Electronic structure of Mo$_{1-x}$Re$_x$ alloys studied through resonant photoemission spectroscopy

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Abstract
We studied the electronic structure of Mo-rich Mo$_{1-x}$Re$_x$ alloys (0 \( \leq x \leq 0.4 \)) using valence band photoemission spectroscopy in the photon energy range 23–70 eV and density of states calculations. Comparison of the photoemission spectra with the density of states calculations suggests that, with respect to the Fermi level \( E_F \), the \( d \) states lie mostly in the binding energy range 0 to \(-6\) eV, whereas \( s \) states lie in the binding energy range \(-4\) to \(-10\) eV. We observed two resonances in the photoemission spectra of each sample, one at about 35 eV photon energy and the other at about 45 eV photon energy. Our analysis suggests that the resonance at 35 eV photon energy is related to the Mo 4p–5s transition and the resonance at 45 eV photon energy is related to the contribution from both the Mo 4p–4d transition (threshold: 42 eV) and the Re 5p–5d transition (threshold: 46 eV). In the constant initial state plot, the resonance at 35 eV incident photon energy for binding energy features in the range \( E_F (BE = 0) \) to \(-5\) eV becomes progressively less prominent with increasing Re concentration \( x \) and vanishes for \( x > 0.2 \). The difference plots obtained by subtracting the valence band photoemission spectrum of Mo from that of Mo$_{1-x}$Re$_x$ alloys, measured at 47 eV photon energy, reveal that the Re \( d \)-like states appear near \( E_F \) when Re is alloyed with Mo. These results indicate that interband \( s–d \) interaction, which is weak in Mo, increases with increasing \( x \) and influences the nature of the superconductivity in alloys with higher \( x \).

Keywords: transition metal binary alloy superconductors, photoemission spectra, electronic structure

(Some figures may appear in colour only in the online journal)

1. Introduction

Discovered in the 1960s, binary Mo–Re alloys are interesting superconductors whose transition temperature \( (T_c) \) is about an order of magnitude higher than that of their constituent elements [1–3]. Experimental studies performed in the mid-1980s and early 1990s suggested the possibility of Re-influenced softening of the phonon spectrum [4] and a change in the electron density of states (DOS) [5] in Mo$_{1-x}$Re$_x$ alloys. But these phenomena could not completely
explain the large non-monotonic enhancement of the \( T_c \) in Mo\(_{1-x}\)Re\(_x\) alloys. The \( T_c \) in Mo\(_{1-x}\)Re\(_x\) alloys increases slowly from 0.90 K for Mo to about 3 K for \( x = 0.10 \) and then rises sharply to about 7 K for \( x = 0.15 \) [6, 7]. With further increases in \( x \), the \( T_c \) increases linearly to about 12.6 K for \( x = 0.40 \) [6, 7]. The composition range in which the \( T_c \) increases sharply in Mo\(_{1-x}\)Re\(_x\) alloys corresponds to the composition range in which the existence of two electronic topological transitions (ETT) have been reported for the critical concentrations \( x_1 = 0.05 \) and \( x_2 = 0.11 \) [8–14]. ETT are associated with the appearance or disappearance of pockets of Fermi surface when an external parameter such as composition, pressure, and/or magnetic field is varied [15]. The coefficient of the thermoelectric power \( \alpha/T \) in the zero temperature limit shows a huge enhancement around \( x_{c2} = 0.11 \) [8, 11, 12]. The \( T_c \) of Mo\(_{1-x}\)Re\(_x\) alloys with \( x > x_{c2} \) is reported to oscillate with pressure [6, 12]. The oscillations in the temperature derivative of \( \alpha/T \) and resistivity were also observed to be maximal at \( x_1 = 0.05 \) and \( x_2 = 0.11 \) [12]. These oscillations were predicted to be due to the localization of electrons at the newly appeared Fermi pockets [12]. Our recent band structure calculation showed that there are substantial changes in the DOS at the Fermi level \( E_F \) for \( x > x_{c2} \) [7]. The x-ray photoelectron spectroscopy revealed that the rigid band model is not applicable in the case of Mo\(_{1-x}\)Re\(_x\) alloys, and the changes in the spectra as a function of \( x \) were assigned to the ETT [16]. Direct evidence of this ETT was provided recently by Okada et al with the help of angle resolved photoemission spectroscopy along the H–N direction of the Brillouin zone [14]. However, their studies could not establish any relation between the ETT and the superconductivity in Mo\(_{1-x}\)Re\(_x\) alloys.

In our recent study, we found evidence of multiband effects in the temperature dependence of the heat capacity and superfluid density (estimated from the temperature dependence of the lower critical field \( H_{c1} \)) in Mo\(_{1-x}\)Re\(_x\) alloys with \( x = 0.25 \) and 0.40 [17]. Our detailed study also revealed that multiband superconductivity appears above \( x > 0.11 \), which is the critical composition corresponding to the ETT [18]. From helium channeling experiments [19] on Mo\(_{1-x}\)Re\(_x\) alloys, Dikiy et al concluded that the new electron sheet that is formed above \( x > x_{c2} \) differs from the main sheets in terms of lower velocity and higher effective mass [20]. Resonant photoemission spectroscopy (RPES) has been shown to be a powerful tool for the determination of the partial density of states (PDOS) in various intermetallic alloys [21–23]. RPES has been used effectively to obtain the details of the electronic structure near \( E_F \) and its role in the superconducting properties in different classes of superconductors, namely, iron pnictides [24–27], YBa\(_2\)Cu\(_{3-x}\)O\(_7\)–\(x\) [28], ZrB\(_2\) [29], PrPt\(_4\)Ge\(_{12}\) [30], and heavy fermion superconductors [31]. Therefore, we expect that RPES studies on Mo\(_{1-x}\)Re\(_x\) alloys may provide useful information regarding the valence band (VB), which in turn will be helpful in understanding the correlation between the ETT and the superconducting properties. In this study, we have therefore performed RPES experiments on \( \beta \)-phase Mo\(_{1-x}\)Re\(_x\) alloys with \( x > 0.1 \) and have compared these results with the results for elemental Mo. Our analysis revealed that substitution of the Re in Mo increases the DOS at \( E_F \), which then develops a Re 5d-like character. These enhanced DOS at \( E_F \) enhance the interband s–d interaction in these alloys with increasing \( x \), which in turn influences the nature of the superconductivity.

2. Experimental and details of the band structural calculations

Polycrystalline samples of Mo\(_{1-x}\)Re\(_x\), where \( x = 0, 0.15, 0.20, 0.25, \) and 0.40, were prepared by melting 99.95% + purity constituent elements in an arc furnace under a 99.999% Ar atmosphere. The samples were flipped and re-melted six times to improve the homogeneity. The x-ray diffraction study of these alloys showed that the samples formed in the body centered cubic (bcc) phase (space group: Im\( \bar{3} \)m) [7, 17, 18].

The RPES measurements on the above samples were performed using the angle-integrated photoemission beamline of the Indus-1 synchrotron radiation source [32]. The VB photoemission spectra were recorded in the 23–70 eV photon energy range. The details of the configuration of the present system and the experimental conditions are available elsewhere [33]. The spectra were normalized by the photon flux estimated from the photocurrent obtained from the post mirror of the beam line. A clean sample surface was obtained by sputtering the sample in situ. Surface cleanliness was confirmed by the absence of the oxygen and carbon contributions in the core level peaks of Mo and Re. The experimental resolution was estimated to be from 0.3–0.4 eV in the present photon energy range. The x-ray photoelectron spectra (XPS) were measured using a Mg K\( _\alpha \), x-ray source (DAR400, Omicron).

The ab initio electronic structure calculations were performed using the spin polarized Korringa–Kohn–Rostoker (KKR) method [34]. The effect of doping was considered under the coherent potential approximation. The exchange correlation functional developed by Vosko Wilk and Nusair was used for the calculation [35]. The number of \( k \)-points used in the irreducible part of the Brillouin zone was 72. The muffin-tin radii for Mo and Re atoms used in the calculations were the same and equal to 2.576 bohr. For the angular momentum expansion, we considered \( l_{\text{max}} = 2 \) for each atom. The potential convergence criterion was set to \( 10^{-6} \).

3. Results and discussion

Figures 1(a) and (b) show the XPS data corresponding to the Mo 4p, Re 4f, and Mo 3d core levels in Mo\(_{1-x}\)Re\(_x\) alloys. These core level spectra are also compared with those of elemental Mo and Re. The inelastic background was subtracted using the standard Tougaard method [36]. In figure 1(a), the 4p\(_{3/2}\) and 4p\(_{1/2}\) peaks for elemental Mo appear at 37 eV and 35 eV BE, respectively, showing a spin orbit splitting of 2 eV. On the other hand, the Re 4f\(_{7/2}\) and 4f\(_{5/2}\) peaks appear at 42.2 eV and 39.8 eV, respectively, showing a spin orbit splitting of 2.4 eV. The interesting observation here is that the Mo 4p\(_{3/2}\) and 4p\(_{1/2}\) core levels in Mo\(_{1-x}\)Re\(_x\) alloys have the same binding energy (BE) positions as the core level of elemental Mo (figure 1(a)). However, the Re 4f\(_{7/2}\) and 4f\(_{5/2}\) show a shift towards higher BE with decreasing \( x \) as compared to elemental Re. Within
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the instrumental resolution, the shift observed for \( x = 0.4 \) is 0.25 eV. For \( x = 0.15, 0.2, \) and 0.25, the shift is about 0.4 eV towards higher BE. In a binary disordered metallic alloy, such a shift appears to be due to the difference in the local chemical environment and/or the charge redistribution, which is related to the hybridization between the valence electron states of the system [37]. In figure 1(b), the BE peak positions for the Mo 3d core levels (Mo 3d\(_{5/2}\) = 227.8 eV and Mo 3d\(_{3/2}\) = 231.0 eV) in Mo\(_1-x\)Re\(_x\) alloys are found to be the same (within the experimental resolution) as those reported for elemental Mo [38]. Similar to the case of the Mo 3d core levels (figure 1(b)), the peak positions for Re 4d core levels in Mo\(_1-x\)Re\(_x\) alloys (not shown here) are also found to be same as those of elemental Re.

The VB spectra for pure Mo in the energy range 23–60 eV are shown in figure 2(a). The background obtained via the Tougaard procedure [36] was subtracted from the raw data. In figure 2(b), we compare the present VB-XPS of elemental Mo measured using Mg K\( \alpha \) radiation with the XPS results reported in the literature for Mo oxides and elemental Mo, where the measurements used Al K\( \alpha \) radiation [38]. From figure 2(b), it is clear that the VB-XPS of elemental Mo is in fairly good agreement with that of the literature and is quite different from that of the oxides of Mo. Therefore, we believe that there is no oxygen in the bulk of the samples. Since the photons with energies such as 20–30 eV are more surface sensitive, in figure 2(c) we compare the photoelectron spectrum (PES) of the VB of Mo obtained using photons of 41 eV energy with the reported PES of the VB of elemental Mo and Mo oxides obtained using a He-II source [39, 40]. The features that correspond to the VB of elemental Mo are distinctly different from those of Mo oxides wherein broad hump-like features are observed centered around \(-5\) eV below \( E_F \). Therefore, we believe that the surfaces of the samples under study here are not contaminated by oxygen. The PES spectra of Mo were taken up to \( BE = -14 \) eV below \( E_F \), and consist of five features: one feature very close to \( E_F \), two features closely spaced around \(-4\) eV below \( E_F \), and then a broad hump ranging from \(-4\) eV to \(-8\) eV, followed by another hump-like feature centered around \(-10\) eV below \( E_F \), in agreement with the measurements [40] at 40.8 eV photon energy (He-II source) and other measurements reported in the literature [41].

The PES spectra of Mo were taken up to \( BE = -14\) eV below \( E_F \), and consist of five features: one feature very close to \( E_F \), two features closely spaced around \(-2\) eV to \(-3\) eV, a broad peak at \(-6\) eV, and a broad hump centered around \(-10\) eV below \( E_F \). All the peaks are quite broad due to the large dispersion of the bands [14]. A systematic shift of
the positions of these peaks is also observed when the incident photon energy is varied. This may be related to the dispersion of the bands along the $k_z$ direction of the Brillouin zone. These results are consistent with many theoretical and experimental studies performed on Mo (1 1 0), (0 1 1), and (1 1 2) face single crystals [42–48]. Since the low-energy photons are surface sensitive, the surface DOS also influence the PES. Weng et al showed that there are two peaks centered around $-0.7$ eV and $-3$ eV below $E_F$ in the DOS corresponding to the Mo surface [42]. We also observed the corresponding features in the PES, which are probably from the admixture of the bulk and surface states. However, we also observed other features at $-2$ eV, $-6$ eV, and $-10$ eV, which are mainly from the bulk of the sample [42]. The resonant enhancement of the PES of the VB is observed as a function of photon energy, which will be discussed later in detail.

A systematic evolution of the VB photoemission spectra of Mo$_{1-x}$Re$_x$ alloys with $x = 0.15, 0.2, 0.25,$ and 0.4 measured at the selected photon energies ranging from 25 eV to 60 eV is shown in figure 3. In comparison with Mo, the intensity of the BE feature in Mo$_{1-x}$Re$_x$ alloys at $-6$ eV decreases monotonically as a function of photon energy and this reduction of intensity is quite significant for the alloys with higher Re content. The features around $BE = -2$ eV become sharp when Re is alloyed with Mo, although the peak positions of these features do not seem to depend on the photon energy. However, when Re is alloyed with Mo, the features in the PES depend on the photon energy quite significantly and the average shift in the peak positions as a function of photon energy increases with increasing Re content. This is due to the enhancement of the dispersion of the bands along the $k_z$ direction of the Brillouin zone when Re is alloyed with Mo [14].

In order to determine the contributions of different orbitals to the PES, in figure 4 we plot the PDOS of Re and Mo in Mo$_{1-x}$Re$_x$ alloys. The $d$ and $p$ states of both Mo and Re lie in the BE range $E_F$ to $-6$ eV, and the $s$ states of both Mo and Re lie below $-4$ eV in the higher BE side. The 4$d$ states of Mo show three peaks around $BE = -2, -3,$ and $-4$ eV below $E_F$, whereas the 5$d$ states of Re show three peaks around $BE = -2.5, -3.5,$ and $-5$ eV below $E_F$. At the Fermi level, a dip is observed in the Mo 4$d$ PDOS. When Re is alloyed with Mo, the contributions of both the Mo and Re $d$ states increase with the increase in $x$ up to $x = 0.25$. In the case of $x = 0.40$, however, the $d$ DOS is reduced once again. The Mo 5$s$ states lie around $-5$ eV below $E_F$, whereas the Re 6$s$ states lie around $-6$ eV below $E_F$. However, the contribution of the $s$ states of both Mo and Re in the energy range $E_F$ to $-4$ eV below $E_F$ is quite small but finite. The Mo 5$p$ and Re 6$p$ states are evenly distributed from $E_F$ to $-4$ eV below $E_F$, but are somewhat smaller in number than the $d$ states. Since Re (5$d^56$s$^2$) has one more valence electron per atom than Mo (4$d^{5}5$s$^1$), the PDOS of both Mo and Re shift towards higher BE with the increase in Re concentration. Therefore, up to about $-4$ eV below $E_F$, the features in the PES are dominated by $d$-like states, while below $-4$ eV towards the higher BE the features represent the $s$-like states.
Figures 2 and 3 show the resonance enhancement of the features in the PES measured using photons with different energies. In all the samples, the feature around \( \text{BE} = -6 \text{ eV} \) below \( E_F \) resonates around 35 eV photon energy, whereas the feature around \( \text{BE} = -2 \text{ eV} \) below \( E_F \) resonates around 45 eV photon energy. A clear picture can be obtained by plotting the constant initial state (CIS) intensities of the VB features as a function of photon energies, as shown in figure 5. The CIS plots of all the samples show two resonances with the peak positions at around 35 eV and 45 eV incident photon energy. In the case of Mo, the resonance corresponding to the incident photon energy of around 35 eV is observed over the entire VB, whereas the resonance corresponding to the incident photon energy of around 45 eV is observed only below the 5 eV BE of the VB. From figure 1, it is clear that the resonance of the VB occurs across the Mo 4p threshold. The band structure calculation (figure 4) suggests that the features of the PES in the BE range from \( E_F \) to \(-5 \text{ eV} \) below \( E_F \) are mainly derived from \( d \)-like states, whereas the features of the PES in the BE range from \(-5 \text{ eV} \) below \( E_F \) to \(-8 \text{ eV} \) below \( E_F \) are mainly derived from \( s \)-like states. Therefore, the resonance around 35 eV photon energy is from the Mo 4p–5s transition via:

1. direct photoemission, 
   \[ 4p^64d^55s^1 + \hbar\nu \rightarrow 4p^64d^55s^0 + e^- , \]
   and

2. Auger emission, 
   \[ 4p^64d^55s^1 + \hbar\nu \rightarrow 4p^54d^55s^2 \rightarrow 4p^64d^55s^0 + e^- . \]

Whereas the resonance around 45 eV photon energy is from the Mo 4p–4d transition via:

1. direct photoemission, 
   \[ 4p^64d^45s^1 + \hbar\nu \rightarrow 4p^64d^45s^0 + e^- , \]
   and

2. Auger emission, 
   \[ 4p^64d^45s^1 + \hbar\nu \rightarrow 4p^54d^55s^1 \rightarrow 4p^64d^45s^1 + e^- . \]

The angle resolved photoemission spectroscopy (ARPES) study on the Mo(1 0 0) surface at various photon energies by Weng et al revealed four resonances at about 15 eV, 30 eV, 38 eV, and 45 eV [42, 43]. They argued that the resonances of the features observed at \( \text{BE} = -0.3 \text{ eV} \) and \(-3.3 \text{ eV} \) below \( E_F \) for photon energies of about 15 eV, 30 eV, and 38 eV are related to surface states. In the present case, both the resonances are observed in the entire VB, indicating that these resonances are related to bulk states. However, the resonances around \( \text{BE} = -0.3 \text{ eV} \) and \(-3.3 \text{ eV} \) below \( E_F \) should be used with care as they might also be influenced by the surface states. It is worth mentioning that the surface resonance feature is extremely sensitive to surface contamination [42, 43]. Both the polycrystalline nature of the samples and the
appearance of these resonances in the alloys suggest that these resonances are mainly related to the bulk states. Similar to Mo, we observe two resonances in Mo$_{1-x}$Re$_x$ alloys. As the Re content is increased (from $x = 0$), the resonance corresponding to the incident photon energy of around 35 eV diminishes below 5 eV and becomes non-existent for $x > 0.25$. The resonance corresponding to the incident photon energy of around 45 eV shifts to higher incident photon energy when Re is alloyed with Mo. This is due to the fact that in these alloys an additional contribution from the Re 5p–5d transition (46 eV) is expected for the resonance at around 45 eV photon energy. This additional contribution originates from the Re 5p–5d transition (46 eV) via:

1. direct photoemission, $5p^65d^66s^2 + h\nu \rightarrow 5p^65d^46s^2 + e^-$, and
2. Auger emission, $5p^65d^56s^2 + h\nu \rightarrow 5p^55d^66s^2 \rightarrow 5p^65d^46s^2 + e^-.$

In order to determine the effect of alloying Re with Mo on the PES, in figure 6 we plot the difference between the spectra for Mo$_{1-x}$Re$_x$ alloys and pure Mo at 47 eV photon energy. The positive contribution implies the enhancement of the intensity of the PES features with respect to that of Mo introduced by the Re states. On the other hand, the negative contribution corresponds to the loss of Mo states due to alloying and/or the absence of Re states at the corresponding BE. The expanded portion of the difference spectra up to $-5$ eV below $E_F$ is shown in figure 6(b). This figure suggests that the contribution of DOS from the Re d states increases near $E_F$ with the increase in $x$ up to 0.25. The width of the Re d states near $E_F$ also increases with the increase in $x$ up to 0.25. For $x = 0.15$ and 0.20, the Re d states are observed up to about $-0.5$ eV below $E_F$, whereas for $x = 0.25$, the Re d states are observed up to about $-1$ eV below $E_F$. On the other hand, the difference spectra for $x = 0.40$ are quite different from those for the rest of the alloys. In this case, the contribution to the difference spectra around $E_F$ is negative, which indicates the loss of DOS in spite of the higher Re content. These results are in agreement with the DOS calculation for $x = 0.4$ (figure 4), which also indicates a decrease in the d PDOS of Mo and Re as compared to the Mo$_{1-x}$Re$_x$ alloys. Additionally, in the higher BE side from $-2$ to $-5$ eV there is a significant contribution from the Re d states.

The ARPES study performed by Okada et al [14] showed that an extra band appears at the Fermi surface of Mo$_{1-x}$Re$_x$ alloys above 10 at.% of Re as a result of ETT in these alloys. When these results are compared with the difference spectra shown in figure 6, it is clear that the extra band that appeared at the Fermi surface above 10 at.% of Re has a Re d-like character. We recently showed that this extra band contributes distinctly to the superconductivity [18]. The temperature dependence of the normal state resistivity of these alloys indicates that the phonon-assisted s-d scattering in Mo is weak compared to the intra-band s-s scattering, and that the s-d

\[ \text{Figure 7. Comparison of the area normalized intensities as a function of incident photon energy at different binding energies of the VB (indicated in the figure) for Mo$_{1-x}$Re$_x$ alloys with } x = 0, 0.15, 0.2, 0.25, \text{ and } 0.4. \]
scattering is enhanced with the increase in $x$ above 10 at.% of Re [7]. In the case of $s$–$d$ scattering, the resistivity is proportional to $N_d(E_F)/N_s(E_F)$ [49], where $N_d(E_F)$ and $N_s(E_F)$ are the partial DOS of the $d$ and $s$ states at the Fermi level. In order to obtain further insight into this, in figure 7 we compared the area normalized intensities as a function of incident photon energy at different binding energies of the VB for the present Mo$_{1−x}$Re$_x$ alloys. The figure reveals that the resonance corresponding to the incident photon energy of around 35 eV is present in Mo over the entire VB. However, when Re is alloyed with Mo, the resonance corresponding to the incident photon energy of around 35 eV diminishes below $BE = −5$ eV and vanishes for $x \geq 0.25$, whereas for $BE > −5$ eV this resonance is present in all the alloy compositions. Note that the $d$ states are present in the range $E_F$ to $−5$ eV below $E_F$ along with a small contribution from the $s$ states. This indicates that in Mo, the photon energy corresponding to the resonance of the PES involving the $s$ states of the VB is distinctly different from that involving the $d$ states, implying negligible $s$–$d$ interaction. This study reveals that there is an enhancement of the $d$ DOS in the vicinity of the Fermi surface when Re is alloyed with Mo, which results in the enhancement of $s$–$d$ scattering in the alloy compositions. Then, the final state $4p^44d^5s^2$formed due to the Auger process at roughly the incident photon energy of 35 eV can return to the original state via $s$–$d$ scattering. This indicates that in Mo, $s$–$d$ scattering is enhanced in Mo$_{0.60}$Re$_{0.40}$ alloy. The present photoemission and band structure calculations showed a decrease in the DOS at the $E_F$ as compared to $x = 0.25$, with the $T_c$ enhanced to 12.6 K compared to 9.6 K for $x = 0.25$. This can be understood in terms of the dispersion of bands along the H–N direction of the Brillouin zone. The momentum $k$ separation between the band that appeared in the H–N direction after alloying and the other band with a Mo-like character reduces with the increase in $x$. Therefore, for alloys with higher concentrations of Re, the low-energy phonons (small $k$) can help in $s$–$d$ scattering. Thus, the multi-band effect is smeared out and the $T_c$ is enhanced in Mo$_{0.60}$Re$_{0.40}$ alloy.

4. Conclusion

We performed resonant photoemission spectroscopy experiments on Mo$_1$,Re$_x$ alloys with $x = 0, 0.15, 0.2, 0.25,$ and 0.4 in the photon energy range 23–70 eV. A resonance enhancement of intensity of the photo-electron spectra corresponding to Mo 4$p$–4$d$ and/or Re 5$p$–5$d$ transitions at about 45 eV incident photon energy was observed in all the alloys. We have observed another resonance in Mo and low-x alloys at about 35 eV incident photon energy. Our analysis reveals that the resonance at 35 eV is related to the Mo 4$p$–5$s$ transition. The two separate resonances at $E_F$ for pure Mo and lower Re content alloys indicate the lack of $s$–$d$ interaction in these alloys. The PES of all the alloys are in agreement with the theoretical DOS estimated from band structure calculations. The analysis suggests that experimentally observed enhancement of $d$-like states at the Fermi level and dispersion upon alloying Re with Mo governs the physical properties of the both normal and superconducting states.

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