PhD project: Discovery of aluminium alloys that can be made from scraps

The mission of the Max-Planck-Institut für Eisenforschung is to understand and design nanostructured materials down to atomic and electronic scales. In this spirit, we conduct basic research on structural and functional materials, mostly metallic alloys, embracing synthesis and processing, characterization and properties, as well as their response in engineering components exposed to real environmental conditions. We work interdisciplinary, with intense mutual stimulation among experimentalists and theoreticians as well as among different groups and departments.

The Helmholtz School for Data Science in Life, Earth and Energy (HDS-LEE) provides an interdisciplinary environment for educating the next generation of data scientists in close contact to domain-specific knowledge and research. All three domains – life & medical sciences, earth sciences, and energy systems/materials – are characterized by the generation of huge heterogeneously structured data sets, which have to be evaluated in order to obtain a holistic understanding of very complex systems. Visit HDS-LEE at: www.hds-lee.de

Project overview:

This project uses artificial intelligence to find new Aluminium (Al) alloys that can be made from scraps. With this it combines two key challenges, namely alloy design and energy-saving recycling of metals.

The number of possible metallic materials and microstructure features that could be made of the ~ 60 relevant elements is practically infinite when including dislocations, interfaces, precipitate phases, and other types of microstructure features. Yet, only a few thousand metallic alloys are currently used. Most of them are not sustainable, i.e., they are only designed for one time use not for multiple recycling and re-melting.

You tackle these challenges with machine learning approaches using the rich data bases that exist for the thermodynamics and kinetics of alloys, for the properties and for scrap compositions. The database data will be augmented by descriptors of the microstructure to be extracted from atom probe analysis and/or “textbook” predictions.

Your Job:

- Scan existing databases and homogenize data that could be used for the project. Also screen existing composition databases for the corresponding types of scraps, which can serve as a sustainable basis for making these or future, more scrap-compatible alloys.
- Explore available atom probe data on Al alloys to derive possible descriptors for mechanical performance and test their predictability from traditional material science approaches. For this, different convolutional reductions of the peculiar structure of APT data shall be attempted.
- Test different machine learning algorithms to predict mechanical performance from available data such as composition, processing, and the microstructure descriptors.
- Use the model to identify scrap-compatible Al alloys.

Your profile

- Masters degree (M. Sc.) in materials science, computer science, physics, mathematics, or a related field
- Highly motivated candidate with strong mathematical skills
- Knowledge in materials science, and/or data analysis
- Good programming skills (preferably Python or C++)
- Good skills in the spoken and written English language: TOEFL or equivalent evidence of English-speaking skills
- You are convincing with your confident attitude and good communication skills
- Outstanding organizational skills and the ability to work independently
- Very good cooperation and communication skills and ability to work as part of a team in an international and interdisciplinary environment
- A high level of scholarship as indicated, for example, by bachelor and master study transcripts and two reference letters
Our offer

The PhD student will be hosted in the Defect Chemistry and Spectroscopy group (C. Freysoldt) in the Department Computational Materials Design at Max-Planck-Institut für Eisenforschung (MPIE), Germany within the Helmholtz School for Data Science in Life, Earth School and Energy (HDS-LEE). Strong collaboration with the Atom probe tomography group of B. Gault at MPIE and the "Mathematical Image and Signal Processing" group of B. Berkels at RWTH Aachen is expected.

- Outstanding scientific and technical infrastructure – ideal conditions for successfully completing a doctoral degree
- Unique HDS-LEE graduate school program
- A highly motivated group as well as an international and interdisciplinary working environment
- Chance of participating in (international) conferences
- Continuous scientific mentoring by your scientific advisor
- Further development of your personal strengths, e.g. via a comprehensive further training program
- Pay in line with 100 % of pay group 13 of the Collective Agreement for the Public Service (TVöD-Bund)
- A contract for the duration of 3 years

The Max-Planck-Institut für Eisenforschung GmbH is committed to employing more handicapped individuals and especially encourages them to apply. The Max Planck Society strives for gender and diversity equality. We welcome applications from all backgrounds.

Become a part of HDS-LEE and apply at https://recruitingapp-5424.de.umantis.com/Vacancies/322/Description/2

Starting date: at the next possible date