Topological transitions of the Fermi surface of osmium under pressure: an LDA+DMFT study

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Abstract

The influence of pressure on the electronic structure of Os has attracted substantial attention recently due to reports on isostructural electronic transitions in this metal. Here, we theoretically investigate the Fermi surface of Os from ambient to high pressure, using density functional theory combined with dynamical mean field theory. We provide a detailed discussion of the calculated Fermi surface and its dependence on the level of theory used for the treatment of the electron–electron interactions.

Although we confirm that Os can be classified as weakly correlated metal, the inclusion of local quantum fluctuations between 5d electrons beyond the local density approximation explains the most recent experimental reports regarding the occurrence of electronic topological transitions in Os.

1. Introduction

Osmium has the highest density of all the known elements. High-pressure experiments and \textit{ab initio} calculations indicate that the bulk modulus of hexagonal close-packed (hcp) Os rivals that of diamond carbon [1–6]. Recently, a combined experimental and theoretical study was presented, identifying two types of electronic transitions under pressure [1]. These transitions expressed themselves as anomalies in the pressure evolution of the measured \(c/a\)-ratio of the hcp structure. At approximately 150 GPa, a so-called electronic topological transition (ETT) was found, which is a topological change of the Fermi surface, also known as a Lifshitz transition [7–9]. Such transitions have previously been demonstrated to cause anomalies in the measured \(c/a\)-ratio [10]. It is worth to mention that a second anomaly seen above 400 GPa could not be identified with any ETT, but was explained by the overlap of core electron levels. Experiments also showed that the hcp structure is stable up to the highest pressure achieved, above 770 GPa.

Earlier experimental and theoretical work has yielded conflicting conclusions regarding the \(c/a\)-anomalies. Measurements by Occelli \textit{et al} [4] reported an anomaly in the \(c/a\)-ratio at 25 GPa. However, a similar study up to 60 GPa by Takemura [5] did not report any such finding. On the theoretical side, Sahu and Kleinman [6] made a fully relativistic \textit{ab initio} calculation of the lattice constants, and predicted a change of slope in the pressure dependence of \(c/a\)-ratio at 9.5 GPa, but they did not consider the evolution of the Fermi surface under pressure. Ma \textit{et al} [11] calculated an equation of state (EOS) based on the generalized gradient approximation (GGA) and found an anomaly in the \(c/a\) ratio at 25 GPa, but without any sign of an ETT up to 80 GPa.

However, high precision calculations by Koduela \textit{et al} [12], demonstrated that although the form of the experimental pressure–volume curve is well reproduced with GGA, it is generally shifted towards larger volumes. Using the local density approximation (LDA), an EOS in closer agreement with experiment was obtained. Three ETTs were identified between 70 and 130 GPa, at different points in the Brillouin zone (BZ). Nevertheless, the observed ETTs were concluded to be unrelated to the \(c/a\) anomaly. Finally, a study by Liang and Fang [14] did not find any peculiarity in \(c/a\)-ratio or any sign of ETTs up to 150 GPa.

In [1], the controversy was resolved. Using a highly accurate experimental EOS, measured up to 770 GPa, and treating electron–electron interactions with the more advanced scheme of combining the LDA with
dynamical mean field theory (the LDA + DMFT method \[15\]), it was demonstrated that the peculiarity of the \(c/a\) ratio does exist at \(\sim 150\) GPa and that it can be related to ETTs. However, no studies of the Fermi surface evolution with pressure in hcp Os which include electron–electron interactions beyond the LDA or the semi-local GGA have been reported so far. The LDA + DMFT method does take dynamical correlation effects into account, and it is capable of interpolating between the metallic regime and the strongly localized Mott-insulating limit.

In this paper, we present further details of the electronic structure of Os in the pressure range where these ETTs were detected, and demonstrate the impact of electron correlations beyond the LDA—local quantum fluctuations on the Fermi surface of this metal.

We calculate the electronic structure of Os within the LDA + DMFT method for the range of pressures, from zero to about 250 GPa, and compare the Fermi surface and charge distributions obtained within LDA + DMFT and LDA. Band structure, Fermi surface, and charge density distribution plots give complementary information on this system from different aspects. In particular, earlier density analysis of Os has suggested the valence charge to be highly localized in the nearest-neighbor bonds \[16\], which could partly explain its high bulk modulus. It is therefore important to investigate what happens to the Os electronic structure and charge density when local quantum fluctuations are included, especially under pressure.

\section{Methods and details of calculation}

\subsection{Lattice constants}

Although DMFT calculations can nowadays be carried out to determine the EOS for a transition metal \[17\], they are still quite time consuming. Therefore, in the present work we have used the experimental lattice constants presented in \[1\] in order to relate the unit cell volume to pressure. To avoid additional complications in comparing LDA + DMFT and LDA results, the latter were obtained at the experimental lattice parameters as well. Besides, the use of experimental lattice parameters allows us to avoid complications related to inaccuracies of the calculated EOS for Os, clearly demonstrated in \[1\], as well as to skip the necessity to compare results of calculations obtained within local (LDA) and semi-local (GGA) approximations of density functional theory. Indeed, it is well documented, that the electronic structure as calculated with either LDA or GGA at the same lattice constants, is practically indistinguishable in nonmagnetic systems \[13\]. The employed values are summarized in table 1.

\begin{table}[h]
\centering
\caption{Lattice constants used in the calculations. All values are experimental and taken from \[1\].}
\begin{tabular}{cccc}
\hline
\(P\) (GPa) & \(V\) (Å\(^3\)) & \(a\) (Å) & \(c/a\) \\
\hline
0 & 27.960 & 2.734 & 1.580 \\
86 & 23.948 & 2.592 & 1.588 \\
134 & 22.572 & 2.540 & 1.590 \\
247 & 20.304 & 2.449 & 1.596 \\
\hline
\end{tabular}
\end{table}

\subsection{LDA calculations}

In our LDA calculations we have used the all-electron full potential band structure method, provided in the Wien2k code \[18\]. We used a \(32 \times 32 \times 32\) \(k\)-mesh, and kept the product \(R_{MT} \cdot K_{\max} = 10\), where we set the muffin-tin radius \(R_{MT} = 2.5\) a.u.

We have also performed calculations using the all-electron full potential local orbital (FPLO) \[19, 20\] method.

\subsection{LDA + DMFT calculations}

For LDA + DMFT calculations, we have used the toolkit implemented in the TRIQS package. References \[21–23\], which is fully self-consistent in both charge and local self-energy in the LDA + DMFT cycles. We have treated the partially filled 5d shell as correlated within the DMFT approximation. The corresponding effective Hamiltonian has the form:

\begin{equation}
\mathcal{H} = \mathcal{H}^{\text{LDA}} + \mathcal{H}^{\text{DC}} + \mathcal{H}^{U},
\end{equation}

\begin{equation}
\mathcal{H}^{U} = \frac{1}{2} \sum_{i=\downarrow,\uparrow} \sum_{l} U_{mm'\sigma\sigma'} \hat{n}_{m\sigma} \hat{n}_{m'\sigma'},
\end{equation}
where $\mathcal{H}^{LDA}$ is the energy of the system in LDA, from which the 5d contribution due to the on-site Coulomb repulsion is subtracted by the double counting term, $\mathcal{H}^{DC}$, which we approximate with the so-called around mean field form [24]:

$$
\mathcal{H}^{DC} = \sum_{mn=mn'} \frac{U_{mn'} - \mu}{2} (n_{mn} - n_{mn'})
\times (\bar{n}_{mn'} - \bar{n}_{mn'}),
$$

where

$$
\bar{n}_{mn} = \frac{1}{(2l + 1)} \sum_m n_{mn},
$$

and finally, $\mathcal{H}^U$ is the Coulomb interaction term.

Within each DMFT iteration, the impurity problem was solved with the hybridization-expansion continuous-time quantum Monte Carlo method [25]. In each DMFT iteration we performed over 512 million Monte Carlo cycles at inverse temperature $1/T = 40$ eV$^{-1}$. The impurity problem was solved for the self-energy on the Matsubara axis, after which an analytical continuation was made to the real axis by a stochastic version of the maximum entropy method [26].

We have used the Coulomb interaction strength $U = 2.80$ eV and Hund’s coupling constant $J = 0.55$ eV, based on the estimations in [27]. It should be noted that the $U$ value may differ slightly, depending on crystal structure and different computational methods [28–30]. However, for a weakly correlated compound as Os, small variations in the $U$ parameter should only slightly affect our quantitative predictions, and not our qualitative conclusions.

LDA+DMFT electronic structure calculations were performed within the scalar-relativistic approximation and using a $k$ mesh with $32 \times 32 \times 32$ points in the full BZ. Since we are interested in comparing the LDA and LDA+DMFT approximations, we used the same parameters as for LDA. As shown in [1], the inclusion of spin–orbit coupling in LDA calculations will split some of the bands, however these features are located far away from the Fermi level, even at high pressure. We have therefore performed our calculations within the scalar-relativistic approximation, neglecting spin–orbit coupling.

### 2.4. Quasiparticle effective mass

We have calculated the ratio of the effective mass of the correlated quasiparticles, $m^*$, to that of uncorrelated electrons, $m$, as:

$$
\frac{m^*}{m} = \frac{\sum \rho_l(E_F)[1 - \partial \text{Im } \Sigma_l(i\omega)/\partial \omega]}{\sum \rho_l(E_F)},
$$

where $l$ is the orbital index, $\rho_l(E_F)$ is the density of states of the $l$th orbital in $\omega$ space at the Fermi level and $E_F$ is the Fermi energy, $\Sigma_l(i\omega)$ is the local self-energy on the Matsubara axis. Since there are several d orbitals and the occupancy of each orbital by the itinerant electrons will vary, we take the averaged value of the effective mass, $\bar{m}^*$, to represent the correlation strength for all the 5d electrons.

### 2.5. Electron density distribution

In order to analyze details of the density distribution we have calculated the Fourier transform of the charge density to $k$-space. We have used a very dense 200 $\times$ 200 $k$-point grid, which is considerably denser than in the Fermi surface calculations. The charge density at each $k$-point was calculated by integrating the $k$-dependent density of states below the Fermi level, i.e., with the following formula:

$$
n(k) = \int_{\omega_{\text{bottom}}}^{E_F} f(\omega) \rho(k, \omega) \mathrm{d}\omega,
$$

where the density of states, $\rho$, was obtained by summing over the orbital channels:

$$
\rho(k, \omega) = \sum_l \rho_l (k, \omega),
$$

labeled by $l$. In turn,

$$
\rho_l (k, \omega) = -\frac{1}{\pi} \text{Im } G_l (k, \omega),
$$

where $G_l (k, \omega)$ is the $k$-dependent Green’s function of the $l$th orbital on the real frequency axis. $f(\omega) = \frac{1}{1 + e^{\beta \omega}}$ is the Fermi–Dirac distribution function with $\beta = 1/k_B T$, where $k_B$ is the Boltzmann constant and $T$ is the temperature. The charge density, $n(k)$, is thus defined on a 2D grid in $k$-space. In fact, $n(k)$ can be measured experimentally as well, e.g., by x-ray scattering.
Figure 1. Averaged quasiparticle mass for the 5d electrons in Os as a function of pressure.

Figure 2. Illustration of relevant high symmetry points on the hcp reciprocal lattice. In (a) and (b), the $\Gamma$ point is at the center of the Brillouin zone. In (c), the center of the cell is at the A-point, and $\Gamma$ is at the top and bottom faces. Figure (b) shows how these are related to each other. This is a more suitable view of the reciprocal lattice for the presentation of our results, and is used in figures 3(b), 6 and 7.
3. Results and discussion

3.1. Correlation strength

We begin by addressing the strength of electron correlations in hcp-Os. In 5d transition metals the effect of electronic correlations is believed to be small. However, previous studies on moderately correlated isoelectronic systems such as hcp-Fe, have shown that a description of correlations beyond the LDA level can lead to new features in the electronic structure \[10\]. More specifically, using the more advanced description provided by LDA+DMFT, an ETT was found for hcp-Fe in precisely the pressure range where an anomaly in \( c/a \) was seen experimentally.

The strength of electron correlations can be quantified by the effective mass of the quasiparticles, which are compared to the mass of uncorrelated electrons with equation (3). As discussed in section 2.4, we express this as a weighted average over all the 5d-orbitals.

In figure 1, we show the averaged effective mass of the quasiparticles plotted against pressure. From the figure, one can observe that the effective mass \( m^* \) is very close to the mass of uncorrelated electrons. Therefore,
Figure 4. Band structure obtained at the experimental lattice constants (from [1]) corresponding to $P = 0$ GPa, using (a) the Wien2k and (b) the FPlo method.

Figure 5. So-called fat bands calculated at ambient pressure. The size of the circles indicate the $d$-electron character of the bands.
this system is a weakly correlated system. Moreover, as expected, we notice that the effective mass decreases as pressure is increased, and kinetic energy starts to be comparable to the Coulomb energy.

3.2. Fermi surface

3.2.1. Ambient pressure
We have calculated the Fermi surface of hcp Os at different pressures using both the LDA and LDA+DMFT approximations. The relevant high symmetry points of the hcp reciprocal lattice are shown in figure 2. In figure 2(a), the standard view of the reciprocal lattice is shown, with the BZ clearly marked. To show our results, it is more illustrative to take the A-point at the center of the cell, as shown in figure 2(c).

In figure 3 we show the Fermi surface of Os at the pressure \( P = 0 \) GPa, as obtained with LDA. Figure 3(a), shows the Fermi surface with the convention of figure 2(a). In figure 3(b), we have replotted the Fermi surface with the convention of figure 2(c). One can see that the Fermi surface consists of four sheets. Two electron sheets surround the \( \Gamma \) point (green and yellow in figure 3(b)), the yellow one having a waist. In addition, one hole sheet is open (red), and disconnected ellipsodials form hole pockets (blue). These are all cut by the L–M–K–H plane. In addition, we see a hole pocket around the \( \Gamma \) point.

This topology of the Fermi surface at ambient pressure is in agreement with the experimental work in [2] and the theoretical work in [11, 12]. However, as discussed in [1], details of the Fermi surface at a given pressure is sensitive to the specific choice of the EOS, which can be obtained by calculations or experiment. For example, at the \( \Gamma \) point, a hole pocket was seen in [14], in contrast to [12]. Nevertheless, calculations at the experimental lattice constants, which we have carried out with the same computational method as in [12] (the FPLO method) clearly show a hole pocket (see figure 4). We therefore believe it is beneficial to compare results at fixed volume, and we therefore use the experimental values presented in table 1.

We now compare results obtained with the LDA and LDA+DMFT methods, to see the impact of correlation effects beyond the LDA. Figure 6 shows a comparative side-view of the Fermi surface obtained with LDA + DMFT (left column) and LDA (right column). Comparing figures 6(a) and (b), we see how LDA+DMFT gives a wider gap at the L point compared to LDA. In addition, the hole pocket around \( \Gamma \) point seen in the LDA calculations, is not present at the Fermi surface calculated within LDA+DMFT. This part of the Fermi surface is not visible in figure 6, but is discussed in section 3.3.1.

In figure 5 we show so-called fat-bands, indicating the d-character of the bands. It is seen that the band edge at the \( \Gamma \) point is of sp-character. At the L-point we also find a large weight of sp-electrons. The main impact of the LDA+DMFT treatment is concerned with the d-states, forming our space of correlated states, which are shifted
along with the chemical potential. Comparing with LDA, the bands at the $\Gamma$ and L-points appear shifted down in energy.

### 3.2.2. 134 GPa

Upon increase of pressure, the LDA+DMFT results in figure 6(c) show how the gap at the L point has only been reduced. This is in contrast to the LDA result shown in figure 6(d), where one of the sheets (red), has become connected, meaning that it has undergone a so-called necking transition at the L–H line. Figure 7 shows the same view of the reciprocal lattice as in 2(c), with the $\Gamma$ point clearly visible. In LDA (figure 7(b)), we see a pronounced pocket at the $\Gamma$ point. There is no topological change of the Fermi surface, as compared to ambient pressure (see figure 3(b)), since the hole pocket is only seen to have become larger. In LDA+DMFT, (figure 7(a)), the pocket is significantly smaller. This pocket is not present at ambient pressure, and the ETT occurs just above 100 GPa [1], in much better agreement with experiment as compared to the LDA calculations.

### 3.2.3. 247 GPa

Increasing pressure further, to 247 GPa, LDA+DMFT also reveals a necking transition of the Fermi surface topology at the L point, as seen in figure 6(e). In this transition, holes pockets appear at the L point, as seen in both LDA and LDA+DMFT. Thus, this ETT consists of a necking transition, followed by the appearance of a hole pocket. We do not observe any of the hole pockets along the L–M line disappearing, which was suggested in [4].

In figure 7 we compare the Fermi surface evolution of hcp Os between the pressure of 134 and 247 GPa. We do not see any additional changes of the Fermi surface topology at the $\Gamma$ point, neither with LDA+DMFT (figure 7(a)) nor with LDA (figure 7(b)). Thus, the only ETT that we see in this pressure range corresponds to the

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**Figure 7.** The Fermi surface of hcp-Os at high pressure, where the left column corresponds to LDA+DMFT (c), (e) and the right to LDA (b), (d). In each column, the figures from top to bottom correspond to $P = 134$ GPa and $P = 247$ GPa. Capital letters label relevant high symmetry points. The arrow in (a) shows the hole pocket at the $\Gamma$ point. In all four cases, the hole pocket is present around the $\Gamma$ point.
one at the L-point in the LDA + DMFT calculations. This result is in agreement with the experimental variation of the \( c/a \) lattice parameters ratio with pressure [1].

Concluding the discussion of the Fermi surface calculations for hcp Os, we see that taking into account local quantum fluctuations with LDA + DMFT, we find the ETTs to occur at higher pressure than in the LDA calculations. Indeed, with LDA + DMFT the transition at the L point is found to occur at around 180 GPa, rather than at 125 GPa, as predicted by LDA [1]. The ETT at the \( \Gamma \) point cannot be seen at all with LDA, since it occurs at a negative pressure. On the contrary, with LDA + DMFT it shows up just above 100 GPa. In this range of pressure, anomalous values of the \( c/a \) ratio were observed in [1].

3.3. Electron density distribution

In order to see the pressure-induced features at the \( \Gamma \) and L points more clearly, we have calculated the Fourier transform of the valence electron charge density distribution on a plane in \( k \)-space containing the \( \Gamma, A, L, \) and \( M \) points. In these 2D calculations one may employ a denser \( k \)-mesh to resolve fine changes due to the ETTs. Figure 8 shows the results.
3.3.1. Ambient pressure
In figure 8 we show the k-resolved charge density at ambient pressure. The \( \Gamma \) point is at the right-bottom corner and the L point is at the upper-left corner. With LDA+DMFT, at 0 GPa (figure 8(a)) the L point is at a medium state density and the \( \Gamma \) point is at a highest state density. With LDA (figure 8(b)), we already see the pocket at the \( \Gamma \) point, with a clear depletion in density. The ETT has thus taken place at a negative pressure.

3.3.2. 134 GPa
At 134 GPa, the L point stays at the same density in our LDA+DMFT calculations (figure 8(c)), reflecting that no ETT has occurred at the L point. However, with LDA, we see a clear depletion in charge density at this point (figure 8(d)). At the \( \Gamma \) point, we note a very small drop in the density with our LDA+DMFT calculations. The drop is hardly visible at the scale of figure 8(c), and the region around the \( \Gamma \) point has therefore been replotted with a finer scale in figure 8(g). The small magnitude of this charge depletion is undoubtedly connected to the small size of the pocket seen in figure 7(a). Within LDA (figure 8(d)) the drop is unmistakable, just as the pocket in figure 7(b).

3.3.3. 247 GPa
At 247 GPa, LDA+DMFT calculations (figure 8(e)) show how the density at the L point has dropped, reflecting the ETT seen at the L point. The density at the \( \Gamma \) point shows a pronounced drop. No qualitative changes are seen in the LDA results (figure 8(f)). These conclusions agree well with accurate estimations of the transition pressure given in [1], 101.5 GPa at the \( \Gamma \) point and 183 GPa at L point. Evidently, these changes for LDA+DMFT calculations also agree well with what is seen in the Fermi surface plots.

3.4. Charge gradient
In figure 9, we examine the LDA+DMFT results for the \( \Gamma \) point in yet greater detail, using a color scheme which allows us to see the gradient of the charge density more easily.

As pressure increases from \( P = 0 \) GPa (figure 9(a)), the high density region around the \( \Gamma \) point becomes narrower in the \( k_x \) direction and wider in the \( k_z \) direction (figure 9(b)). At 134 GPa (figure 9(b)), there is a clear loss of electrons, which is connected to the ETT. As pressure increases further to 247 GPa (figure 9(d)), the drop at the \( \Gamma \) point is clear.

The Fourier transform of the charge density distribution gives additional valuable information and has its advantages. It gives information about the charge density at each \( k \)-point, instead of the isoenergetic Fermi surface. Therefore, it is easier to notice subtle changes. For example, from figure 9, one can already see an early sign of an ETT at 86 GPa from the charge depletion as compared with 0 GPa. As pressure increases, we observe the ETT at the \( \Gamma \) point between 86 and 134 GPa.
4. Summary and conclusions

In this work a theoretical investigation of hcp-Os Fermi surface under pressure was performed using the LDA + DMFT technique. Details about the pressure-induced ETTs of its topology are presented.

Although we find from the effective mass of the quasiparticles that Os should be classified as weakly correlated systems, the beyond-LDA treatment of electron correlations provided by the LDA + DMFT method leads to noticeable changes in the predicted pressure evolution of its electronic structure.

The previously suggested ETT at the $\Gamma$ point is not observed with LDA calculations if the experimental lattice constants are used. However, including correlations beyond LDA, by means of the LDA + DMFT method, we clearly see this ETT. Calculations with the LDA + DMFT method also see the other ETT at the L point, which is observed in LDA at a substantially lower pressure. Moreover, these ETTs can also be clearly seen in the Fourier transform of the charge density distribution. We have demonstrated how early signs of an ETT at the $\Gamma$ point can be seen already at 86 GPa. Thus, LDA + DMFT calculations put theoretical predictions in much better agreement with the experimentally detected anomalies connected with ETTs. Our results thus confirm that local dynamical quantum correlation effects may be important even in weakly correlated transition metals.

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