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Quarterly Management Document – FY17, 1st Quarter, Physics-based Creep Simulations of Thick Section Welds in High Temperature and Pressure Applications

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Quarterly Management Document – FY17, 1st Quarter, Physics-based Creep Simulations of Thick Section Welds in High Temperature and Pressure Applications

Document # INL/EXT-17-40950

WBS Element	Project Title	Contract Number	Contract Start	Contract End
C.B.10.02.02.40	Physics-based Creep Simulations of Thick Section Welds in High Temperature and Pressure Applications	FEAA90	10/01/16	09/30/2017
Performer Name and Address Thomas Lillo Idaho National Laboratory P.O. Box 1625 Idaho Falls, ID 83415			**Principal Investigator(s)** Thomas Lillo	

BUDGET AND COST REPORT

Prior Year Funds ($K)				**56**								
Total Current Year Commitment ($K)				**361**								
Projected Current Year Costs ($K)				**317**								
	O	**N**	**D**	**J**	**F**	**M**	**A**	**M**	**J**	**J**	**A**	**S**
Planned Costs	**15**	**15**	**15**	**23**	**25**	**33**	**28**	**28**	**30**	**35**	**35**	**35**
Actual Costs	**14.4**	**7.9**	**14.8**									
Variance	**0.6**	**7.1**	**0.2**									

MILESTONE REPORT

Milestone Designation	Milestone Description	Due Date	Revised Due Date	Completion Date
A	Evaluate current MOOSE capabilities	09/30/2015		09/30/2015
B	Complete Alloy 617 weld characterization	10/30/2015		11/18/2015
C	Receipt of Alloy 740H plates	10/30/2015		11/05/2015
D	Complete welds in Alloy 740H	11/16/2015	7/31/2016	7/31/2016
E	Characterize Alloy 740H welds	02/01/2016	09/30/2016	9/02/2016
F	Creep model development – Stage 1	09/30/2016		9/30/2016
G	Creep Model Development – Stage 2	8/29/2017		

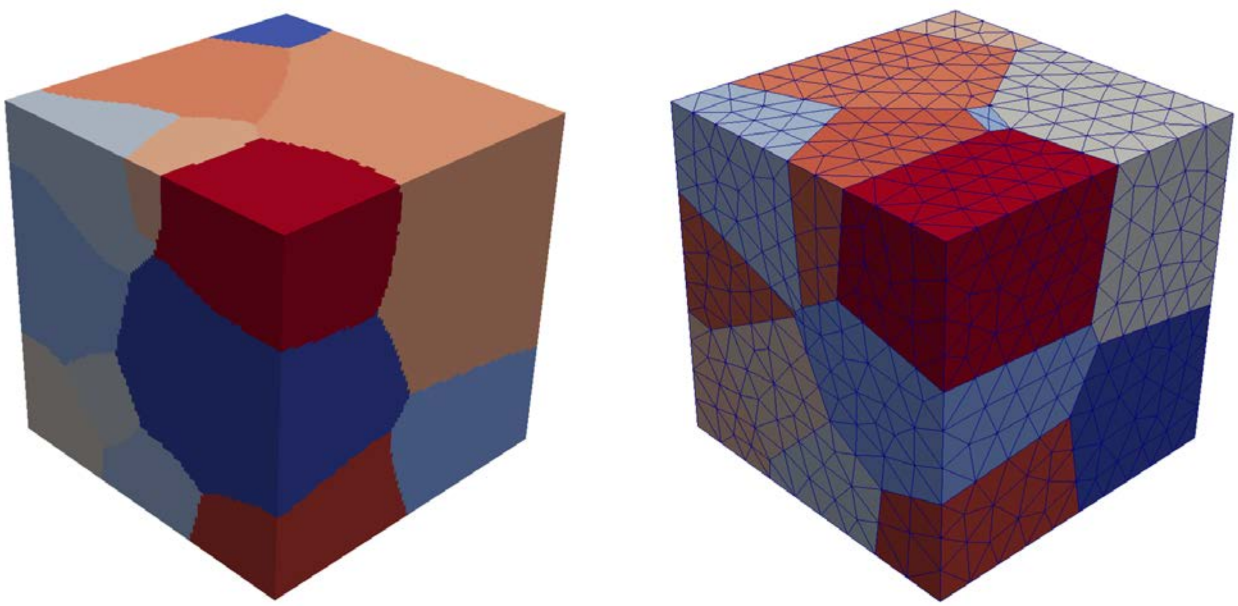
H	Calibration of Secondary creep	9/30/2017		
I	Stress Drop Tests	2/01/2017	9/30/2017	
J	Characterization of creep failure mechanisms	4/01/2017		

TECHNICAL HIGHLIGHTS

Milestone G, "Creep Model Development – Stage 2"

This will include generation of synthetic microstructures in the weld, heat affected zone and base metal based on the experimental characterization of the Alloy 740H welds that was started in FY16. The Orowan loop model for dislocation/γ' particle interactions will be implemented. Presently a model exists in Grizzly within the MOOSE architecture. We will re-implement the model in the user-object based CP model. Incorporation of the evolution of γ' particles will be handled through scalar equations and will be coupled to the material models by evolving the volume fraction and channel width parameters. This γ' evolution model will be compared to the aged base metal and weld metal. A summary of the first quarter efforts is given below.

1. Preliminary work on generation of synthetic microstructures



(a) (b)

Figure 1. Microstructure generation and meshing: (a) microstructure generated in DREAM.3D (b) volume mesh.

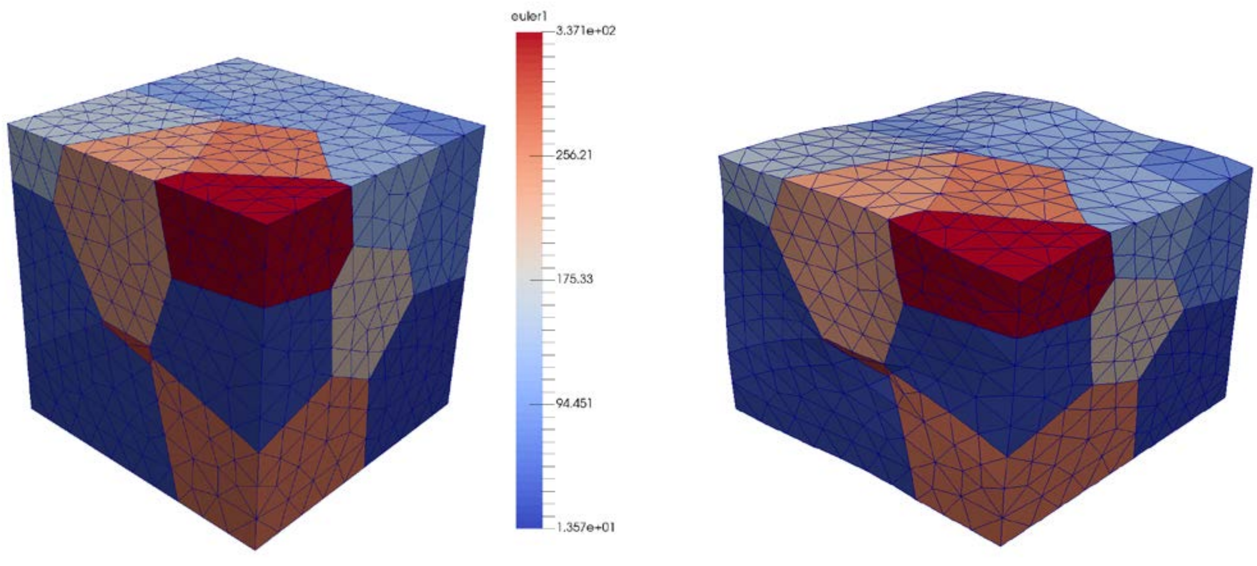
DREAM.3D [1] software will be used to generate synthetic microstructures using experimentally characterized microstructure morphological and crystallographic statistics. Grain size, distribution and orientation collected from microstructure observations will provide inputs for DREAM.3D to generate statically equivalent polycrystalline structures, see Figure 1(a).

The Voro++ software [2] will be used to carry out three-dimensional computations of the Voronoi tessellation based on the grain centroids coordinates taken from DREAM.3D. A meshing script will then utilize the outputs from Voro++ and generate a volume mesh of the microstructure using Cubit [3], see Figure 1 (b).

This discretization work flow (DREAM3D → Voro++ → Cubit) will be used to generate synthetic microstructure of Alloy 617 and 740H welds based on the information obtained from SEM and OIM microstructure characterization techniques.

2. Numerical Examples

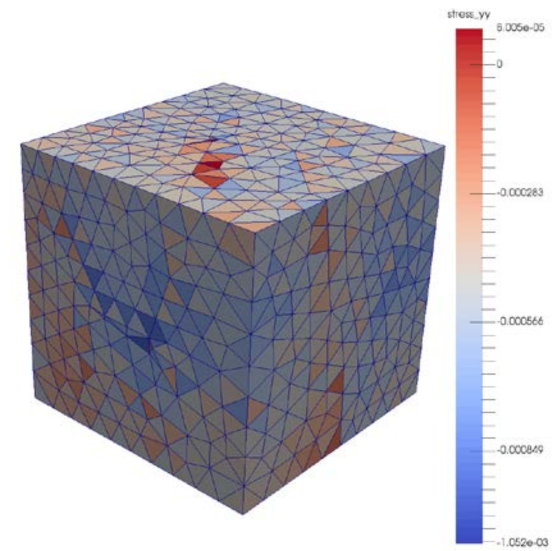
Several numerical robustness issues are raised when the crystal plasticity model applies to polycrystalline microstructures. Efforts have been made to resolve these issues. A cube of size 20x20x20 μm^3 with 18 grains is used to verify the dislocation density model of the glide component. A pressure of 500MP is applied on the top surface and symmetric boundary conditions are used to restrain the rigid body motion. Random orientations are assigned to every grain as shown in Figure. 2(a). The deformation is shown in Figure. 2(b).



(a) (b)

Figure 2: (a) Euler angle 1 component θ in the representative polycrystalline microstructure. (b) Deformation (exaggerated by 25 times).

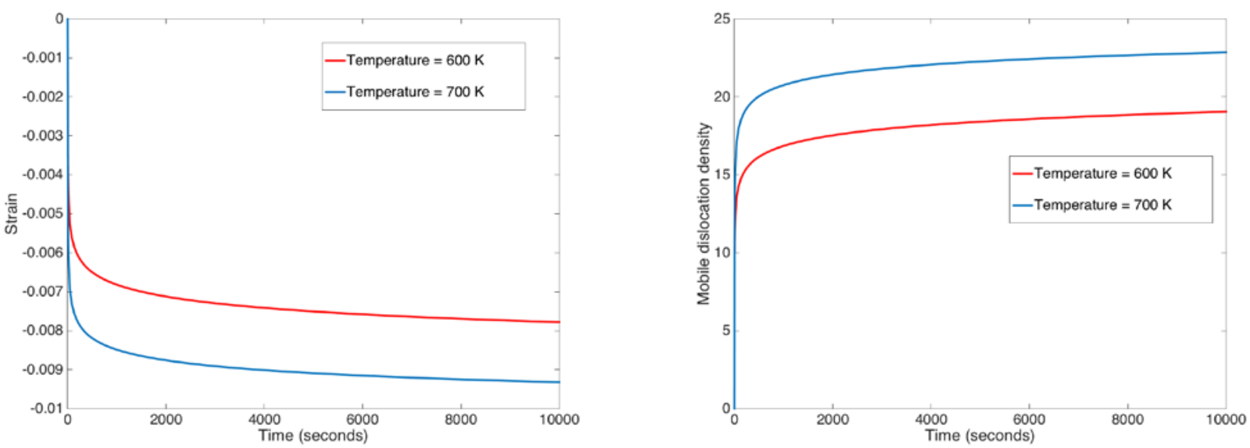
The effect of grain orientation and strain compatibility leads to heterogeneous distribution of stress and plastic strain as shown in Figure. 3.



(a) (b)

Figure 3: Response at time = 10,000 seconds: (a) Stress and (b) plastic deformation gradient component normal to loading direction.

The creep strain and mobile dislocation density evolution on (11-1)[011] system for all the grain are shown in Figure. 4. As can be seen from the figure, with increasing temperature, the glide slip rate at initial stages is higher. This is due a larger thermal activation for glide at higher temperatures. The mobile dislocation density is higher with increasing temperature.



(a) (b)

Figure 4: Creep at stress 500 MPa and temperature 600K and 700K. (a) Creep strain; (b) Mobile dislocation density (11-1)[011] system.

References:

[1] Groeber M and Jackson M, DREAM.3D: a digital representation environment for the analysis of microstructure in 3D. Integr. Mater. Manuf. Innov: **3** 5-19, 2014

[2] Chris H. Rycroft, Voro++: A three-dimensional Voronoi cell library in C++, Chaos **19**, 041111, 2009.

[3] CUBIT, Geometry and Mesh Generation Toolkit, https://cubit.sandia.gov

Milestone H, "Calibration of Secondary creep"

The secondary creep rate data obtained from existing creep data on Alloy 617 will be used to assess the accuracy of the model and then calibrate the model. Work is not scheduled to start on this task until 7/2017 after significant progress has been made on Milestone G.

Milestone I, "Stress Drop Tests"

The effectiveness of γ' particles at pinning mobile dislocations and, thus, imparting creep resistance is dependent on γ' particle size and volume fraction. Stress drop tests are used to evaluate the threshold stress generated by the γ' particle distribution. Long term service can lead to coarsening of the γ' particle distribution and may also alter the volume fraction of particles present, both of which alter the threshold stress and, therefore, the creep behavior. In order to accurately model and simulate creep behavior, threshold stress as a function of particle size and volume fraction must be determined. To this end base metal is being aged at 750ºC for 4000 and 8000 hours to generate different γ' particle distributions. The threshold stress for these two γ' particle sizes and the initial post-weld heat treated γ' particle size will be determined. Aging of a sufficient amount of material was begun in the 4th quarter of FY16 and is scheduled to be removed according the information in Table 1. Again, the goal of this aging treatment is to produce base metal with significantly different γ' particle sizes (and, perhaps, volume fractions) so that the dependency of the threshold stress on γ' particle size can be determined and incorporated into the simulation of welded material. This relationship will be used in the simulation of long term creep behavior where the γ' particle size is coarsening in base metal, weld metal and heat affected zone. This data will yield the threshold stress as a function of γ' particle size.

The due date for this milestone was moved to a later date due to a late start in the aging of base metal. The first material, SD-1 in Table 1 was originally planned to be removed after 4500 hours while the second material, SD-2, was originally planned to be removed after 8800 hours. However, due to the late start on aging, the duration for SD-1 will be aged only 4000 hrs while SD-2 will be only aged for 8000 hrs, to allow for fabrication of samples and stress drop testing prior to the end of the fiscal year. Stress drop testing of SD-1 is expected to commence 6-8 weeks after aging is complete (aging projected to be complete on 2/15/2017 in Table 1).

Table 1. Base Metal Aging Information for Stress Drop Tests

Sample ID	Aging Temperature	Target Aging Time, hours	Insertion Date	Expected Removal date
SD-1	750	4000	9/1/2016	2/15/2017
SD-2	750	8000	9/1/2016	7/31/2017

Milestone J, "Characterization of creep failure mechanisms"

As of the end of the first quarter, six creep tests have been completed, see Table 2. They are being prepared for optical metallography and characterization of these samples using optical metallography and SEM will start early in the second quarter of FY17.

Other highlights

Short Term Creep Tests
Shorter term creep testing of welded Alloy 740H for development of model parameters is continuing and six tests have been completed with one currently running, 740-Q1-06 at 700°C and 395 MPa. Upon arrival of the FY17 funding additional creep samples will be fabricated from the welds made in the 4th quarter of FY16. Eighteen cross weld creep samples will be made as well as four all-weld metal samples will be made to finish off the test matrix in Table 2. (Some creep tests with conditions that duplicate some of the tests in Table 2 will be run to assess variability of the creep behavior, due possibly to weld defects which can range in size and number from sample to sample.)

Table 2. Short term creep testing parameters for modeling development

Specimen ID	Test temperature, °C	Test type	Initial Stress, MPa	Orientation	Expected rupture life, hrs	Start date	Finish date	Rupture life, Hrs
740-Q1-01	700	Rupt	413	CW*	200	8/24/2016	9/21/2016	639
740-Q1-08	700	Rupt	413	CW	500	11/28/2016	12/27/2016	670.8
740-Q1-06	700	Rupt	395	CW	1000	01/09/2017		
	700	Rupt	344	CW	1000			
740-Q1-03	750	Rupt	350	CW	200	9/29/2016	10/07/2016	184
740-Q1-05	750	Rupt	305	CW	500	10/18/2016	11/06/2016	450
	750	Rupt	213	CW	1000			
740-Q1-04	800	Rupt	240	CW	200	10/10/2016	10/15/2016	123.6
740-Q1-02	800	Rupt	200	CW	500	11/08/2016	11/22/2016	326.8
	800	Rupt	138	CW	1000			
	700	Rupt	400	AWM**	500			
	750	Rupt	248	AWM	500			
	800	Rupt	144	AWM	500			

* CW = Cross weld
** AWM = All Weld Metal

Long Term Creep Tests
Presently, two long term creep tests are underway for verification of the final creep simulation. The test at 800°C and 83 MPa has surpassed 3500 hours (the expected rupture time is on the order of 9700 hours) while the test at 750°C and 141 MPa has surpassed 3600 hours (the expected rupture time is also on the order of 9700 hours).

γ' Aging Study
Aging of welds at 700, 750 and 800°C continues. Table 3 summarizes the current progress on aging. TEM samples will be made from base metal, weld metal and metal in the heat affected zone at each aging time and temperature Table 3. The γ' size, morphology and volume fraction will be characterized to understand

coarsening behavior during extended times at elevated temperatures. Changes in size, shape and volume fraction can have a significant impact on creep behavior which will need to be addressed in the developing creep simulations with the coarsening relationships documented under this task. Characterization efforts will begin early in the second quarter of FY17.

Table 3. Aging Conditions for γ' Coarsening Study

Aging Temperature, °C	Aging Time, hrs	Insert Date	Removal Target date	Date/time out	Actual aging hours
700	50	9/6/2016 8:56	9/8/2016 10:56	9/8/2016 10:55	50.0
	100	9/12/2016 9:34	9/14/2016 11:34	9/14/2016 11:30	99.9
	200	9/22/2016 9:35	9/26/2016 13:35	9/26/2016 13:38	200.0
	400	9/29/2016 9:15	10/7/2016 17:15	10/7/2016 15:00	397.7
	1000	10/13/2016 8:20	11/7/2016 8:20	11/4/2016 8:45	926.1
	3000	11/14/2016 10:39	2/8/2017 20:31		
	6000				
	10000				
750	50	9/6/2016 8:56	9/8/2016 10:56	9/8/2016 10:56	50.0
	100	9/12/2016 9:34	9/14/2016 11:34	9/14/2016 11:30	99.9
	200	9/22/2016 9:35	9/26/2016 13:35	9/26/2016 13:38	200.0
	400	9/29/2016 9:15	10/7/2016 17:15	10/7/2016 15:00	397.7
	1000	10/13/2016 8:20	11/7/2016 8:20	11/4/2016 8:45	926.2
	3000	11/14/2016 10:39	2/8/2017 20:30		
	6000				
	10000				
800	50	9/6/2016 8:56	9/8/2016 10:56	9/8/2016 10:56	50.0
	100	9/12/2016 9:34	9/14/2016 11:34	9/14/2016 11:30	99.9
	200	9/22/2016 9:35	9/26/2016 13:35	9/26/2016 13:38	200.0
	400	9/29/2016 9:15	10/7/2016 17:15	10/7/2016 15:00	397.7
	1000	10/13/2016 8:20	11/7/2016 8:20	11/4/2016 8:45	926.2
	3000	11/14/2016 10:39	2/8/2017 20:30		
	6000				
	10000				

ISSUES

Funding issues in FY16 and, to a lesser extent, FY17 have adversely impacted schedule and some task completion dates have been pushed back while the impact on the completion dates of other tasks is being evaluated.

Report Prepared By	Date
Thomas M. Lillo	01/27/2017