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LINEAR APPROXIMATIONS FOR DETERMINING ATOMIC SUBLATTICE OCCUPANCIES BY ALCHEMI

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The orientation dependence of inner-shell ionization that arises due to dynamical diffraction, or 'channeling,' provides the underlying basis for atom-location by channeling-enhanced microanalysis (ALCHEMI), a technique for the characterization of atomic sublattice occupancies in ordered crystals. Since its introduction two decades ago, the formulation of the ALCHEMI technique has been modified by a variety of authors, in both its traditional algebraic 'ratio' and multivariate 'statistical' forms.

However, these formulations are predicated upon a common linear approximation that the channeling responses of all elements occupying a common sublattice are proportional to one another. In this case, the channeling response of an 'alloying' or 'impurity' element can always be expressed as a unique linear combination of the channeling responses of 'marker' elements that are independently distributed among the sublattices occupied by the alloying element. The essential ALCHEMI results are the linear algebraic coefficients. Various ALCHEMI formulations typically differ only in the interpretation of these linear coefficients, addressing the effects of so-called 'ionization delocalization' or of anti-site defects in determining the elemental sublattice occupancies.

An alternative methods for interpreting channeling data during the past several years has been the development of software for first-principles calculation of orientation-dependent inner-shell ionization cross sections. Simulations of channeling response suggest the limitations of a linear approximation such as ALCHEMI. The purpose of this paper is to compare various formulations of ALCHEMI, and to assess the viability of linear approaches given the availability of simulation software.

Keywords: ALCHEMI CHANNELING SUBLATTICE

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ALCHEMI STUDIES ON Al-Ni-Co DECAGONAL QUASICRYSTALS

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Al-Ni-Co alloy forms decagonal quasicrystals with various superlattice orders as the composition and temperature are changed. The superlattice ordered phases always have a very weak order of a 0.8 nm periodicity along the decagonal axis, whereas decagonal $Al_{72}Ni_{20}Co_8$, which shows only fundamental reflections, has a 0.4 nm periodicity. It had been considered that the 0.8 nm periodicity is attributed to a chemical order between Ni and Co, though no experimental confirmation had been made. We first applied ALCHEMI (atom location by channeling enhanced microanalysis) technique on $Al_{72}Ni_{20}Co_8$ and revealed that Ni and Co occupy at a common site in disorder. In the present study, we have applied the ALCHEMI technique for decagonal $Al_{70}Ni_{18}Co_{12}$ with a superlattice order to reveal the chemical order of the constituent elements. Channeling patterns, which measure characteristic X-ray emissions as a function of the incident direction of the electron beam, were taken at incidences perpendicular and parallel to the decagonal zone axis. The ratio patterns between the constituent elements clearly show that Al occupies at a definite site different from the transition metals and that the transition metals occupy at common site in disorder Therefore, it has been found that the superlattice order is not attributed with a chemical order but with a topological order.

Keywords: DECAGONAL QUASICRYSTAL, ALCHEMI, CHEMICAL ORDER

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DETECTOR NEEDS AT A THIRD GENERATION SYNCHROTRON SOURCE

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Even though the last decades have seen a significant improvement in x-ray detector performance, the developments in this area have been much less spectacular than the ones for the synchrotron sources. As a consequence, the detector is now often the limiting factor in the experiment. This mismatch between source and detector performance is particularly evident for area detectors.

In areas like protein crystallography, the detector is mainly limiting the throughput. Only in special cases, like severe radiation damage, is the detector limiting the science that can be done. This situation is different in quickly developing areas like time resolved diffraction, where better (i.e. Faster) detectors could open up complete new fields of science. Time resolved (small angle) scattering has always been an area where the detector is limiting the science and new detectors are desperately needed. Another rapidly developing field at the third generation synchrotron sources is x-ray imaging, covering many different x-ray energies (few keV to few 100 keV), different spatial resolutions (few tens of microns to sub micron) and many different time scales, seconds to hours). An overview of the current detector systems will be given, followed by a summary of the requirements for today's science.

An attempt will be made to illustrate which (kinds of) science would be possible if we could make full use of the available flux and brilliance of third generation sources.

Keywords: X-RAY DETECTORS SYNCHROTRON RADIATION DEVELOPMENTS

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PILATUS: A 2-DIMENSIONAL X-RAY DETECTOR FOR MACROMOLECULAR CRYSTALLOGRAPHY

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A large quantum-limited area x-ray detector for protein crystallography is under development at the Swiss Light Source. The final detector will be 2k x 2k pixels covering 40 x 40 cm^2. A three-module prototype with 1120 x 157 pixels covering an active area of 24.3 x 3.6 cm^2 has been tested. X-rays above 6 keV with peak count rates exceeding 500 kBq/pixel could be detected in single photon counting mode. Statistics of module production and results of threshold trimming are presented. To demonstrate the potential of this new detector, protein crystal data were collected at beamline 6S of the SLS.

Keywords: PIXEL DETECTOR SINGLE PHOTON COUNTING