Comment on “Electronic structure of Mo(1−x)Rex alloys studied through resonant photoemission spectroscopy”

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Comment on “Electronic structure of Mo\(_{1-x}\)Re\(_x\) alloys studied through resonant photoemission spectroscopy”

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Abstract

Further analysis of the resonant photoemission data, found within Sundar et al (2016 J. Phys.: Condens. Matter 28 315502), show the intensities do not follow the elemental composition in the Mo\(_{1-x}\)Re\(_x\) alloy. Similar trends are observed in the published data for Gd\(_{1-x}\)Ni\(_x\) alloy films. The analysis of the resonant photoemission intensities suggests that Mo in the Mo\(_{1-x}\)Re\(_x\) alloy and Gd in the Gd\(_{1-x}\)Ni\(_x\) alloy have nearest neighbor bonds to Re and Ni respectively. This means the A–B bond is favored over the average of the A–A bond and the B–B bond in these binary alloys, so that the short range order favors strong local ordering rather than clustering alloys.

Keywords: resonant photoemission, screening, short range order, alloys

The resonant photoemission intensities, found within ‘Electronic structure of Mo\(_{1-x}\)Re\(_x\) alloys studied through resonant photoemission spectroscopy’, have implications beyond those discussed, by Sundar et al [1]. The suppression of the resonant photoemission intensities, as a function of Mo\(_{1-x}\)Re\(_x\) alloy composition [1], parallel similar trends to those found for Gd\(_{1-x}\)Ni\(_x\) alloy films [2], and imply strong hybridization, considerable short-range in the Mo\(_{1-x}\)Re\(_x\) alloy system.

The similarities in the resonant photoemission data collected for both Gd\(_{1-x}\)Ni\(_x\) and Mo\(_{1-x}\)Re\(_x\) alloy is evident by plotting the Gd 5\(p^4f^75d^16s^2\) → 5\(p^5f^75d^26s^2\) → 5\(p^6f^75d^06s^2\) + e\(^-\) (figure 3 of [2]) and Mo 4\(p^6d^55s^1\) → 4\(p^5d^55s^1\) → 4\(p^64d^45s^1\) + e\(^-\) (figure 7(a) of [1]) super Coster Kronig resonance intensities, obtained near the Fermi level, as has been done in the figure. There is a significant decrease in the photoemission resonance intensities for alloys occurs far faster than the decrease in Mo or Gd concentrations in the Mo\(_{1-x}\)Re\(_x\) and Gd\(_{1-x}\)Ni\(_x\) alloys respectively, as seen in figure 1 created from data abstracted from [1] and [2]. Similar data is seen from the resonant photoemission intensities from the mid of the valence band for the Mo\(_{1-x}\)Re\(_x\) alloy as well [1] and plotted here also as a raw normalized intensity versus alloy composition.

Resonant photoemission intensities are greatest in insulators, as the screening of the photohole is suppressed [3, 4], but strong hybridization between nearest neighbors, within an alloy, can also influence the resonant photoemission intensities even in metals [2]. The simple fact that the resonant intensities fall faster than the elemental composition suggests that both Mo in the Mo\(_{1-x}\)Re\(_x\) alloy [1] and Gd the Gd\(_{1-x}\)Ni\(_x\) alloy [2] are increasingly bonded to Re and Ni respectively. This is consistent with strong local ordering, rather than strongly clustering alloys, i.e. the A–B bond is favored energetically over the average of the
A–A bond and the B–B bond in these binary alloys. Such local short range ordering is expected from the Mo$_{1-x}$Re$_x$ alloy [5–7] and Gd$_{1-x}$Ni$_x$ alloy [8, 9] phase diagrams. In summary, the data of [1] implies considerable short range ordering in the Mo$_{1-x}$Re$_x$ alloy samples studied and strong Mo-Re orbital hybridization.

References


Figure 1. The normalized peak resonant photoemission intensities, as a function of alloy composition, for the Mo$_{1-x}$Re$_x$ alloy [1] and the Gd$_{1-x}$Ni$_x$ alloy [2]. From [1], the resonant photoemission intensities, at the Fermi level, for the Mo$_{1-x}$Re$_x$ alloy (squares) and Gd$_{1-x}$Ni$_x$ alloy (circles) are compared with the resonant photoemission intensities in the mid valence band region for the for the Mo$_{1-x}$Re$_x$ alloy (triangles). Linear trend lines for each are shown and are meant to guide the eye.