

### 3d and 4d resonant photoemission in Pr and Nd metal

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Photoemission (PE) data for Pr and Nd metal around the 4d and 3d threshold have been measured. The experiments were performed at beamline 7.0.1 at the ALS in Berkeley. The samples were films evaporated on a W(100) single crystal. Here only the data for Nd metal are discussed, those for Pr metal are similar. Fig. 1 shows the "on resonance" and "off resonance" spectra of Nd metal at the 3d threshold. They exhibit the expected features. In the simplest approach to resonant photoemission of Nd metal,

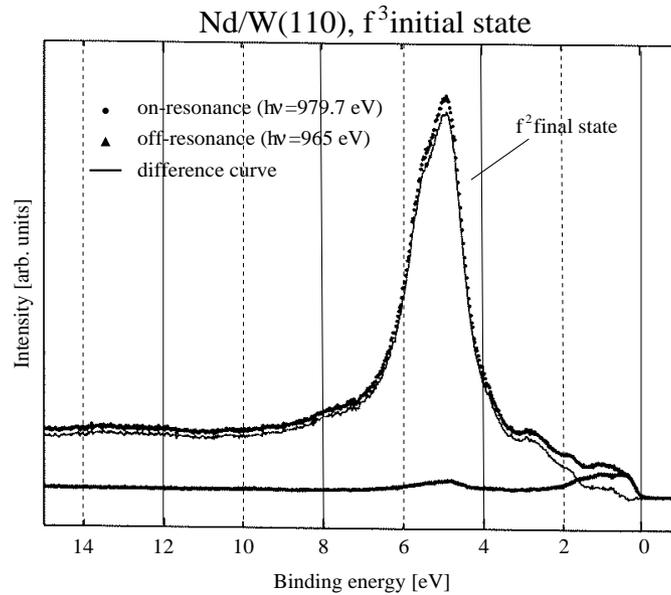
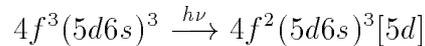


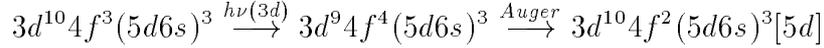
Figure 1: "On" (979.7 eV) and "off" (965 eV) resonance spectra for Nd metal at the 3d  $\rightarrow$  4f resonance.

there are two channels that contribute to the spectra:

direct PES:

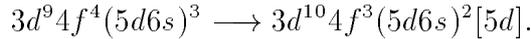


resonant PES:



where the screening electron in the valence band has been indicated by square brackets. The two equations show that an enhancement in the  $4f^2$  structure should be observed as is actually the case.

Additional structures in the "on" spectra is most likely produced by a  $4f^3$  final state which can occur via two mechanisms. Because the correlation energy  $U$  of the  $4f$  electrons is finite, there is a mixing of the  $f^4$  configuration (above the Fermi energy) into the  $f^3$  groundstate configuration of Nd. This, via direct photoemission, results in a  $f^3$  final state configuration. A second possibility for the occurrence of a  $f^3$  final state is by a different decay channel of the intermediate state into the final state in the resonant channel, namely:



It is difficult to determine the relative strength of the two processes. However, since in Fig. 1 the valence band changes its shape in going from the "off" to the "on" condition the second process must play a distinct role.

The data at the  $4d$  edge (see Fig. 2) have higher resolution and are therefore analysed in more detail. In order to come to analyse these data a smoothed version of the data at

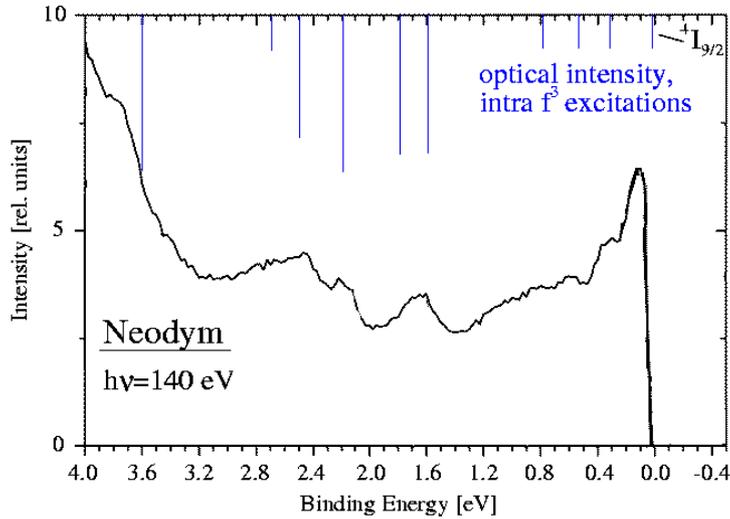


Figure 2: Subtraction of smoothed and raw data for Nd metal at the  $4d$  threshold. Bar diagrams are the energies of the optical absorption maxima of  $\text{Nd}^{3+}$  ions in solution and a calculation of the intensities of these transitions, where in many cases a number of transitions have been summed to make the general picture clearer [1,2].

the  $4d$  edge is produced and used for subtraction from the raw data in order to enhance the contrast.

Assuming that in Nd metal the  $4f^3(5d6s)^3$  configuration is a possible final state, as outlined above, it will be of the form  $4f^{3*}(5d6s)^2[5d]$ , where the star indicates the excitation within the  $4f$  manifold. This excitation process may be thought to be similar to the one in optical experiments. Therefore one may take the intensities from optical experiments [1,2] and check how far they reproduce those measured in the present experiment. In analyzing intensities in rare earth optical spectra often a number of close lying transitions have been lumped together. In addition the transition strength within the ground state manifold is not very well known and an arbitrary number is attached to it. With these reservations the optical intensities are shown in an additional bar diagram in Fig. 2, and the agreement with the resonance photoemission data is quite convincing. More high accuracy photoemission data are needed to substantiate the findings of this experiment.

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## References

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