New XRD Data Based Approaches to Soil Mineralogy

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Soils are complex materials formed at the interface of the geosphere, the biosphere and the atmosphere, they perform many functions relating to biomass production, environmental interactions and biodiversity. In addition to various forms of organic matter, living organisms, gases, water and solutes, most soils consist largely of a mixture of primary minerals derived from the soils geological ‘parent materials’, along with secondary minerals such as clay minerals and iron oxides, often formed by weathering. Additionally, the suite of minerals present in any given soil may be variously distributed amongst the sand, silt and clay particle size fractions, whilst also varying widely in chemical composition, crystal structure, surface area and solubility. Thus it has long been recognised that soil minerals are intimately related, both directly and indirectly, to many of the physical, chemical and biological properties of a soil which in turn govern the functions it may perform. Given the complexity of soil, however, it has been notoriously challenging to systematise soil property/mineralogy relationships.

Conventional approaches to the assessment of soil mineralogy by X-ray diffraction (XRD) typically involve a first stage of identification of the minerals present and a subsequent stage that seeks to quantify the relative abundance of the different minerals identified in the soil. In recent years the availability of archived digital XRD patterns from soil has increased, and attempts are now being made to generate datasets containing thousands of spatially referenced XRD measurements [e.g. those collected for the National Soil Inventory of Scotland (NSIS) and the Africa Soil Information Service (AfSIS)]. Since many soil properties are closely related to soil mineralogy, such datasets in combination with computational data analysis represent unique opportunities to advance the understanding of the role of soil minerals in governing or influencing many soil properties, processes and functions.

Use of data approaches such as cluster analysis and data mining allow soil XRD patterns to be treated simply as digital signatures which encode information on soil mineral (peaks) and amorphous (background) components. Viewed like this, conventional expert analysis and interpretation involving the steps of mineral identification and quantification become somewhat redundant, at least in the early stages of processing large data sets. Examples of these data based approaches to unravelling and advancing understanding of soil property - mineralogy relationships will be illustrated using the NSIS and AfSiS data sets. Additionally, approaches to high throughput conventional quantitative mineralogical analyses that can be applied to large and mineralogically diverse sets of soils will also be outlined. Together these approaches begin to define a vision for an emerging field of ‘digital soil mineralogy’ aimed at helping to inform the sustainable soil use and management of the future.