Uncertainty quantification of a graphite nitridation experiment using a Bayesian approach


1. Introduction

Experiments are performed to test physical theories or to estimate parameters of widely used theoretical models. An experimentalist usually prescribes the measurement uncertainties while reporting the results. The theorists or the users of theoretical models need to estimate parameters appearing in their models using the experimental data (i.e., a calibration process). There are various methods of parameter estimation that can be found in many textbooks on data analysis, under the category of inverse problems (for example [2] and many others). Inverse problems can be very ill-conditioned and in many cases special numerical techniques are required. In this work, we focus on the Bayesian method that is a robust method when there are uncertainties due to the experimental measurements as well as uncertainties in the model used to reduce the measured data [3]. We consider an experiment for the nitridation of graphite conducted by Zhang et al. [1]. The quantity that needs to be calibrated is the reaction probability of the graphite–nitrogen atom surface reaction. This reaction is of great importance for modeling the thermo-chemical processes (for example [2] and many others). Inverse problems, parameter estimation, Bayesian method, and uncertainty quantification are topics of great importance for modeling the thermo-chemical processes.

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