

f-OCCUPANCY AT THE γ - α PHASE TRANSITION IN Ce ALLOYS

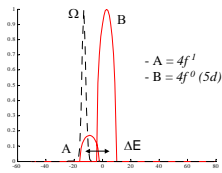
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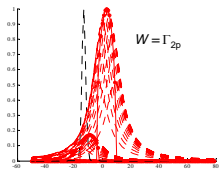
Phenomenological model

1- Initial parameters



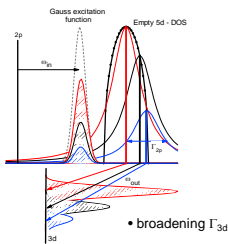
- 2 sem-elliptical bands
- Same width W
- Gaussian excitation at Ω

2- Intermediate states construction



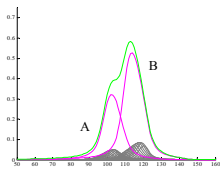
- equally spaced Lorentzian
- overlap excitation / intermediate states

3- Final states calculation



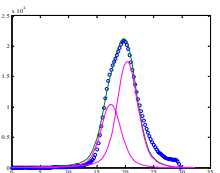
- broadening Γ_{3d}

4- Emission spectra reconstructed



Individual contribution from intermediate states

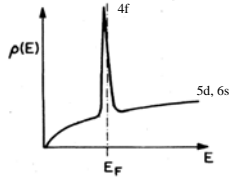
5- Comparison with experiment



- broadening by experimental function
- complete series of spectra computed by changing Ω only

INTRODUCTION

Ce α - γ transition : role of 4f hybridization

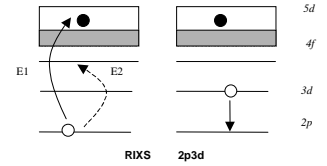


The Ce α - γ transition is one of the most intriguing phenomena in condensed matter physics. It embraces a variety of complex mechanisms yielding anomalous behavior on a structural level (lattice parameter), but also more fundamentally in the magnetic (magnetization) and electronic properties (specific heat, etc). Beyond the widely discussed theoretical paradigms, namely the **Mott transition scenario** and the **Kondo volume collapse** approach, there is a solid consensus that **hybridization** between 4f and valence electrons plays a key-role in the Ce α - γ transition.

How to estimate hybridization of f electrons ?

Resonant Inelastic X-ray Scattering

RIXS

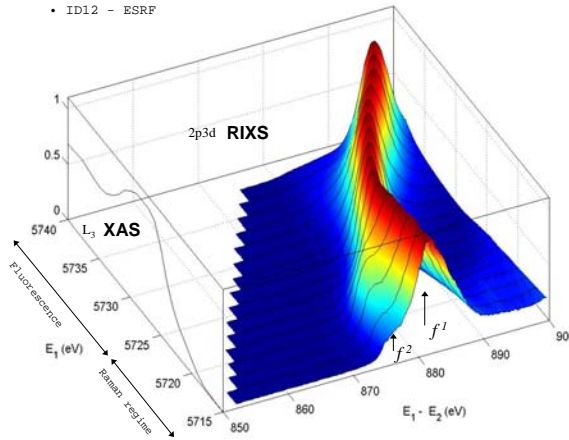


EXPERIMENTS

➤ Cerium solid solution:

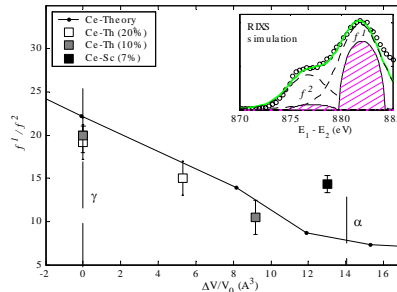
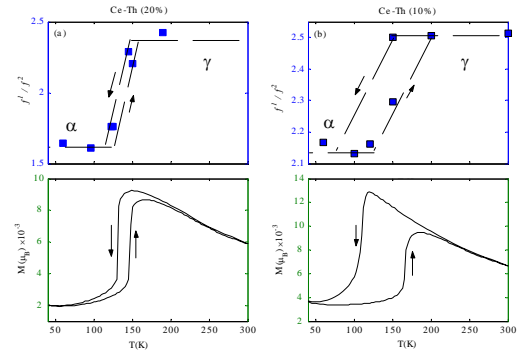
- Temperature-induced transition by substitution of Ce with Th or Sc

- Ce-Th (10%), 60 K
- ID12 - ESRF



- f^1 / f^2 intensity ratio derived from RIXS spectra scales with ground state properties (magnetization) at the α - γ transition

- Concentration-dependent hysteresis



[†] Mc Mahan et al., Phys. Rev. B **67**, 075108, (2003)

- corrected f^1 / f^2 intensity ratio from simulation of the RIXS spectra (phenomenological model)

- comparison with first principle calculations in pure Ce (DMFT + LDA)

- Good agreement in Ce-Th when renormalized to the volume change

Comments

- f^2 contribution hidden in XAS but visible by RIXS
- no contamination by α -like surface contribution such as in XPS
- f^2 relates to the 4f correlation strength in the ground state
- strongly supports Kondo volume collapse model

CONCLUSIONS

- 2p3d RIXS in light rare-earth systems is able to reveal structures hidden in XAS measurements below threshold.
- XAS cannot be used as a straightforward method to estimate the 4f count in the ground state.
- The 4f hybridization in intermetallic compounds is deduced from RIXS using a simple model.
- Next step : RIXS in pure Ce under pressure.