DATA DRIVEN DESIGN OF AL ALLOYS

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Modern High-throughput methods make it possible to obtain large volumes of data. This "Big Data" approach allows not only to find trends and dependencies, but also opens up fundamentally new methods of research.

Today less than 200,000 materials are known, but only for a few of these "known" materials basic properties have been studied, and in fact there is an infinite number of compounds that need further research.

Therefore it is likely that new materials with excellent and still unknown properties exist that could help to solve fundamental problems in energy, transportation, security, information and health.

One of the most widely studied and practically useful problems is the creation of new aluminum alloys. Therefore binary aluminum alloys with 1% impurity concentration were selected for our High-throughput analysis. To do this we have developed a comprehensive automated system for physical properties computation. The software handles creation of configuration files, executes calculations, processes and visualises the results.

We had reviewed binary aluminum alloys with 63 alloying components. For each alloy we built its equation of state, determined the lattice parameters and the bulk modulus, computed the elastic constants, the Young's modulus and the shear modulus. Finally we had compared these results with the available experimental data.