

Faculty of Engineering

Summer Research Program 2023-2024

Project Title: Making Aluminium Sustainable

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Objective

Scientific objective: Designing new aluminium alloys with passive cross-contaminant alloying elements

Learning objective: Introduction to (1) high performance massively parallel computing and (2) atomic-scale modelling of materials

Project Details

Aluminium alloys are extensively used in applications as varied as packaging, construction, automobile and aerospace. The extraction of aluminium from bauxite is an energy intensive process, so to minimize the amount of new aluminium produced and the associated energy cost, it is paramount to improve the recycling of aluminium alloys. One key problem in the recycling of aluminium is the cross-contamination of alloying elements from different alloy types [1]. This project will investigate ways to neutralise or even exploit such contaminants in alloys. This will be carried out by simulating the interaction between alloying contaminants and well-known precipitate phases in strategically selected aluminium alloys. The methodology will be that used in previous studies on precipitation and solute segregation in high-strength aluminium alloys, and will employ first principles methods on massively parallel high performance computing facilities [2-3].

- [1] D. Raabe et al., "Making sustainable aluminum by recycling scrap: the science of 'dirty' alloy", Prog. Mater. Sci. 128 (2022) 100947.
- [2] S. Su, L. Bourgeois and N.W. Medhekar, "Predicting the early stages of solid-state precipitation in Al-rich Al-Pt alloys", Acta Mater. 255 (2023) 119048.
- [3] L. Bourgeois, Y. Zhang, Z. Zhang, Y. Chen and N.V. Medhekar, "Transforming solid-state precipitates via excess vacancies", Nature Comm. 11 (2020) 1248.

Prerequisites

Undergraduate knowledge of crystal structure, phase transformations, eg via MTE2101, MTE2102.