 20.5Å$^3$ to 22.5Å$^3$, which corresponds to the intermediate pressure region, the results obtained by LDA, GGA and LDA+G are quite different. First of all, all the three methods predict that all the three phases appear as the locally stable phases in the intermediate pressure region. While LDA results indicate that the $\alpha''$ phase is only the meta stable phase in almost the whole intermediate pressure region except for volume being 21Å$^3$. 


And GGA can give a very small region, within which the $\alpha''$ phase is the most stable phase. Only LDA+G predicts that the $\alpha''$ phase is the most stable one of all the three phases in the whole intermediate pressure region. For volume larger than 23Å³, the three methods again reach the same conclusion that the $\alpha$ phase is more stable and all the other meta stable states including $\alpha''$ and high pressure bct phases disappear completely, which is again quite consistent with the existing experiments[8–10].

The optimized $c/a$ ratio as the function of volume obtained from our LDA, GGA and LDA+G calculations are plotted in Fig. 3 together with the experimental results[8]. We can find clearly that the LDA+G calculation obtains the stable region of $\alpha''$-Ce to be from 20.5Å³ to 22.5Å³, which is in good agreement with the experimental data[8]. While LDA and GGA only get a much narrow region for $\alpha''$-Ce stable as shown in Fig. 3.

The next issue to be addressed is the relative energy of the $\alpha'$ phase compared with the other three phases discussed in the previous paragraph. The $\alpha'$ phase has a orthorhombic $\alpha$-U structure which can be viewed as distorted fcc with some of the face-centered atoms being shifted from their original positions, as described by the parameter 2y[11]. The 2y value obtained experimentally by McMahon and Nelmes[9] is 0.2028Å. If 2y=0.5 Å and $a=b=c$, the standard fcc structure can be restored. Therefore we can calculate the energy of $\alpha$-Ce(fcc) and $\alpha'$-Ce within the same $\alpha$-U structure. We use $a/b = 0.5115, c/b = 0.8756$ as obtained from the experiment[9] and optimize the 2y value for any given volume. We find that 2y=0.21 gives the minimum-energy for volume being 22.5Å³, which is in good agreement with experiment[9]. We calculated the energy of $\alpha$-Ce(fcc) and $\alpha'$-Ce within the $\alpha$-U structure frame for a volume region: $18\text{Å}^3 \leq \text{volume} \leq 28\text{Å}^3$. The energy difference between them($E_{\alpha'} - E_\alpha$) is plotted in Fig. 4 together with the energy difference of $E_{\alpha''} - E_\alpha$ and $E_{\text{bct}} - E_\alpha$ obtained previously. Our results confirm that $\alpha'$ phase is always higher in energy. We thus rule out the $\alpha'$ structure as an stable intermediate pressure phase of cerium. This conclusion is in good agreement with the FPLMTO method calculations[14]. From Fig. 4 we can also see that $\alpha''$ structure is the most stable phase among the above mentioned four possible phases within the volume region: $20.5\text{Å}^3 \leq \text{volume} \leq 22.5\text{Å}^3$. Therefore based on the LDA+G calculation, we conclude that $\alpha''$ phase is the most stable phase for cerium in the intermediate pressure region. This conclusion is quite consistent with the most recent experiments[9, 10].

In Fig. 5 we plot the renormalization factor of the 4f bands in the $\alpha$, $\alpha''$ and high
pressure bct phases as the function of volume. We can find that the renormalization factor of the 4f bands decreases monotonically with the increment of the volume for all the three phases, which can be easily explained by the fact that increasing volume reduces the hopping integral between the neighboring f orbitals which enhances the correlation effect among 4f electrons and thus reduces the corresponding renormalization factor. From the present LDA+G calculation, we find that the main consequence of the correlation effect in the total energy is to reduce the kinetic energy. Since the fcc structure is close packed, compared with the α" phase, the α phase has relatively higher kinetic energy gain, which is over counted by LDA. Because of that, the reduction of kinetic energy gain captured by LDA+G is also more pronounced in the α phase, which raises the total energy of the α phase relative to the α" phase and makes it unstable in the intermediate pressure region.

IV. CONCLUSIONS

In summary, using the newly developed LDA+G technic, we have carried out systematical numerical study on the phase diagram of cerium metal under pressure. We found that the correlation effect among f electrons in cerium plays a crucial role to determine the most stable phase of cerium in the intermediate pressure region. The LDA calculation over estimates the chemical bonding contributed by the 4f electrons, which leads to smaller equilibrium volume and larger bulk modulus comparing to the experimental data. With the increment of pressure, the overlap between 4f orbitals becomes more and more pronounced, which reduces the correction to the total energy caused by the correlation effect. Therefore the correct description of the correlation effect which evolves with the pressure becomes one of the key issues to obtain the correct phase diagram in the intermediate pressure region. Our numerical results obtained by the LDA+G method conclude that the α" phase is the most stable phase in the intermediate pressure region, which is quite consistent with the recent experiments.

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FIG. 1: The relationship between the $\alpha$ phase (face-centered cubic, dashed lines with hatched circles—main cell), bct phase (body centered tetragonal, dash dot line subcell with unfilled circles) and the $\alpha''$ phase (C-face-centered monoclinic, solid line subcell with black circles).
FIG. 2: The total energy of body-centered tetragonal structure as a function of $c/a$ axial ratio. LDA, GGA and LDA+G results are marked with black, red and blue line respectively. $\alpha, \alpha''$ and bct phase are marked with purple, orange and green arrows.
TABLE I: Theoretical and experimental values of the equilibrium volume $V$ and bulk modulus $B$ for $\alpha$-Ce from our LDA+G calculations, some LDA/GGA calculations\cite{15, 26} and experimental data\cite{5, 8}

|            | $V(\text{Å}^3)$ | $B(\text{GPa})$ |
|------------|-----------------|-----------------|
| LDA        | 22.74\cite{26}, 23.3\cite{15} | 60.5\cite{26}, 58.7\cite{15} |
| GGA        | 26.05\cite{26}, 26.3\cite{15} | 48.7\cite{26}, 43.0\cite{15} |
| Present(LDA+G) | 28.91           | 36.2            |
| Experiment\cite{5, 8} | 28-29           | 20-35           |

FIG. 3: The $c/a$ axial ratio for the body-centered tetragonal structure as a function of volume for Ce. LDA+G results are marked with red solid line and filled circles, LDA results are marked with green solid line and filled triangle, GGA results are marked with blue dash line and filled triangle, experimental data (Ref. 8) are marked with black open squares.
FIG. 4: The relative total-energy curves with respect to the α phase (fcc).

FIG. 5: The average quasi-particle weight as a function of c/a axial ratio for angular momentum J=5/2 and J=7/2 f-electrons of Ce.