Atomistic Simulations of Diffusion Induced Grain Boundary Migration in Aluminium

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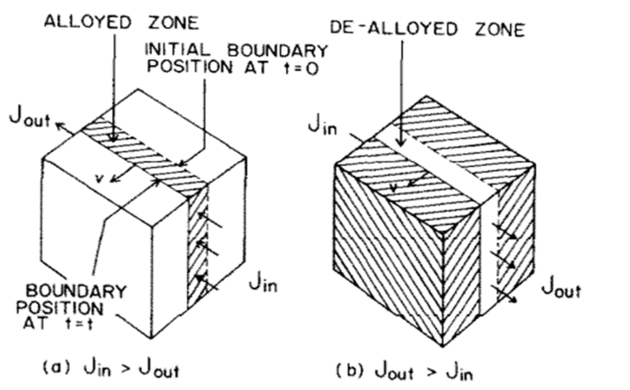
Introduction

Diffusion-induced grain boundary motion (DIGM) can be caused when solute atoms diffused out of grain boundary (GB) in the presence of solute sink or diffuse into the GB in the presence of solute source thereby causing the boundary to migrate and produce de-alloyed (solute depleted) and alloyed zones (solute enriched).



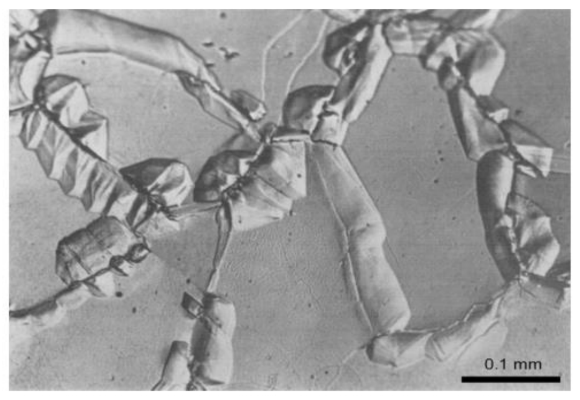


Fig. 6-14—Photomicrograph illustrating the surface relief accompanying the local zincification of an iron foil 40 microns thick by DIGM. [M. Hillert, G. Purdy, Acta Met. 26 (1978) 333.]

Objective

- To simulate grain boundary migration induced by diffusion by using Molecular Dynamic Simulations.
- The present study is focused on DIGM when solute sink is present.

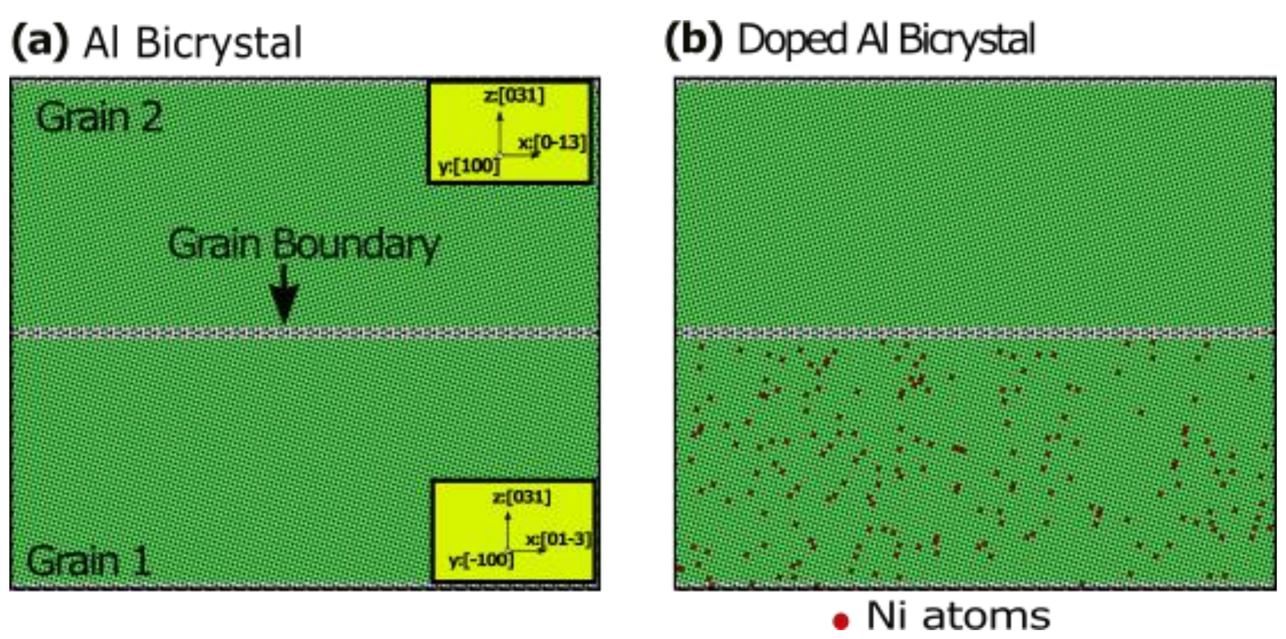
Technological Applications

- Surface Alloying
- Improving creep resistance
- DIGM can reduce fatigue lifetimes.
- DIGM can cause premature failure in electrical interconnects.

Motivation

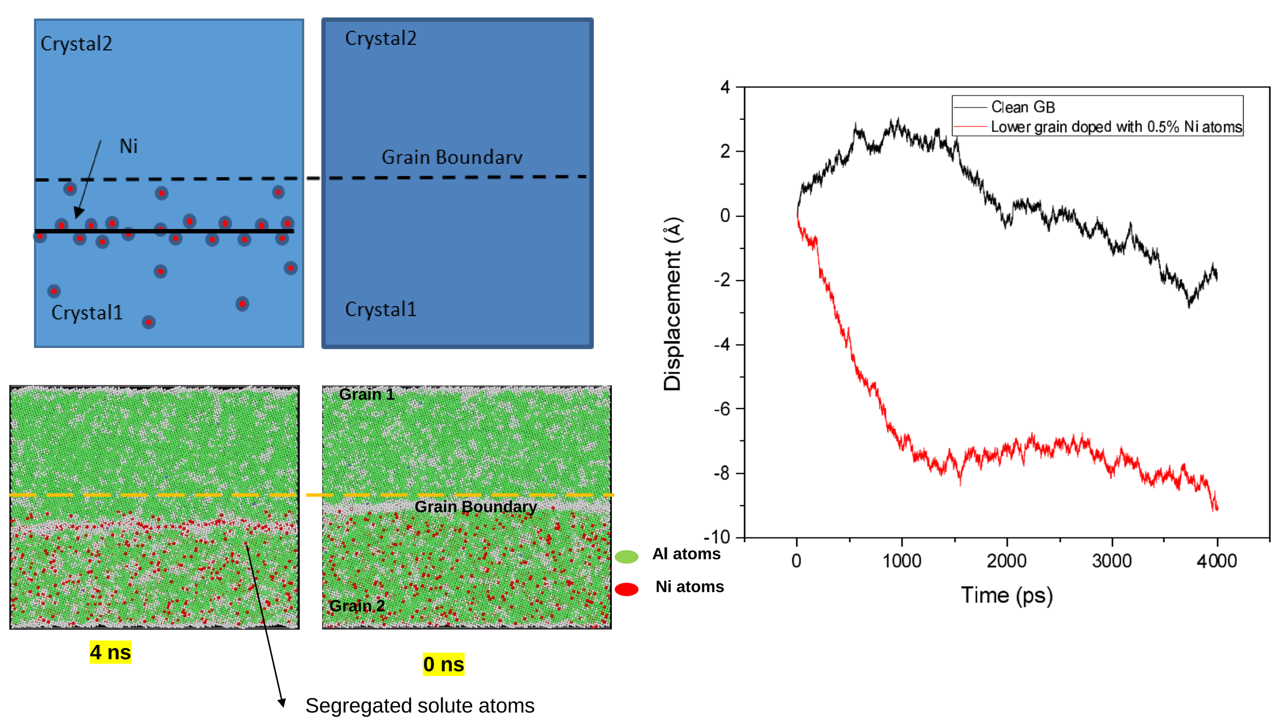
To control DIGM, operating driving forces and mechanisms needs to be understood

Model Approach

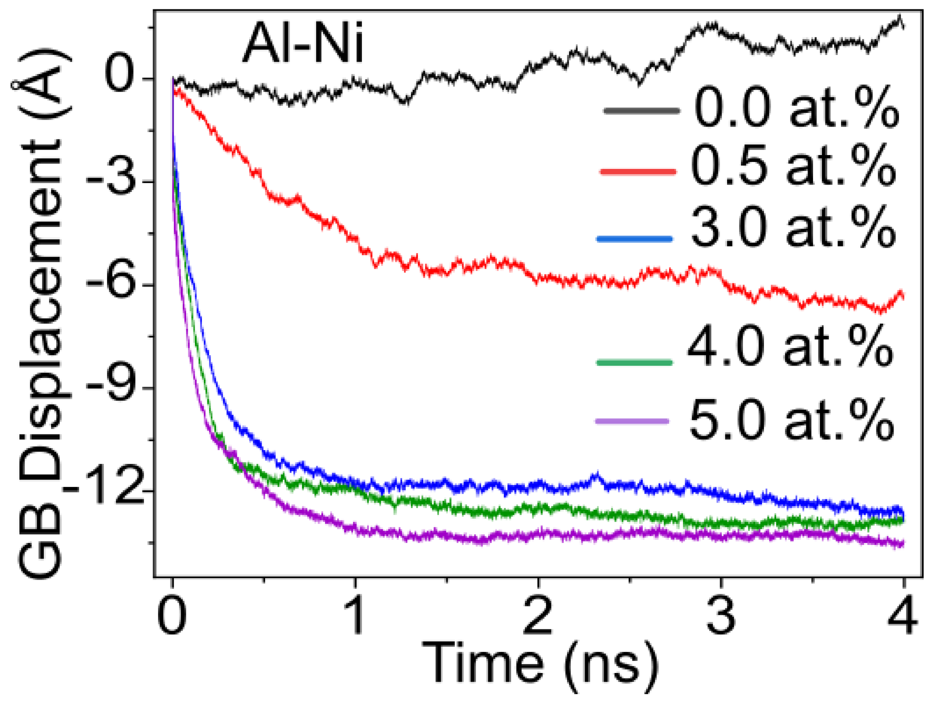


Assumption: It is assumed that solute sink is present which depleted GB from solute atoms.

Grain Boundary (GB) displacement in Al bicrystal models



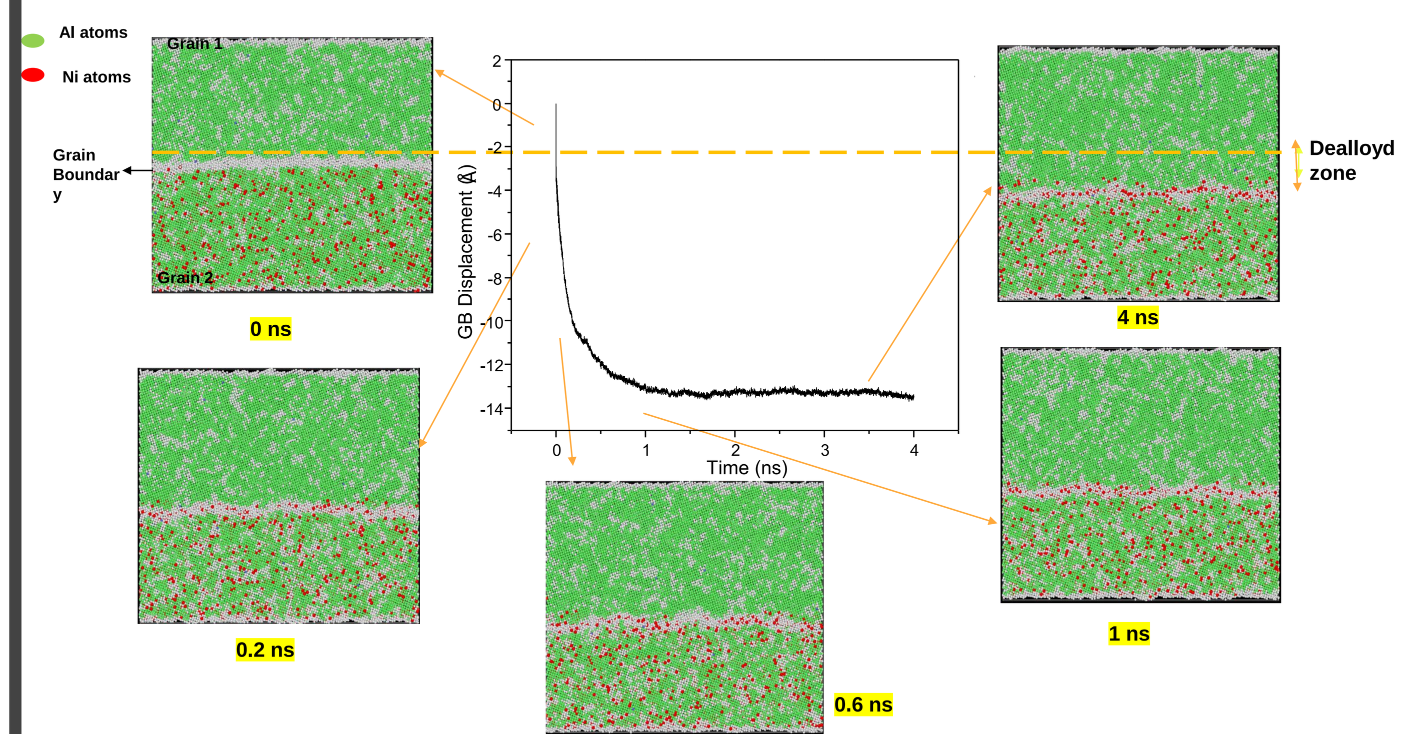
Effect of solute (Ni) concentration on GB displacement



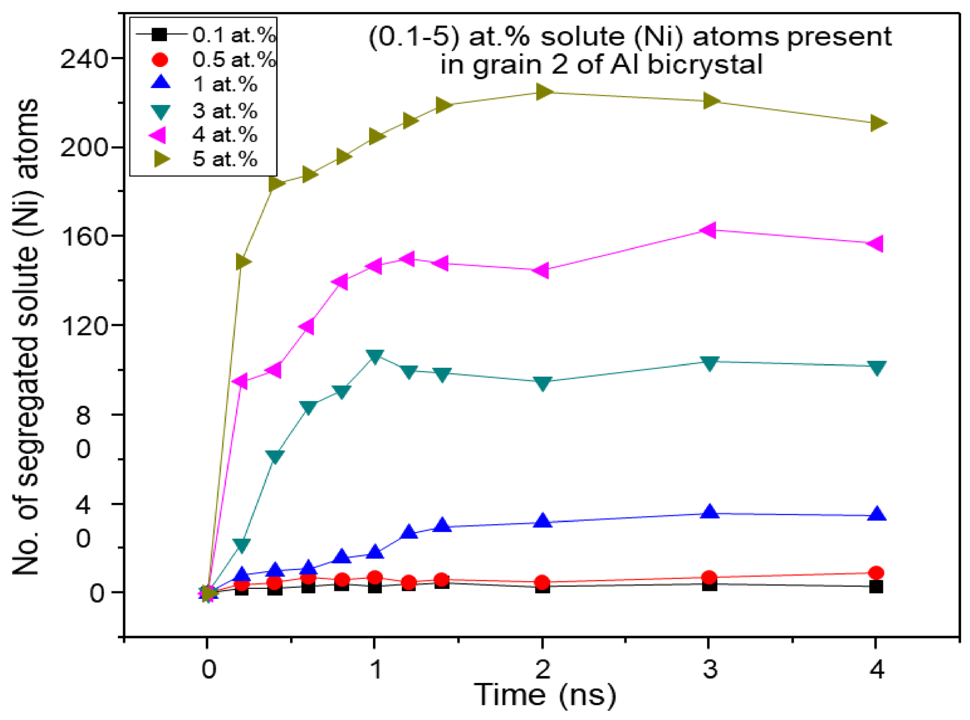
GB displacement increases with increase in solute concentration.

Atomic (View) of the mechanism

- When concentration of solute atoms fall below equilibrium due to solute depletion, GB moves toward solute atoms trying to regain equilibrium and creating a dealloyed zone in its wake.

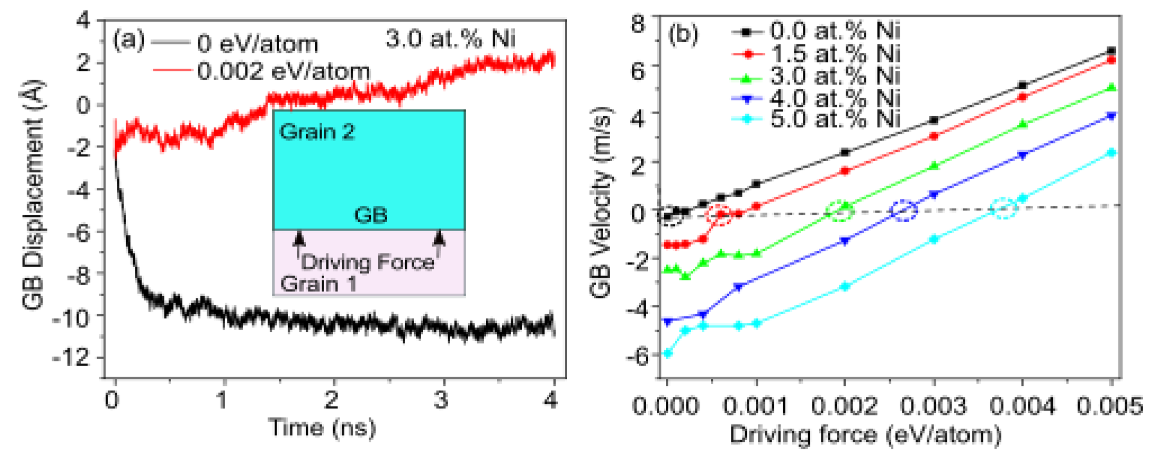


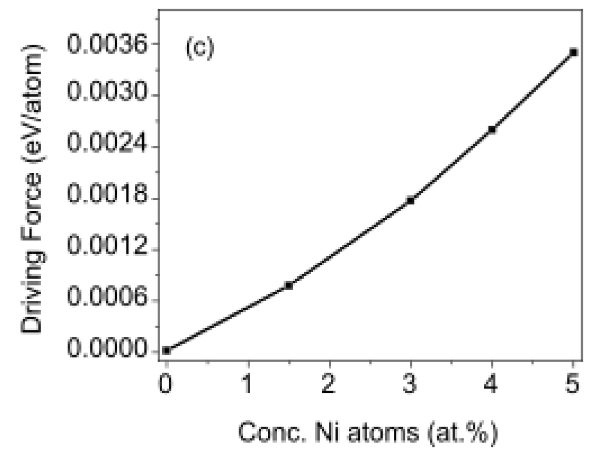
Effect of solute segregation on GB displacement



- Solute segregation increases as the grain boundary moves with time.
- No. of segregates solute atoms also increase with increasing concentration of solute atoms in grain 2 of Al bicrystal.

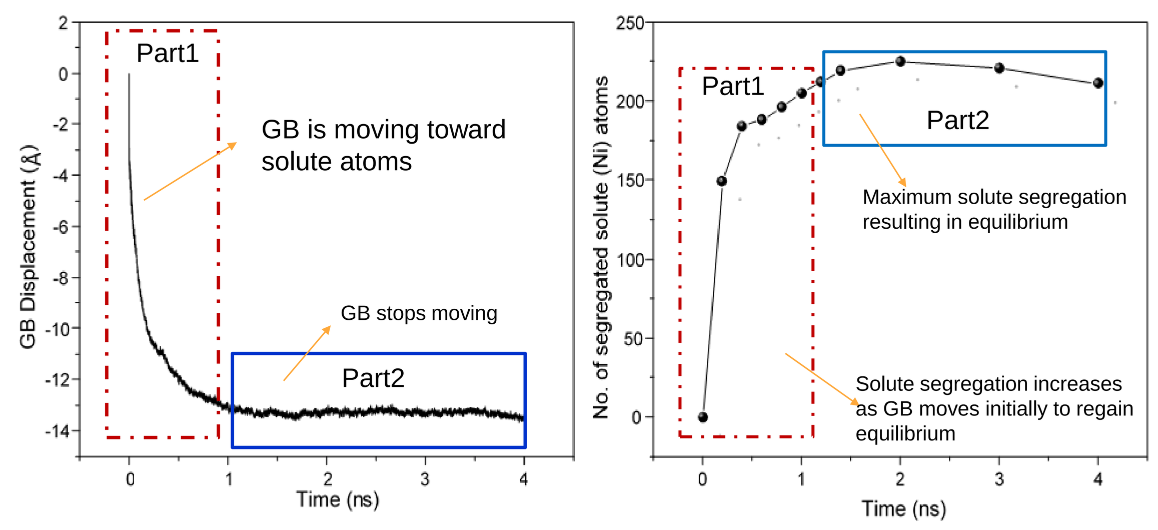
Driving force for DIGM

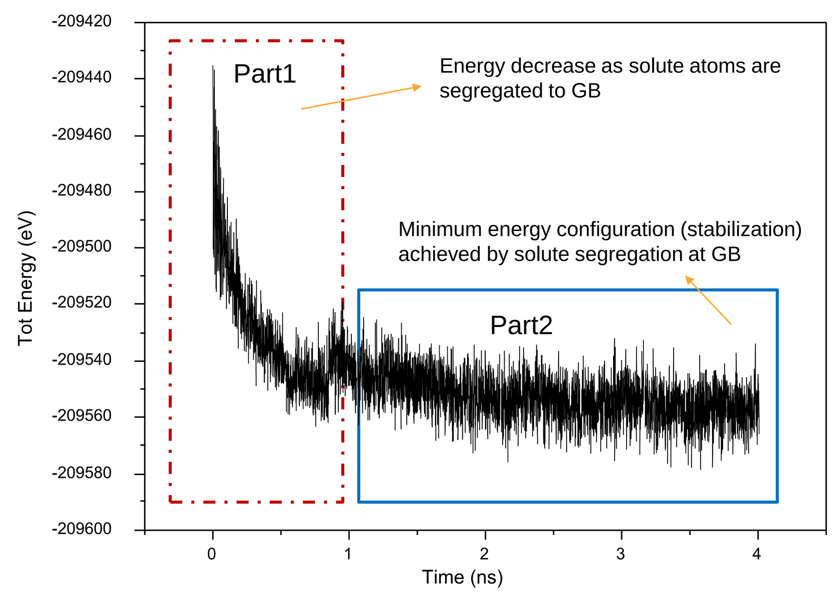




Driving force needed to move GB increases with increasing conc. of solute atoms.

Conclusions





- It is observed that when solute sink is present, depletion of GB solute content to below the equilibrium level (due to diffusion of solute from GB to sink), causes the boundary to move through high solute field to regain equilibrium thereby creating de-alloyed zone.
- Part 1. GB migration is driven by the need to reduce total energy of the system which is achieved by solute segregation.
- Part 2.This is dynamic process, continuing until the boundary has returned to its stabilized position and stops when equilibrium is regained.
- Segregation plays a crucial role in promoting DIGM.

Acknowledgement

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