

parameters for the major 3d elements could only be found from the SR data sets. While site-occupation parameters obtained for the binary Cr-Fe  $\sigma$  crystal studied with SR were more precise by a factor of 3 than those recovered from conventional data, precisions of parameters for the binary  $\tau$  crystal with  $x = 0.74$  were not materially improved. In both cases, differences between parameters obtained from conventional and SR data were of marginal significance.

This work has confirmed that the success of SR diffraction experiments using dispersion to differentiate scattering cross sections depends on the precision with which dispersion correction terms can be measured or predicted. Results of analyses of SR data measured just below the Cr K edge energy from the binary  $\tau$  crystal with  $x = 0.74$  show that reasonable agreement factors can only be obtained if  $f'(\text{Cr})$  is allowed to decrease in magnitude with  $\sin\theta/\lambda$ . There is need for improved theoretical treatments and expanded experimental estimates of dispersion terms for particular elements in particular crystallographic environments.

Descriptions of local departures from average structures should also be improved if SR tuned near absorption edge energies is used to measure diffuse scattering from crystals whose components have similar atomic numbers. Methods will be presented that use variations in anomalous dispersion terms at multiple wavelengths to separate data sets into functions from which short-range structural parameters of binary and ternary alloys can be derived.

**15.X-8 BAND STRUCTURE APPROACH TO THE X-RAY SPECTRA OF METALS.** By J.E. Müller, Institut für Festkörperforschung der Kernforschungsanlage Jülich, D-5170 Jülich, West Germany.

A formalism to compute X-ray spectra due to core excitations in metals using single-particle band structure techniques is presented and illustrated with a calculation of the K and L absorption edges of transition and rare-earth metals. The scheme is based on a new linearized version of the augmented plane wave method specifically designed to cover large energy ranges (200 eV).

The main features of the spectra are interpreted in terms of band structure and EXAFS concepts and the connection between both forms of description is discussed.

The calculated spectra are compared with available experimental data: All the experimental features are reproduced by the calculation. However, for the heavier elements the actual placement of the features shows discrepancies, which point to a limitation of the ground state potentials for calculating high energy states.

**15.X-9 X-RAY EXCITED OPTICAL LUMINESCENCE (XEOL) : POTENTIALITY AND LIMITATIONS FOR THE DETECTION OF SITE SELECTIVE EXAFS SPECTRA**

by  
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The optical luminescence induced in various materials by X-ray excitation has been used for many years as a sensitive analytical tool. This phenomenon however deserves further attention from the spectroscopist because :

- (i) the differences between UV or X-ray excited spectra can be very useful in the assignment of weak transitions in multiple site systems : e.g. in  $\text{C-Y}_2\text{O}_3$  doped with  $\text{Eu}^{3+}$  cations, three lines assigned to transitions occurring at the centrosymmetrical  $\text{Eu}^{3+}$  ( $\text{C}_{3i}$ ) site are strongly enhanced in the XEOL spectrum.
- (ii) X-ray excitation spectra were reported to reproduce, in few cases (e.g.  $\text{CaF}_2$ ,  $\text{ZnO}$ ...) either positive or negative edges and EXAFS oscillations.
- (iii) we have recently established that in the case of mixtures of different species (e.g.  $\text{ZnO} + \text{Zn:porphyrin}$ ), the X-ray absorption spectrum of one specific species (i.e.  $\text{ZnO}$ ) could be obtained by this method.

The XEOL and optical EXAFS/XANES spectra of several inorganic or organometallic systems will be presented. Time resolved XEOL spectra have also been obtained, taking advantage of the pulsed structure of the synchrotron radiation light. Finally a simple formulation of the phenomenon predicting either positive or negative edges will be developed and the requirements for site selectivity discussed.

**15.1-1 A NEW INSTRUMENT FOR PROTEIN CRYSTALLOGRAPHY ON THE WIGGLER BEAM LINE AT THE SRS PROVIDING A FOCUSED, TUNABLE BEAM AT SHORT X-RAY WAVELENGTHS.** By J R Helliwell<sup>1</sup>, M Papiz<sup>2</sup>, P R Moore<sup>1</sup> and A W Thompson<sup>1</sup>.

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A new instrument has been constructed on the wiggler beam line at the Daresbury Synchrotron Radiation Source (SRS). The wiggler provides much harder x-radiation wavelengths than are available on an ordinary bending magnet at the SRS; the critical wavelengths of the emitted spectrum of radiation being 1Å and 4Å respectively for the SRS operating at 2 GeV. Hence, the new instrument provides shorter wavelengths than the first protein crystallography workstation at the SRS which has been routinely operational from 1981 (Helliwell et al (1982) J.Phys.E. 15, 1363). The optimization of the anomalous dispersion coefficients  $f'$  and  $f''$  for those elements with absorption edges with wavelengths  $0.8\text{Å} < \lambda < 3\text{Å}$  is possible. The range  $0.8 < \lambda < 1.1\text{Å}$  encompasses the L absorption edges of the heavy atoms which are usually used as derivatives in protein crystallography (eg Pt, Au, Hg). We present details of the spectral characteristics of the new wiggler magnet source, the parameters of the x-ray optics, the remote control alignment system and the computer configuration. In addition, an electronic area detector diffractometer (the FAST) has been supplied by Enraf-Nonius whose performance has been successfully tested. The diffractometer is capable of being mounted 'on its side' to move the detector in a vertical plane on the workstation to allow for the horizontal polarization of the SRS beam. Data collected on the system at Daresbury will be described.