

# Contribution to the electronic density of states in the valence band of AlPdMn

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In spite of more than a decade of intense research, the intriguing physical properties of quasicrystalline alloys still await explanation in terms of the characteristics of the states involved in the valence level electronic structure. Conventional notions of electronic structure in translationally periodic solids have to be adapted to the unique order and symmetry of quasicrystalline solids to understand properties such as the extremely low electrical conductivity, an unusual optical conductivity  $\sigma(\omega)$ , and the low electronic contribution to the specific heat, among others<sup>1</sup>. Photoelectron spectroscopy has developed into an extremely useful tool for the detailed study of the electronic structure of solids, and thus has also been applied to quasicrystalline materials; an overview of photoemission work performed until 1998 is given by Stadnik<sup>2</sup>.

Here we report on a core and valence level photoemission study of the AlPdMn quasicrystalline alloy in order to distinguish contributions from each atomic species to the valence level region of the spectrum, and to the density of states at  $E_F$  in particular. We use photoemission from specific regions in the valence band, resonantly enhanced upon crossing an excitation threshold for a deep core level, in order to establish the contribution of the Mn-derived states. Consider the data in Figure 1, which show a set of valence level spectra from i-AlPdMn recorded in the region of photon energies near the

Mn  $2p$  core excitation; a Mn L-edge absorption spectrum is plotted against the vertical axis on the right, recorded in the same experiment by means of total yield (solid line) and “partial yield” (dots, explained below) spectroscopy. The spectra (solid lines) consist of a dominant Pd  $4d$ -derived peak at about 4 eV, and a region extending towards the Fermi level  $E_F$ ; arrows indicate the photon energy used for excitation. The dotted spectra on the left indicate the difference between an off-resonance and on-resonance spectrum. An enhancement of the region between 3 eV binding energy and  $E_F$  is observed already in the raw data. The difference spectra clearly show the shape of the resonantly enhanced Mn valence states; their origin is additionally clarified by the fact that the final spectrum (669 eV) again has no enhancement near  $E_F$ , as has the first (bottom) spectrum. Furthermore, a partial-yield NEXAFS

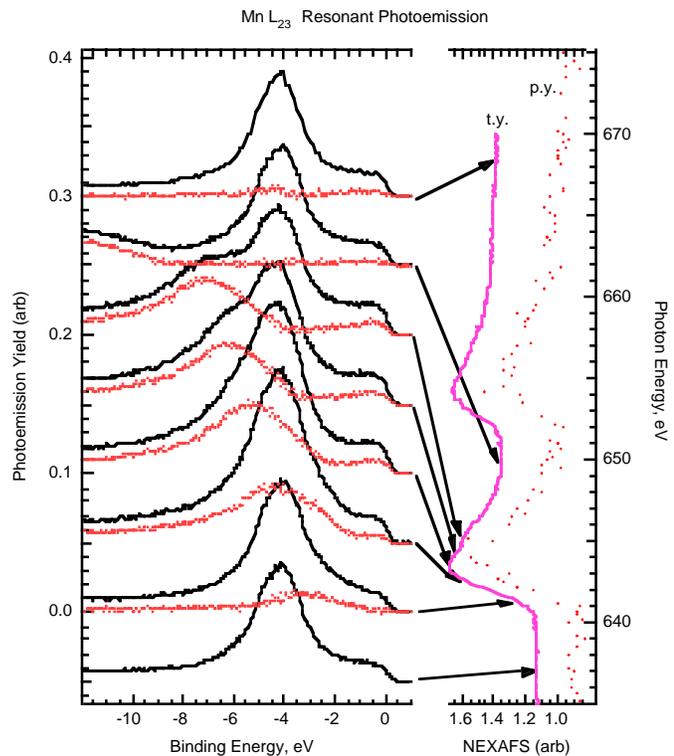
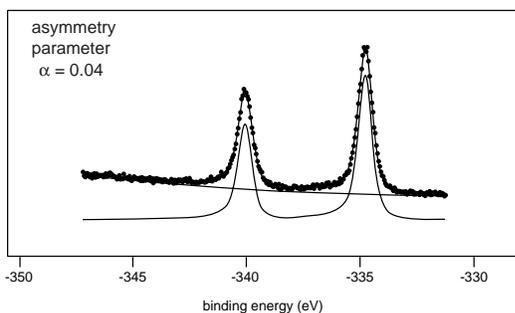


Figure 1: Resonant photoemission from the valence band of i-AlPdMn in the region of the Mn  $2p$  core excitation.

spectrum (shown as dots on the right hand part of the figure), acquired by windowing the detector about 1 eV below  $E_F$  closely follows the total yield spectrum, further supporting that these states are Mn-like. The enhancement extends from  $E_F$  down to about 2.5 eV binding energy. The large peak which develops at about 3 eV binding energy in the first on-resonance spectrum and moves further down with photon energy stems from the Mn LMM Auger deexcitation of the Mn  $2p$  hole. This set of data shows the strong contribution of the Mn  $d$  states near  $E_F$ , since the resonant enhancement concentrates on these.

The contributions of the other constituents to the states near  $E_F$  can be inferred in a more indirect way, from the shape of the respective core level photoemission lines. Upon photoionization, the positively charged ion is screened by the surrounding electrons from filled conduction band states, producing electron-hole pairs. This leads to the well-known asymmetry of core level lines from metallic systems, where the strength of the asymmetry parameter  $\alpha$  is related to the density of states at  $E_F$ .<sup>3</sup> Pd serves as an interesting case in point, since its 3d

Pd 3d core level photoemission from i-AIPdMn



Pd 3d core level photoemission from Pd metal

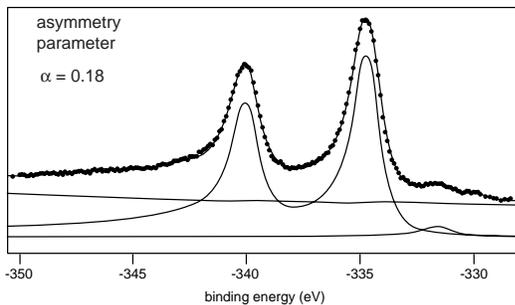


Figure 2: Comparison of the core level line shape of Pd 3d from Pd metal (bottom) and i-AIPdMn (top).

spectrum exhibits a large asymmetry. Consider the bottom spectrum in Figure 2, which shows a Pd 3d spectrum from Pd metal, recorded with Mg  $K\alpha$  radiation (1253.6 eV). This doublet was fitted with a convolution of a Gaussian and the Doniach-Sunjc line shape which describes the effect of core hole screening from a constant density of states near  $E_F$ . The asymmetry parameter derived from this fit is  $\alpha = 0.18$ . The upper part shows a similar fit for a Pd 3d spectrum from i-AIPdMn, recorded with synchrotron radiation at 420 eV. Here the large asymmetric tail has almost vanished; the fit results in  $\alpha = 0.04$ . Thus metallic screening of the Pd 3d hole through Pd valence states is strongly reduced in i-AIPdMn, implying that the density of states of Pd states at  $E_F$  is much reduced compared to the Pd metal case. From the valence spectrum in Figure 1 it is found that the dominant peak at 4 eV is Pd  $4d$ -derived, such that the contribution of  $d$  electrons near  $E_F$  is small in any case. Since core hole screening mostly occurs through the mobile  $s$  electrons, these results indicate that not only the  $d$  density, but also the Pd-derived  $s$  density near  $E_F$  is quite small.

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