FINAL TECHNICAL REPORT

Project Title: Development of integrated methodology for thermomechanical processing of Al alloys

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Recipient: Drs. Ben Q. Li and Dave Field, School of Mechanical and Materials Engineering, Washington State University, Pullman, WA 99164

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Executive Summary:

The objective of the research project is to develop an integrated methodology for modeling local structural evolution during thermomechanical processing of rolled aluminum sheet for alloy design and manufacturing. The integrated methodology resulting from this project provides a computer-aided, science-based tool to the engineers in the aluminum industry for the design of alloys and their processing systems that have been considered over-engineered at a substantial energy and material cost to aluminum producers. The development of the integrated methodology is based on finite element modeling of large scale plasticity deformations, with full integration of thermomechanical and microstructural models for process understanding and design sensitivity analyses. The models, either individual or integrated, are validated performance through experimental measurements in a small experimental forging press. The project has resulted in an enhanced fundamental of the physics of deformation and structure development will result in the opportunity to reduce alloy content, minimize processing steps, and improve performance of existing products. The project was carried out in close collaboration with the Aluminum Company of America (Alcoa). Four students were trained through this project, and graduated at the end of this project: two with Ph.D. and two with M.S. degrees. These

students now are working as researchers or research fellows at other Universities and/or private companies in the United States. The integrated model, obtained from this research project, is now being used by engineers at Alcoa and researchers at other metal deformation research centers to help design novel Al alloys and processing systems that provide substantial energy and material savings to aluminum producers.

Comparison of Actual Accomplishments with the Goals of the Project:

The work was performed based on the subtasks that are defined to achieve the goals and objectives of the project. The table below compares the performance of the work tasks with the goals. As it can be seen from the table, all the tasks, as proposed and defined in the final contract, were performed and finished satisfactorily for this project.

ID Number	Task / Milestone Description	Planned Completion	Actual Completion	Comments
Sub_T1	Build crystal plasticity into the FEM code	9/30/02	10/5/02	
Sub_T2	Develop first order constitutive model	9/30/02	9/31/02	
Sub_T3	Select recrystallization models	7/31/02	8/15/02	
Sub_T4	Compare deformation model with experiments	7/31/02	9/30/02	
Sub_T5	Integrate FEM/Microstructure models	9/30/03	12/31/03	
Sub_T6	Refine integrated model through iteration	9/30/03	10/15/04	
Sub_T7	Verify recrystallization models by experiments	9/30/03	9/30/03	
Sub_T8	Implement parallel computing scheme	12/31/03	12/31/03	
Sub_T9	Refine the structure evolution models	5/15/05	5/15/05	
Sub_T10	Optimize the parallel computations	8/15/04	8/05/04	
Sub_T11	Verify integrated model by additional experiments	5/15/05	7/15/05	
Sub_T12	Outline plans to including chemistry effect in the model	5/15/05	7/15/05	

Summary of Project Activities:

This project is aimed at developing an integrated methodology for modeling metal rolling or extrusion processes in order to design better aluminum alloys. The developed integrated methodology involves the coupling of thermomechanical deformation mechanics with materials microstructure evolution during deformation processing. The development is based on our current understanding of the interaction between macro and micro mechanics that governs the deformation processes. The approaches are based on the solution of mechanical equilibrium equations governing the plastic deformation processes by the use of non-linear finite element method, taking into account the geometric and kinematic effects caused by the large deformation, which occurs in extrusion and rolling processes. Materials microstructure models are developed based on the internal state variable approaches as well as micromechanics based on the dislocation and crystal plasticity. The parameters for materials models are obtained from the experimental measurements. The materials models, which occur at local scale, are coupled with the macroscale finite element model, through macro/micro coupling. Extension

numerical simulations were made using the coupled model. To validate the model predictions, channel die experiments were conducted for both single and polycrystal samples. Experimental measurements are compared well with the predictions for samples with single crystal. The comparisons of the model predictions with the measurements on polycrystal samples and real samples taken from rolling processes are considered reasonably good, as shown in Figures 1-2 below. Additional results are published in literature, which can be found in the session of publications below. The detailed assumptions, methods and experimental procedures used in this project also can be found in these publications.

Figure 1a. Schematic of channel die deformation setup with relative positions of the single crystal and multicrystal specimens. The mating surfaces are those that were polished for characterization.

Figure 1b. The bi-crystal aluminum specimen used in the channel die experiments.

Figure 1c. Comparison of measurements and predictions from integrated macro/micro finite element model for Grain A of bi-crystal sample from 0 to 10% deformation: a) Experimental measurements, b) Asaro's hardening model, c) Power law model, d) Bassani's model.

Figure 2a. Initial random orientations of 500 grains - (111) pole figure

Figure 2b. Plane strain compression texture obtained after 60% deformation

Products developed under the award:

a) Publications:

- 1) PB Trivedi, DP Field, RS Yassar, and R Alldredge, "Microstructural evolution and observed stress response during hot deformation of 5005 and 6022 Al alloys," Mat. Sci. Eng, A 425 (2006) pp. 205-212.

- 2) R.S. Yassar, D.P. Field, and H. Weiland, "TEM and DSC Studies on the precipitation sequence in an Al-Mg-Si alloy; AA6022," *J. Mat. Res.* 20 (2005) pp. 2705-2711.
- 3) R.S. Yassar, D.P. Field, and H. Weiland, "The Effect of Cold Deformation on the Kinetics of the Precipitates in an Al-Mg-Si Alloy," *Metall. Mater. Trans.* 36A (2005) pp. 2059-2065.
- 4) R.S. Yassar, D.P. Field, and H. Weiland, "The effect of predeformation on the β' and β'' precipitates and the role of Q' phase in an Al-Mg-Si alloy; AA6022," *Scripta Materialia* 53 (2005) pp. 299-303.
- 5) R. Prasannavenkatesan, B.Q. Li, D.P. Field, and H. Weiland, "A Parallel Macro/Micro Elastoplasticity Model for Aluminum Deformation and Comparison with Experiments," *Metall. Mater. Trans.* 36A (2005) pp. 241-256.
- 6) D.P. Field, P. Trivedi, S.I. Wright, and M. Kumar, "Analysis of Local Orientation Gradients in Deformed Single Crystals," *Ultramicroscopy*, 103 (2005) pp 33-39.
- 7) R.S. Yassar, P. Trivedi, and D.P. Field, "Characterization of Dislocation Structures in the Presence of Precipitates in Precipitation Hardening Aluminum Alloys," in *Proceedings of Second International Conference on Multiscale Materials Modeling*, N.M. Ghoniem, Ed, UCLA publishing, 2004, pp. 198-200.
- 8) R.S. Yassar and D.P. Field, "Influence of Predeformation on Precipitation Kinetics and Aging Behavior of the AA6022 Alloy," *TMS Letters*, 1 (2004) pp. 83-84.
- 9) P.B. Trivedi and D.P. Field, "Experimental Analysis of Local Orientation Gradient using EBSD," *TMS Letters*, 1 (2004) pp. 9-10.
- 10) P. Trivedi, D.P. Field and H. Weiland, "Alloying Effects on Dislocation Substructure Evolution of Aluminum Alloys," *Intl. J. Plasticity*, 50 (2004) pp. 459-476.
- 11) D.P. Field, S.I. Wright, and P. Trivedi, "Microtextural Analysis of Grain Fragmentation in Aluminum," *Mater. Sci. Forum*, Vols. 426-432, (2003) pp. 3739-3744.
- 12) R. Prasannavenkatesan, B.Q. Li, D.P. Field and H. Weiland, "A Finite Element Model for Crystal Plasticity During Large Deformation and Comparison with Experimental Measurements," in *Hot Deformation of Aluminum Alloys III*, Edited by Z. Jin, A. Beaudoin, T. Bieler, and B. Radhakrishnan, TMS, Pittsburgh, 2003, pp. 279-288.
- 13) P. Trivedi, D.P. Field, and H. Weiland, "Effect of alloy chemistry on microstructural evolution during deformation of Al alloys," in *Hot Deformation of Aluminum Alloys III*, Edited by Z. Jin, A. Beaudoin, T. Bieler, and B. Radhakrishnan, TMS, Pittsburgh, 2003, pp. 51-59.
- 14) B.Q. Li, *Discontinuous Finite Element Method in Computational Fluid Mechanics and Heat Transfer*. Springer-Verlag, January, 2006, 578 pages.
- 15) R. Akarapu, B. Q. Li and A. Seagall, "A thermal stress and failure model for laser cutting and forming operations," *J. Failure Analysis Prevention*, Vol. 45, 2004, pp. 45-56.
- 16) R. Akarapu, B. Q. Li and A. E. Segall, "A 3-D model for thermal ablation and stress evolution during laser machining," *National Heat Transfer Conference*, Las Vegas, July, 2003, Paper #: HT2003-40298.
- 17) R. Akarapu, B. Q. Li and A. E. Segall, "Finite element modeling of ablation phenomena and thermal stress evolution during a unique application of dual laser cutting of ceramics," *Energy Efficient Manufacturing Processes, Fourth MPMD International Symposium on Global Innovations (Ed. I. Anderson, T. Marechaux, and C. Cockrill)*, *TMS Annual Conference*, San Diego, CA, 20003, pp. 87-98.

b) **Students:**

The work has produced 2 Ph.D. dissertations and 2 M.S. theses. These students are now employed either by the other U.S. universities as senior researchers or research fellows or by the U.S. companies as engineers.

c) **Collaborations Fostered:**

The work has helped strengthen the collaboration between Drs. Ben Q. Li and David Field at Washington State University with researchers at Alcoa. Routine meetings between research team at Washington State University and Alcoa were held. Students went to work as summer intern at Alcoa. The models developed are now also being used by Alcoa researchers for the purpose of developing new aluminum alloys and alloy processing technologies.

d) **Other Products:**

The channel die deformation equipment, developed and used for this project, is now part of the materials lab equipment for both education and research at Washington State University.