



Calculation of the XPS Mg 2p spectrum

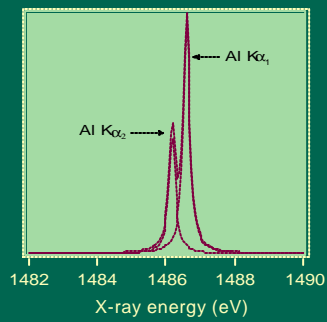
M. Kurth and P.C.J. Graat

Max Planck Institute for Metals Research, Stuttgart, Germany

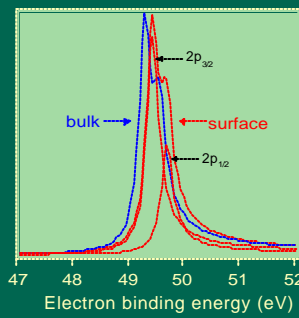
Introduction

Part of the intrinsic intensity of XPS spectra may not be contained in the main peak. Particularly, free-electron metals, like Mg and Al, have a significant intrinsic contribution in the plasmon-loss peaks. In this work the intrinsic and extrinsic contributions to the Mg 2p spectrum of pure Mg have been determined, accounting for surface effects.

X-ray energy distribution (Lorentz)

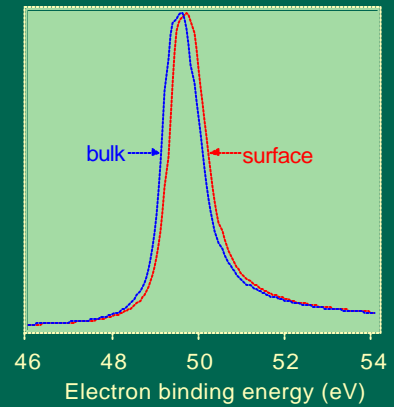


Core-level excitations (Doniach-Sunjić)

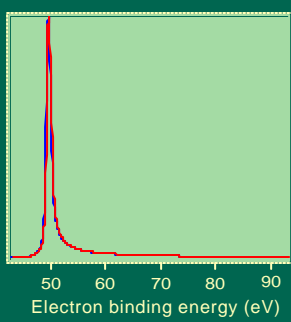


Fitparameter	
position of 2p _{3/2} bulk peak	= 49.27 eV
width	= 0.12 eV
asymmetry	= 0.12

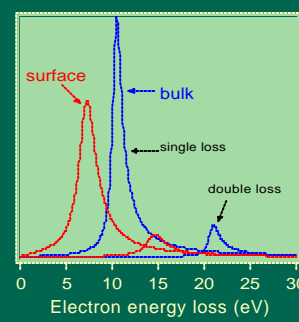
Main peak



Main peak

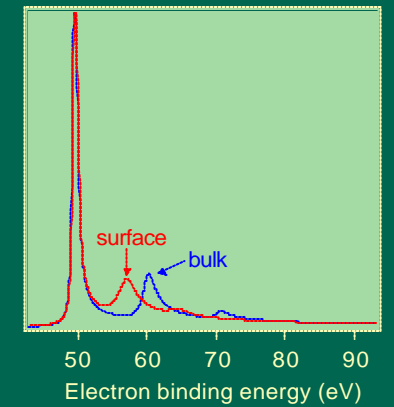


Intrinsic loss function (Drude-Lindhard)

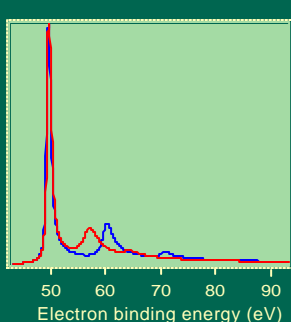


Fitparameter	
position bulk plasmon peak	= 10.35 eV
width	= 0.91 eV
position surface plasmon peak	= 7.14 eV
width	= 1.61 eV
area intrinsic loss function	= 0.36

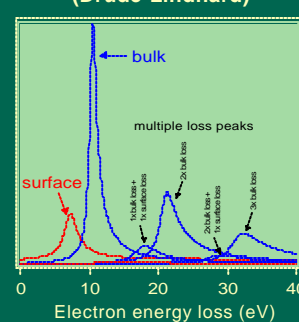
Intrinsic spectrum



Intrinsic spectrum

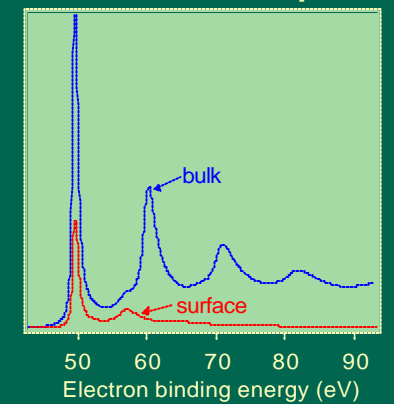


Extrinsic loss function (Drude-Lindhard)

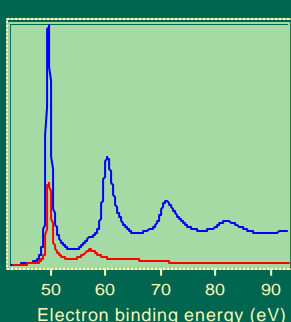


Fitparameter	
area extrinsic loss function	= 0.77
thickness of surface layer	= 0.63 nm

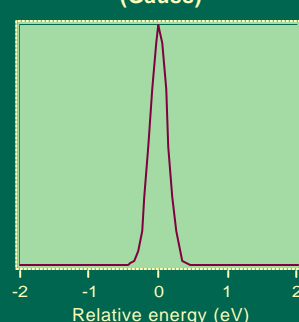
Intrinsic + extrinsic spectrum



Intrinsic + extrinsic spectrum



Instrumental broadening (Gauss)



Fitparameter	

Total vs. experimental spectrum

