Modeling of M23C6 Carbide Precipitation in Relation to Ductility Dip Cracking Alloy 690

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1. Problem Statement

- DDC is a solid-state cracking phenomenon known to form during multi-pass welding of austenitic alloys.
- The exact mechanism is still in discussion, but susceptible materials exhibit a solid-state Ductility Dip Temperature range.
- Alloy 690 is a nickel-based alloy used in fabrication of nuclear reactors that exhibits DDC in multipass welds.

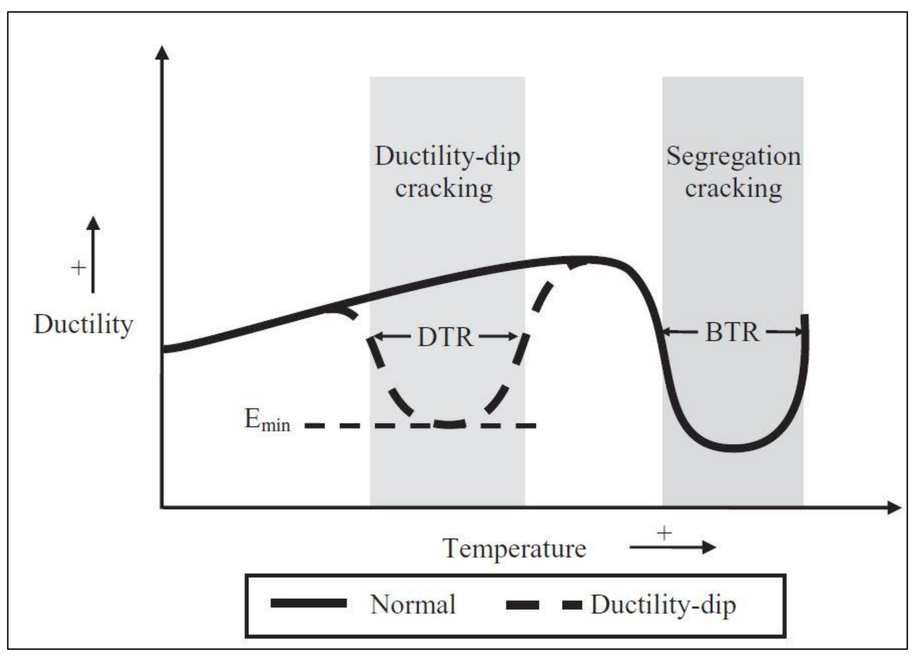


Figure 1: Ductility vs. temperature graph for a material prone to DDC [1].

- It has been theorized that sulfur and phosphorous segregate at the grain boundary during welding and contribute to DDC formation or propagation.[2-3]
- Model the microstructural dynamic precipitate behavior of Nickel-based alloy 690 during transient thermal cycles

2. Computational Modeling Procedures

- To supplement future experimental results a precipitation modeling of Alloy 690 was conducted in Thermo-Calc's Prisma module.
- Two different thermal cycles were used in the simulation: 1) a thermal history of a multi-pass weld in alloy 690 shown in Figure 2 and 2) a 2 hour hold in the DDC temperature range, shown in Figure 3.
- The DDC hold thermal cycle was simulated with three different hold temperatures: 850C, 900C, and 1000C.
- DIS_FCC_A1, the disordered austenite phase, was selected as the matrix phase with the M23C6 carbide as the sole precipitate.
- The carbide was selected to form along grain boundaries, and with an interfacial energy of .207 J/m^2 [4].
- A simplified elemental composition of alloy 690 was used.

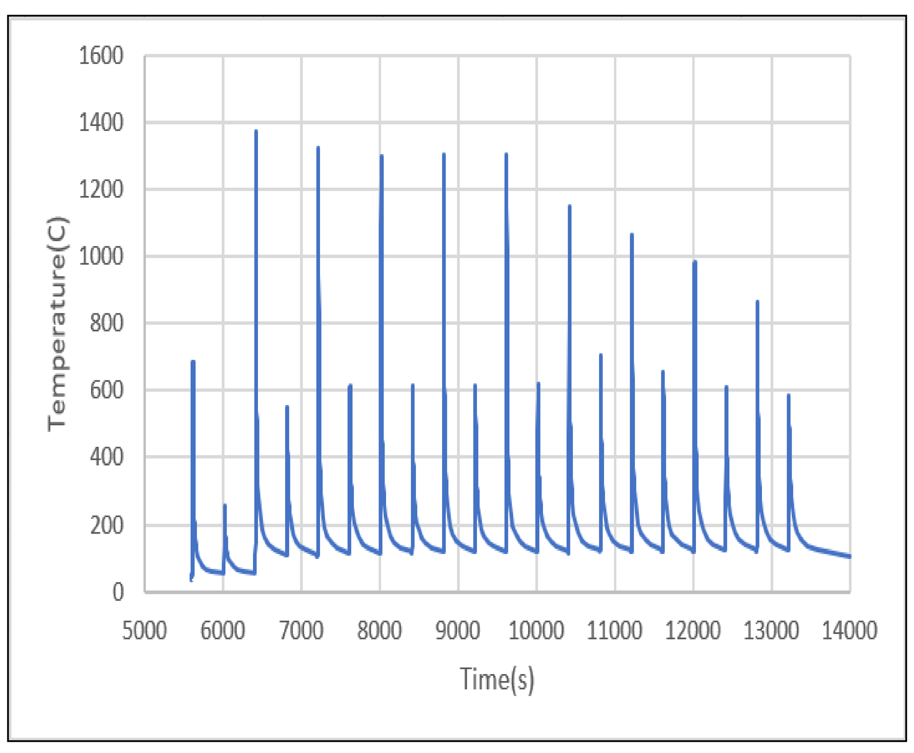


Figure 2: Thermal history generated SysWeld model

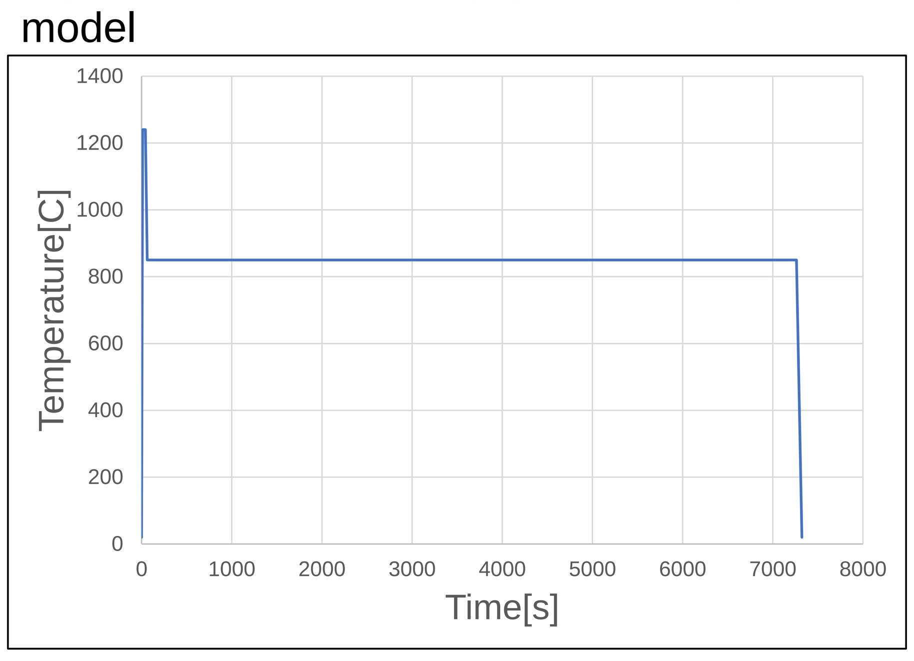


Figure 3: Thermal cycle for a hold in the DDC range at 850C

Simplified Composition of Alloy 690 (wt-%)			
Nickel	Iron	Chromium	Carbon
58.735	10.54	30.68	0.045

Table 1

3. Results

DDC Hold Thermal Cycle

Figure 4: M23C6 Critical Radius at 850C

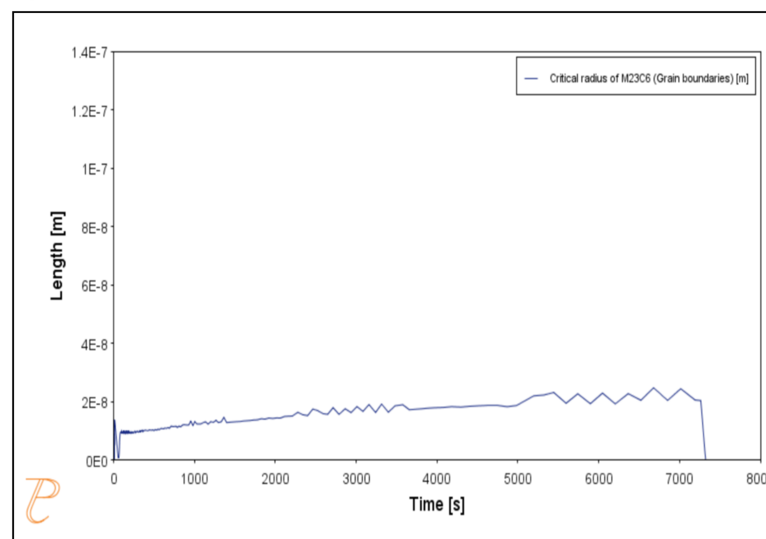
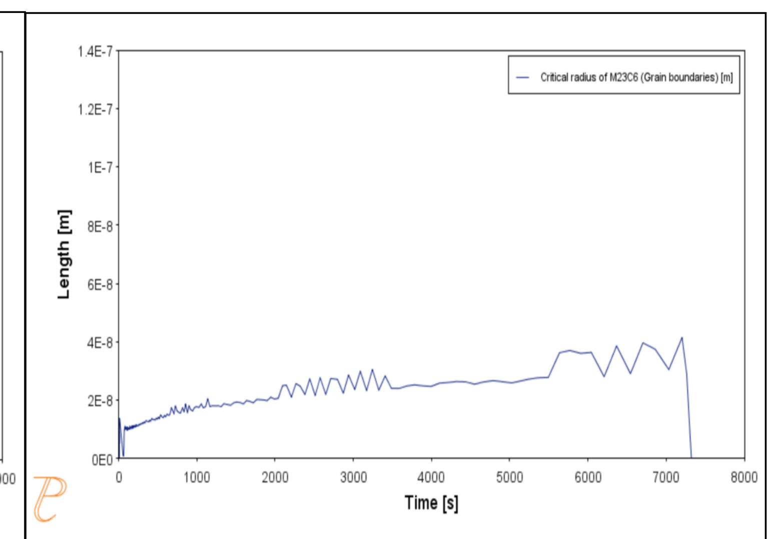


Figure 5: M23C6 Critical Radius at 900C



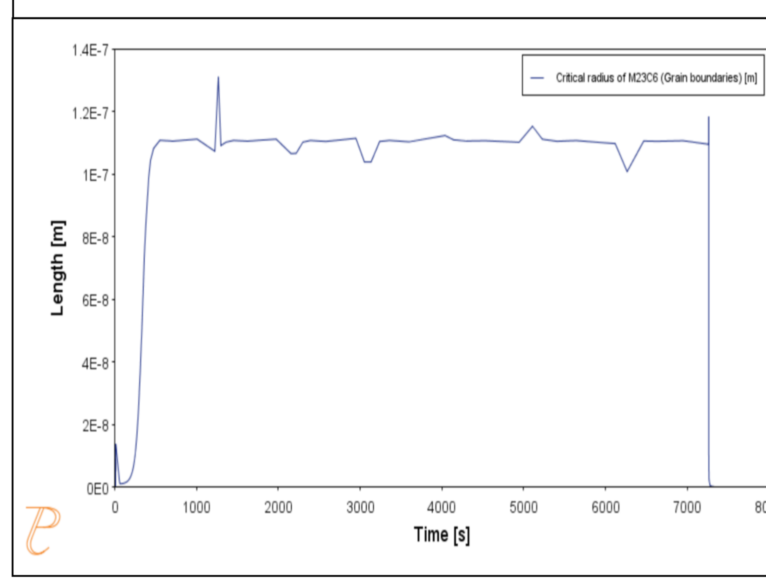


Figure 6: M23C6 Critical Radius at 1000C

- The critical radius is the required radius length for a particle to be stable.
- The critical radius of M23C6 particles, and the particles size increased with increasing hold temperature.
- The time taken for reaching critical radius increased with the increase in hold temperature.

SysWeld Simulated Weld Thermal History

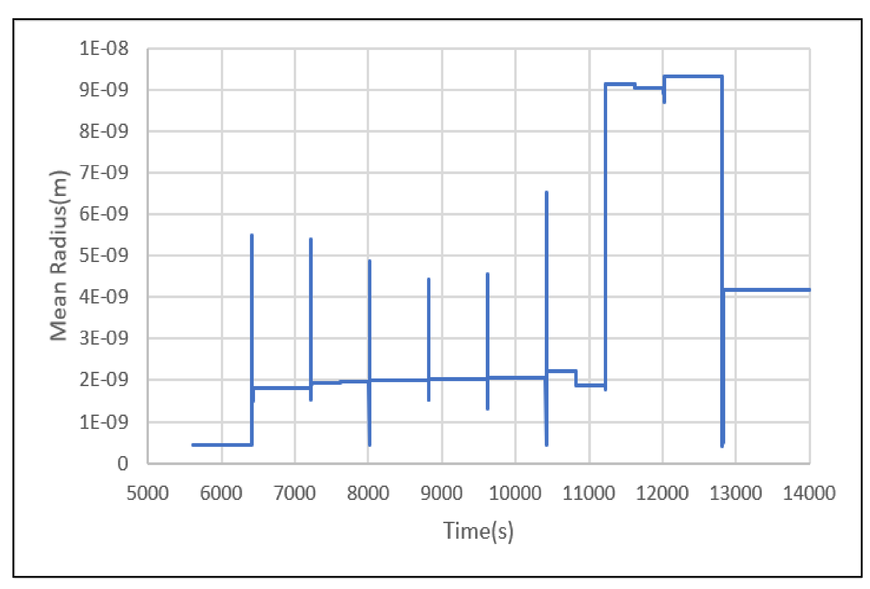


Figure 7: M23C6 Mean Radius in Simulated Weld Thermal History

- The simulation returned critical and mean radius measurements that spiked with temperature and dropped with temperature.
- The last 5 cycles did not follow this trend, and did not fully drop until the last cycle. This is due to an error in the T-C simulation.

4. Discussion

- As the hold temperature neared the precipitation temperature of M23C6 the initial rate of precipitation became lower as shown by the critical radius requiring more time to grow on the higher temperatures.
- The 850C and 900C have critical radius measurements that continually increase during holding, while the 1000C does not.
- The SysWeld cycle shows sharp drops and increases. However despite the peak temperature decreasing across cycles the maximum mean radius continues increasing.

Tempera ture [°C]	Amount of BCC_B2 [mol]	Amount of FCC_L12 [mol]	Amount of LIQUID [mol]	Amount of M23C6 [mol]
1160		1		
1150		1		
1146.5001		1		
1146.501		1		0
1140		0.99963		0.00037
1130		0.99907		0.00093
1120		0.99853		0.00147
1110		0.99802		0.00198
1100		0.99753		0.00247
1090		0.99706		0.00294
1080		0.99661		0.00339
1070		0.99618		0.00382
1060		0.99577		0.00423
1050		0.99538		0.00462
1040		0.99501		0.00499
1030		0.99466		0.00534
1020		0.99433		0.00567
1010		0.99401		0.00599
1000		0.99371		0.00629
990		0.99343		0.00657
980		0.99316		0.00684
970		0.99291		0.00709
960		0.99267		0.00733
950		0.99245		0.00755
940		0.99224		0.00776
930		0.99204		0.00796
920		0.99186		0.00814
910		0.99169		0.00831
900		0.99153		0.00847
890		0.99138		0.00862
880		0.99124		0.00876
870		0.99111		0.00889
860		0.99099		0.00901
850		0.99089		0.00911
840		0.99078		0.00922
830		0.99069		0.00931
820		0.99061		0.00939
810		0.99053		0.00947
800		0.99046		0.00954

Table 2: Single Axis Equilibrium

5. Conclusions

- The size of M23C6's critical radius increases with increasing hold temperature.
- As the hold temperature increases, the time is takes for the critical radius of M23C6 to reach a maximum also increases.
- At 1000C the critical radius of M23C6 does not increase during a hold, but at 850 and 900C it does.
- These simulations provide baseline trends however future work with the alloy's full elemental composition is needed.

References: [1] J. DuPont, et al., *Welding Metallurgy and Weldability of Nickel-Base Alloys*, Hoboken, NJ: Wiley, 2013. [2] Saida, K., Nomoto, Y., Okauchi, H., Ogiwara, H., & Nishimoto, K. (2012). Influences of phosphorus and sulphur on ductility dip cracking susceptibility in multipass weld metal of alloy 690. *Science & Technology of Welding & Joining*, *17*(1), 1–8. [3] Masatake Yamaguchi, Motoyuki Shiga, & Hideo Kaburaki. (2005). Grain Boundary Decohesion by Impurity Segregation in a Nickel-Sulfur System. *Science*, *307*(5708), 393. [4] Jiang, L., Hu, R., Kou, H., Li, J., Bai, G., & Fu, H. (n.d.). The effect of M23C6 carbides on the formation of grain boundary serrations in a wrought Ni-based superalloy. *MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING*, *536*, 37–44. https://doi-org.proxy.lib.ohio-state.edu/10.1016/j.msea.2011.11.060

Acknowledgements

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