A MODEL OF MIGRATING GRAIN-BOUNDARY GROOVES WITH APPLICATION TO TWO MOBILITY MEASUREMENT METHODS

Donghong Min
Ph.D. Candidate
Faculty Advisor: Dr. Harris Wong

ABSTRACT
A grain boundary intercepting a free surface forms a groove at the tip to reduce the combined surface energy. Previous work has solved the groove profile for grain boundaries that migrate at constant speed assuming small groove slopes. This work extends the analysis to finite slopes. Quasi-steady groove profiles developed by surface diffusion are computed by shooting methods. It is found that the grain-boundary tip is inclined in the migration direction. The inclination angle \( \theta \) depends on the supplementary dihedral angle \( \sigma \), and is found for \( 0 \leq \sigma \leq 180^\circ \). An asymptotic solution is derived in the limit \( \sigma \to 0 \) that agrees with the numerical results. The inclination angle \( \theta(\sigma) \) applies to the "quarter-loop" and Sun-Bauer methods of measuring grain-boundary mobility. In both cases, we not only capture known features, but also make new predictions.

Figure 8 Comparison of two Sun-Bauer experiments with theory. The NaCl grain boundary is taken from Fig. 2 (b) of Sun and Bauer [5]. The Fe-3%Si grain boundary comes from Fig. 2 (\( \Sigma 9, 600 \)) of Tsurekawa et al. [6]. The inclination angles \( \theta \) and \( \beta \) are first measured from the figures and then adjusted slightly for better fitting. For the NaCl grain boundary \( \theta = 30^\circ \) and \( \beta = 60.3^\circ \), and for the Fe-3%Si grain boundary, \( \theta = 18^\circ \) and \( \beta = 78.9^\circ \). Predictions of the Sun-Bauer model (\( \theta = 0 \)) are also plotted in dashed lined. To conform to the traditional way of viewing grain boundaries, \(-y\) is plotted against \(-x\).

Figure 4. (a) Groove surface angles \( \alpha_+ \) and \( \alpha_- \) and grain boundary inclination angle \( \theta \) (Fig. 2(a)) as functions of the supplementary dihedral angle \( \sigma \). The asymptotic solutions in (16), (17) and (21) obtained in the limit \( \sigma \to 0 \) agree well with the numerical predictions, even at \( \sigma \) close to \( 180^\circ \). (b) Normalized surface depth \( Y_0 \), curvature \( C_0 \), and mass

\[ \sigma(\theta) \]
flux $M_0$ at the groove root as functions of the supplementary dihedral angle $\sigma$. The asymptotic solutions in (18), (19) and (20) are obtained in the limit $\sigma \to 0$.

ACKNOWLEDGMENTS

This work was supported by NSF under the CAREER program (DMR-998450 to HW) and by the Louisiana Board of regents through the Research Competitiveness Subprogram (LEQSF1999-02-RD-A-21 to HW). Acknowledgment is also made to the Donors of The Petroleum Research Fund, administered by the American Chemical Society (PRF#34049-G5 to HW).

REFERENCES