XPS Limit in Soft X-Ray Photoemission Spectroscopy of Ag(001)

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Abstract. PhotoEmission Spectroscopy (PES) is a surface sensitive technique within the Ultra-Violet regime. A way to make it more bulk sensitive consists in increasing the photon energy for entering the X-ray regime. As a counterpart, this increase breaks the k-conserving dipole selection rule and results in a smearing of the measured electronic band structure caused by phonon-assisted electronic transitions. It is therefore essential to model this physical effect within *ab-initio* calculations. We herewith sketch the implementation of lattice vibrations within the one-step model of photoemission through the Coherent Potential Approximation (CPA). Moreover, we show a practical example with the case of Ag(001) on which the influence of photon energy and/or temperature is benchmarked and interpreted.