MEASUREMENT OF COEFFICIENT OF THERMAL EXPANSION BY X-RAY DIFFRACTION: A METHOD FOR ACCURATE FITTING OF LATTICE CONSTANT DATA

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Abstract

The use of in-situ heating and cooling of samples via a thermal stage mounted on a diffractometer is a common practice employed to measure thermal expansion of materials by x-ray diffraction. When using a simple least squares fitting of lattice constant measurements to a quartic function in order to yield a thermal expansion that is cubic in temperature, the thermal expansion function oscillates in an unphysical way. In order to accurately fit the lattice constant data taken during x-ray diffraction thermal expansion measurements, a new method for fitting the data is required. We report on a modified method of fitting using a penalized least squares method, the theoretical and experimental analyses of the method, and the limitations of the technique.