Solid solution strengthening in aluminium alloys from first-principles and machine learning interatomic potentials

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Aluminum alloys provide attractive characteristics like low density, high specific strength, excellent oxidation and
corrosion resistance. By injecting foreign elements into the stable aluminium phase, mechanical properties can be improved. This is dictated by the mechanism of solid solution strengthening, which has its origin on the nanoscale. The identification and tailored design of promising alloys bears the potential to outperform known materials and opens new perspectives for target advanced applications. However, first-principle
calculations are limited by computational ressources due to the large configuration space.

In this study, strengthening of aluminium solid solutions containing magnesium and zirconium is investigated using Density functional theory and Molecular dynamics. From stress-strain curves, elastic and plastic properties are derived. Additionally locking mechanism are studied to understand the interaction between solute atoms and dislocations. The ab-initio calculations show, that desired properties are dependent on the concentration of alloying elements and their relative position inside the bulk. It is therefore sufficient to analyze the whole phase space up to the solubility limit of impurities. In order to do this in a computational feasible manner, a machine learning interatomic potential (MLIP) is trained on the fly based on kernel ridge regression and Bayesian statistics.

The approach accelerates first-principle investigation of solid solution strengthening in alpha-aluminium alloys by maintaining the underlying accuracy.