

s7.m7.o3 **Diffraction Anomalous Fine Structure for probing local structure: strain, ordering, low dimensionality effects.** M.G. Proietti^{#§}, H. Renevier[#], S. Grenier[#], G. Subias[§], L. Gonzalez⁺, J.M. Garcia^{+§}, J.L. Hodeau[#], J.Garcia[§]. [#]*Laboratoire de Cristallographie, C.N.R.S.-UJF*, B.P. 166, 38042 Grenoble Cedex 09, France. [§]*Departamento de Fisica de la Materia Condensada - I.C.M.A., Universidad de Zaragoza, pza S. Francisco s.n., 50003 Zaragoza, Spain.* ⁺*I.C.M.M., C.S.I.C., I. Newton 8, 28760 Tres Cantos, Spain.*
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The extended fine structure appearing above an Anomalous Diffraction edge can be described in terms of interference of the virtual outgoing photoelectron wave function with the partial waves scattered by the atoms surrounding the anomalous scatterers. The oscillating behaviour of the diffracted intensity reflects, as in the case of Extended Absorption Fine Structure (EXAFS), the local structure of matter and provides, in addition to the absorption chemical selectivity of EXAFS, spatial and site selectivity. This renders DAFS a powerful local order probe that is complementary and even alternative to EXAFS. We will give examples of the application of DAFS to systems which could not be investigated on a local scale by other EXAFS-like techniques: the strained III-V semiconductors, so popular in the telecommunication materials world, and magnetite, that is a reference system for modeling the complex properties of transition metal oxides. We report the results obtained for a partially relaxed epitaxial semiconductor alloy¹, GaAs_xP_{1-x}/GaAs(001), and show how the extended DAFS can be treated to extract the EXAFS-like information. We determine the strain content, the validity of the macroscopic elastic theory and the presence of an ordering mechanism of P. Another relevant example is the study of self-growth nanostructured materials as Quantum Dots (QD) and Quantum Wires (QW). We have studied InAs QW and QD arrays, grown by MBE onto InP(001) and GaAs(001) substrates, with and without a capping layer. We report at last on the analysis of the extended part of the Fe₃O₄ DAFS spectrum, measured at the Fe K-edge of the 002 and 006 forbidden reflections². The scattered intensity is due to the anisotropy of the dipolar scattering factor of the octahedral Fe atoms and the oscillation frequencies that show above the Fe K-edge, depend on the distance difference between successive coordination shells. In such a way tiny distortions, induced by charge fluctuation and charge ordering mechanism, can be detected.

s7.m7.o4 **Multiple Scattering approach to DAFS: Surface and Interface applications** R. Felici (1), M. Benfatto (2) and V. Formoso (3), (1) *INFM-OGG, c/o ESRF, BP 220, F-38043 Grenoble, France*, (2) *INFN-Laboratori Nazionali di Frascati, PB 40, I-00044 Frascati, Italy* and (3) *INFM-UdR Cosenza, Universita' della Calabria, 87036 Arcavacata di Rende, Italy*
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The structural characterization of reconstructed surface is of fundamental importance for the determination of most of their properties. Several techniques employing x-ray beams are normally used for this purpose as Grazing Incident X-Ray Diffraction (GIXD), Surface Extended X-Ray Absorption Fine Structure (SEXAFS) and X-Ray Standing Waves (XSW). Recently, a different approach based on the measurements of the scattered intensity as a function of the energy near and above an absorption edge, usually referred as Diffracted Absorption Fine Structure (DAFS), has been proposed and used to determine bulk structure. In principle this technique joins the advantages of the x-ray diffraction and the x-ray absorption (XAS) methods and, for this reason, can be a very powerful structural technique.

In the case of clean reconstructed surfaces the measurement of DAFS intensities of non integer peaks leads to extract the contribution to the XAS signal of the atoms participating in the reconstruction only. Moreover, in the case of deposition of different atomic species, the signal coming from atoms in ordered positions can be derived without any problems.

In spite of these possibilities, very few examples of this kind of experiments appeared in the literature because of difficulties either in the experimental setup and in the data interpretation. The data are usually analyzed by separating the form factor in a smooth part plus an oscillating contribution. The oscillating term is interpreted by following an EXAFS-like approach. In general this method is not valid due to the presence of two different polarizations directions in the resonant correction to the Thompson scattering amplitude.

In this work we give general analytical expressions, using multiple scattering theory, for the DAFS cross section and we discuss their relation with the standard EXAFS formulation. Applications to the Ge bulk will be shown as test cases for theoretical and experimental methods. DAFS signals measured onto reconstruction peaks of the clean Ge(001)2x1 and of the Sb-Ge(001)-2x1 surfaces will be discussed in term of the local atomic arrangement.

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