Atomistic Simulations of Grain Boundary Diffusion in Magnesium

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Motivation

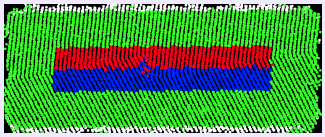
Grain boundary diffusion is a key mechanism that contributes to thermally activated evolution of microstructures. The predictability of microstructure evolution models depends critically on the availability of accurate estimates of kinetic parameters such as grain boundary diffusivity. The long-term goal of this research is to develop a database of kinetic parameters for magnesium alloys. The present effort represents the preliminary phase of this effort and focuses on computing the grain boundary diffusivity in magnesium bicrystals containing [10-10] tilt boundaries that are known to be present in high population. We specifically investigate three types of tilt boundaries - an asymmetric 34.2° boundary and a general 40.3° tilt boundary and a 34.2°symmetric tilt doundary. The calculated diffusion coefficient and the activation energies are compared with available experimental data.

Computational Methodology – Molecular Dynamics

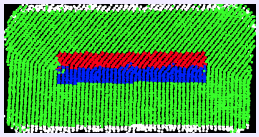
- The Sandia code LAMMPS code was for the simulations
- Bi-crystals generated by rotating single crystals to the required orientations and assembling them
- Initial energy minimization carried out using a low simulation anneal
- Bi-crystal then expanded uniformly in all directions using thermal expansion coefficient at the diffusion temperature and equilibrated at the highest temperature investigated (750K)

- The motion of free-surface atoms constrained to a plane parallel to the grain boundary
- Mean square displacement of atoms measured in a 2 -3 nm wide region centered on the grain boundary
- Grain boundary diffusion coefficient calculated from the slope of the mean square displacement versus time
- Activation energy for grain boundary diffusion calculated from an Arrhenius plot of the diffusion coefficient versus 1/T

34.2° asymmetric tilt boundary

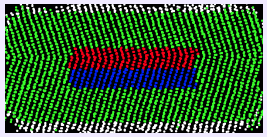


40.3° general boundary



Atomic structure of the asymmetric tilt (left) and general (right) boundary after expansion and equilibration at 750K. The red and blue atoms correspond to the ones used for measuring MSD. The white atoms at the free surface are constrained to move parallel to grain boundary

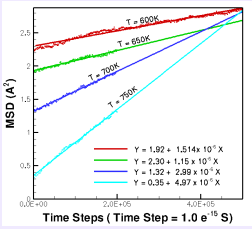
34.2° symmetric tilt boundary

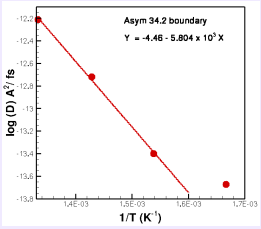


Atomic structure of the symmetric tilt boundary after expansion and equilibration at 750K.

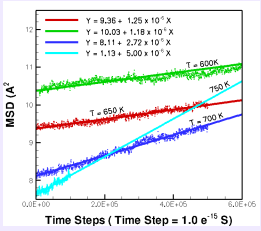
Calculation of Grain Boundary Diffusivity using MSD

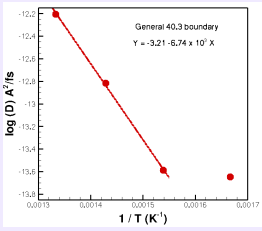
34.2° asymmetric tilt boundary



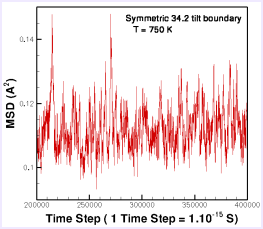


40.3° general tilt boundary





34.2° symmetric tilt boundary



Grain Boundary Type	Activation Energy (Cal/mole)	D at 750K (cm^2/s)
34.2 asymmetric	11,680	4.97×10^{-7}
40.3 general	13,480	5.0×10^{-7}
34.2 symmetric	----	-----

Summary

- The symmetric 34.2° boundary did not show any appreciable MSD at the highest temperature studied
- Both the asymmetric 34.2° boundary and the general 40.3° boundaries showed measurable MSD in the temperature range of investigation
- At higher temperatures, the boundaries were not stable; showed lateral migration and new facet formation
- At low temperatures (600K) the boundaries again showed facet formation and the MSD measurements are not reliable; therefore, the 600K measurements were not included in the MSD measurements
- The computed activation energies for the two tilt boundaries were roughly the same and the simulated diffusion coefficients at 750 K were at least three orders of magnitude higher than the value for polycrystalline magnesium at 741K experimentally measured by Shewman and Rhines (Trans. AIME, 1954).

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