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Machine Learning Assisted Mineral Analysis: Case Studies on X-ray diffraction and Resonant Ultrasound Spectroscopy

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Predicting structures and thermodynamic properties of minerals and ceramics is important for many aspects, including ore genesis, mineral alteration, new material fabrication, etc. The traditional way to obtain such information is through manual analysis of experimental data from different characterization techniques, e.g., XRD, calorimetry, and ultrasonic spectroscopy, which are common to geochemist and mineralogist. However, it is often time consuming and requiring profound understanding to the materials and techniques. To overcome these barriers and improve the efficiency for materials research, we introduced a series of automatic methods based on neural network (NN) to solve XRD and resonant ultrasound spectroscopy (RUS) data and obtain structural, physical, and thermodynamic properties without human intervention. For solving XRD data and retrieving structural information, we successfully developed models to identify phases of REE minerals from the in-situ hydrothermal fluid experiment involving $LaCl_3$ and calcite. For solving RUS data and obtaining elastic moduli from ceramics, we trained models based on the computed RUS data modulated into image-like format. The resulting models successfully solved the experimental RUS data from a steel cylinder and three Ce doped yttrium aluminum garnets. We demonstrated that these machine learning methods are promising to automatically analyze experimental data and retrieve structural, physical, and thermodynamical information making mineral and material analysis accessible.