

1-2017

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

Prescott Evans

University of Nebraska-Lincoln, prescott.evans@huskers.unl.edu

Peter A. Dowben

University of Nebraska-Lincoln, pdowben@unl.edu

Follow this and additional works at: <http://digitalcommons.unl.edu/physicsdowben>

 Part of the [Atomic, Molecular and Optical Physics Commons](#), [Condensed Matter Physics Commons](#), [Engineering Physics Commons](#), and the [Other Physics Commons](#)

Evans, Prescott and Dowben, Peter A., "Comment on “Electronic structure of Mo(1-x)Rex alloys studied through resonant photoemission spectroscopy”" (2017). *Peter Dowben Publications*. 272.
<http://digitalcommons.unl.edu/physicsdowben/272>

This Article is brought to you for free and open access by the Research Papers in Physics and Astronomy at DigitalCommons@University of Nebraska - Lincoln. It has been accepted for inclusion in Peter Dowben Publications by an authorized administrator of DigitalCommons@University of Nebraska - Lincoln.

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

Prescott Evans and P. A. Dowben

Department of Physics and Astronomy, Jorgensen Hall, University of Nebraska–Lincoln, Lincoln, NE 68588, USA

Email: prescott.evans@huskers.unl.edu and pdowben1@unl.edu

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 $\text{Mo}_{1-x}\text{Re}_x$ alloy. Similar trends are observed in the published data for $\text{Gd}_{1-x}\text{Ni}_x$ alloy films. The analysis of the resonant photoemission intensities suggests that Mo in the $\text{Mo}_{1-x}\text{Re}_x$ alloy and Gd in the $\text{Gd}_{1-x}\text{Ni}_x$ 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 $\text{Mo}_{1-x}\text{Re}_x$ 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 functional of $\text{Mo}_{1-x}\text{Re}_x$ alloy composition [1], parallel similar trends to those found for $\text{Gd}_{1-x}\text{Ni}_x$ alloy films [2], and imply strong hybridization, considerable short-range in the $\text{Mo}_{1-x}\text{Re}_x$ alloy system.

The similarities in the resonant photoemission data collected for both $\text{Gd}_{1-x}\text{Ni}_x$ and $\text{Mo}_{1-x}\text{Re}_x$ alloy is evident by plotting the Gd $5p^6 4f^7 5d^1 6s^2 \rightarrow 5p^5 4f^7 5d^2 6s^2 \rightarrow 5p^6 4f^7 5d^0 6s^2 + e^-$ (figure 3 of [2]) and Mo $4p^6 4d^5 5s^1 \rightarrow 4p^5 4d^5 5s^1 \rightarrow 4p^6 4d^4 5s^1 + e^-$ (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 as alloy Re [1] or Ni [2] composition increases. What is important here is that the fall in photoemission resonant

intensities for alloys occurs far faster than the decrease in Mo or Gd concentrations in the $\text{Mo}_{1-x}\text{Re}_x$ and $\text{Gd}_{1-x}\text{Ni}_x$ 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 $\text{Mo}_{1-x}\text{Re}_x$ 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 $\text{Mo}_{1-x}\text{Re}_x$ alloy [1] and Gd the $\text{Gd}_{1-x}\text{Ni}_x$ 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

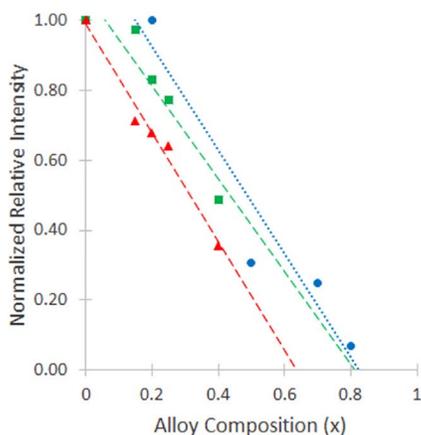


Figure 1. The normalized peak resonant photoemission intensities, as a function of alloy composition, for the $\text{Mo}_{1-x}\text{Re}_x$ alloy [1] and the $\text{Gd}_{1-x}\text{Ni}_x$ alloy [2]. From [1], the resonant photoemission intensities, at the Fermi level, for the $\text{Mo}_{1-x}\text{Re}_x$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

A–A bond and the B–B bond in these binary alloys. Such local short range ordering is expected from the $\text{Mo}_{1-x}\text{Re}_x$ alloy [5–7] and $\text{Gd}_{1-x}\text{Ni}_x$ alloy [8, 9] phase diagrams. In summary, the data of [1] implies considerable short range ordering in the $\text{Mo}_{1-x}\text{Re}_x$ alloy samples studied and strong Mo–Re orbital hybridization.

References

- [1] Sundar S, Banik S, Chandra L S S, Chattopadhyay M K, Ganguli T, Lodha G S, Pandey S K, Phase D M and Roy S B 2016 *J. Phys.: Condens. Matter* **28** 315502
- [2] Wu N, LaGraffe D, Yakovkin I N and Dowber P A 2001 *Phys. Status Solidi b* **248** 1253
- [3] Li D, Zhang J, Lee S and Dowben P A 1992 *Phys. Rev. B* **45** 11876
- [4] Dowben P A 2000 *Surf. Sci. Rep.* **40** 151–247
- [5] Knapton A G 1958–1959 *J. Inst. Met.* **87** 62
- [6] Savitskii E M, Tylkina M A and Povarova K B 1959 *Russ. J. Inorg. Chem.* **4** 190
- [7] Arzadfar S A, Levesque M, Phejar M and Joubert J-M 2009 *CALPHAD, Comput. Coupling Phase Diagr. Thermochem.* **33** 502
- [8] Opeland M I, Krug M and Armantrout C E 1964 Nickel—gadolinium phase diagram *Report of Investigations* 6566 U.S. Department of the Interior, Bureau of Mines
- [9] Pan Y Y, Zheng J X, Li M and Yang H 1986 *Acta Phys. Sin.* **35** 677