Department of
Mechanical Engineering
The University of Hong Kong

DEPARTMENT OF
MECHANICAL ENGINEERING
THE UNIVERSITY OF HONG KONG

SEMINAR

(onsite and online)

Molecular Dynamics Study of Segregation and Diffusion at Al-Mg Grain Boundaries

Date: 25 April, 2025 (Friday)
Time: 11:00 a.m.
Venue: Room 7-34 and 7-35, Haking Wong Building, HKU

Speaker: Miss Xiaofan Shi (PhD candidate)
Department of Mechanical Engineering
The University of Hong Kong

Join Zoom Meeting:
https://us05web.zoom.us/j/87151808402?pwd=9LaYQsQVztMU7bNswzPouTIrCCcne3.1

Meeting ID: 871 5180 8402
Password: MC34ti

Abstract:

Al-Mg alloys are widely utilized in aerospace and automotive industries due to their excellent combination of strength, workability, corrosion resistance, and reduced density. Previous experimental studies have shown that, in Al-Mg alloys with low magnesium concentrations, magnesium atoms segregate at grain boundaries, significantly influencing the thermodynamic, mechanical, and kinetic properties of the alloy.

This study investigates magnesium segregation at high-angle tilt grain boundaries in Al-Mg alloys using molecular dynamics simulations within a semi-grand canonical ensemble. The results demonstrate that magnesium segregation decreases with increasing temperature, in agreement with the Langmuir-McLean theorem. The structural characteristics of the grain boundaries were found to play a critical role in modifying the segregation behaviour by affecting the competition between enthalpy and entropy. Magnesium atoms were observed to form clusters at the grain boundaries, distributing mostly along the tilt axis. These clusters were analyzed to determine their geometric and

structural characteristics. By altering the diffusion mechanisms, the presence of these clusters was found to reduce the diffusivity of aluminum atoms, potentially impacting the microstructural evolution of the material.

This work refines and expands the simulation methods presented in prior studies, providing deeper insights into the temperature-dependent and structural effects of grain boundary segregation and clustering. These findings contribute to the design and optimization of Al-Mg alloys for advanced industrial applications.

ALL INTERESTED ARE WELCOME

For further information, please contact Prof. David J. Srolovitz at 3917 2800.