# Data mining of Ti–Al semi-empirical parameters for developing reduced order models

Broderick, Scott R.; Aourag, Hafid; Rajan, Krishna

**Abstract :**

A focus of materials design is determining the minimum amount of information necessary to fully describe a system, thus reducing the number of empirical results required and simplifying the data analysis. Screening descriptors calculated through a semi-empirical model, we demonstrate how an informatics-based analysis can be used to address this issue with no prior assumptions. We have developed a unique approach for identifying the minimum number of descriptors necessary to capture all the information of a system. Using Ti–Al alloys of varying compositions and crystal chemistries as the test bed, 5 of the 21 original descriptors from electronic structure calculations are found to capture all the information from the calculation, thereby reducing the structure–chemistry-property search space. Additionally, by combining electronic structure calculations with data mining, we classify the systems by chemistries and structures, based on the electronic structure inputs, and thereby rank the impact of change in chemistry and crystal structure on the electronic structure.