CompuMat

Compumat Technologies Ltd. is a London-based tech startup building data-driven discovery tools for clients in the materials and chemicals industries. This white paper presents a case study of the methodology applied to the problem of predicting corrosion rates of arbitrary steel grades in various chemical environments.

Introduction

Machine Learning, a subfield of Artificial Intelligence, has over the past few years powered predictive modelling breakthroughs in fields such as web technology and ecommerce, due to its capacity to adapt to highly nonlinear, correlated and high-dimensional data. Recently, techniques from Machine Learning have started to find use in the hard sciences, starting with the pharmaceutical and petroleum industries. The common factor is the use of cutting-edge algorithms and large amounts of data to provide significant speedups and cost reductions to previously time-consuming tasks.

The materials industry has lagged behind in this development, even though materials testing is a slow and expensive process, impacting both materials R&D and materials selection.

Compumat Technologies was founded to address this problem. We are developing software tools that enable clients to reduce their reliance on physical testing of materials, speeding up the process of discovery and optimization of novel materials, as well as helping solve materials selection problems. Our Machine Learning models integrate three types of data:

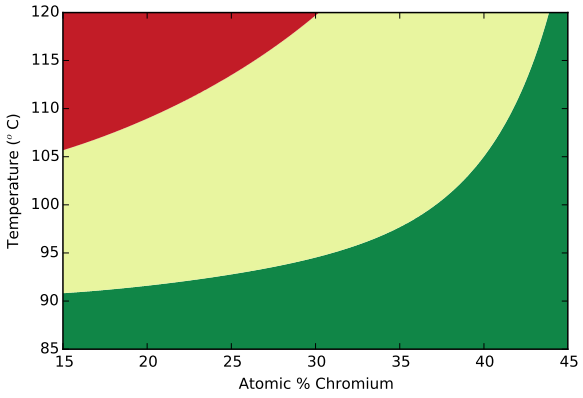
- publicly available data (publications and databases)
- private, internal data
- Custom generated data from large sets of ab-initio simulations

By leveraging this data, our tools can predict the suitability of a material for a given application more quickly, and at a much lower cost than it would take to validate experimentally. Compared to generic analysis tools, Compumat offers domain expertise in materials physics, which is essential for achieving optimal performance in terms of data selection and feature engineering. In addition, for certain applications, the ability to set up and interpret large sets of physics simulations can enable clients to explore the materials design space much more efficiently.

Case Study: Data-driven Corrosion Prediction

Corrosion of metal structures and components accounts for an estimated $270bn of costs annually in the US alone. Prediction of the corrosion rate of a given material in a given environment is not always straightforward, since there can be uncertainty as to which of several competing mechanisms is causing the corrosion, and also because the dependency on certain process parameters can be highly nonlinear. Many steel producers provide tabular corrosion rate data on their products in various environments, but if the environment differs from the points in the table, the best an engineer can do is make an educated guess.

We have built a software tool based on a predictive model for corrosion rate estimation by using corrosion tables which are freely available online. Using this tool, we can finely explore the composition space, rather than having to rely on a finite number of measurements. An example is illustrated below for steel grades with varying Chromium content in a 80% phosphoric acid environment (green: not corrosive, yellow: moderately corrosive, red: highly corrosive).



This type of tool allows R&D professionals to precisely see the effects of changing various composition and processing parameters, but it is also indispensible for materials selection: given a specific environment that may not be included in the tablular data, the tool can provide valuable information as to which products are expected to perform to specification.

Contact Us

Please contact info@compumat.io for further information.