

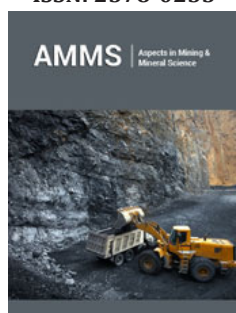
Synchrotron-(XRF, XRD, XAFS) Techniques in Advanced Mineralogy

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Abstract

Advent of high-intense x-ray synchrotrons has significantly empowered detection capabilities and stimulated diverse atomic-scale characterization experiments with wide application spectrum extending to under-explored fields such as structural biology and environment. We review the utilization of synchrotron-based techniques (XRF, XRD, XAFS) in mineralogy. While (XRF, XRD) are more regularly employed for basic speciation of minerals, the exploitation of versatile XAFS technique to address advanced problems in mineralogy is clearly limited. We suggest a host of advanced problems that could be addressed by these techniques and should inspire ambitious research for advancing the scope of mineralogy in future.

Keywords: XAFS; XRF; XRD; Minerals; Synchrotron

Introduction

X-ray and electron probe-based characterizations of minerals have traditionally addressed scientific problems of micro- and macro- length scales [1]. However, recent advancements in mineral applications e.g. nano-drugs [2], novel functional materials [3-5] demand nano-scale characterization for better understanding and control of this field. In this article, we review the scope of synchrotron-based x-ray techniques [XRF, XRD, XAFS] to address this requirement. The advantage of synchrotron-based research approach derives from (i) high x-ray flux (10^{11-14} ph/s), enabling the detection of elements in ppm concentrations; (ii) wide energy spectrum (5-30keV) covering the binding energies of all elements and enabling their detection; (iii) short wavelengths (0.5-2.5Å) to probe atomic length-scale phenomena. Synchrotrons around the world are listed in [6]. All of these techniques are non-destructive and undemanding wrt sample requirements. Laboratory-based XRF is widely employed in mineralogy for elemental speciation and XRD for characterization of crystalline phases and detection of crystalline-amorphous phase transitions. These techniques are significantly empowered by synchrotron as detection limits are extended towards dilute hidden phases. Advanced scientific problems can be addressed with (relatively recent) versatile XAFS technique [7], that reveals chemical state of any selected element in the material and structural information within 10\AA of the element. Unique advantages of XAFS are (i) simultaneous structural and chemical information, (ii) detection of ppm elemental concentrations, (iii) sensitivity to amorphous structure (e.g. liquid, glass, soil), (iv) site-resolved information (e.g. structure around dilute dopants). (XRF, XRD, XAFS) in conjunction can provide the most comprehensive information for any mineral. We review the present utilization and future scope of these techniques in mineralogy.

Application

Many current works are limited to basic speciation [8-11]. Advanced problems include bioavailability of essential minerals [12], remediation of toxic contaminated soil [13,14], fuel

behavior in reactors and synthesis of novel catalysts [15]. These studies reveal correlation between (oxidation state/bond-length) parameters and (mobility/solubility/sorption), with implications for reclamation/remediation/reactor technology. Our recent investigation of gadolinite revealed the role of structural disorder in flexible accommodation of radioactive waste. These citations cover the current utilization range of these techniques in mineralogy, which is clearly limited. Future role of these techniques lies in guiding the development of mineral nano-drugs [16] and mineral extraction nanotechnology [17,18]. Advanced adaptations of these techniques e.g. structure-pressure correlation from High Pressure-(XRD, XAFS) could be exploited to locate minerals beneath earth [19]. Magnetic measurement with XAFS-based "X-ray Magnetic Circular Dichroism" (XMCD) technique [20] should be envisaged to explore novel magnetic materials. These novel problems will greatly advance the scope of mineralogy.

Conclusion

The review reveals the comprehensive potential of synchrotron-based (XRF, XRD, XAFS) techniques for nano-scale characterization, which is clearly under-utilized in mineralogy. Their current utilization in mineralogy is limited mostly to basic speciation of minerals and a few advanced problems with implications for mineral reclamation/ soil remediation/ waste immobilization technologies. We suggest a host of novel problems that can be undertaken by these techniques and that can broaden the scope of mineralogy significantly.

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