

CALCULATION OF PHASE AND POURBAIX DIAGRAMS FOR HPCRM ALLOYS (DSTAR case #6534)

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The development of High Performance Corrosion Resistant Materials(HPCRM) alloys that are damage tolerant and applicable as a coating to a wide variety of substrates under a wide range of conditions is a remarkable achievement that has been accomplished is just over two years by the dedicated efforts of experienced scientists who made judicious choices in charting the direction of their work. and engineers(1).The reduction to practice based on amorphous metal alloys has left some gaps in in knowledge,which has been filled by using **Computational Thermodynamics** based on **CALPHAD Methods**(2)which were used to define the unstable Fe₃B phase as the nucleation site(3) to define the glass transition and transformation limiting temperatures as shown in Figures 1 and 2.The TCFE3 database and Thermo-Calc database were adapted to perform the calculations for a series of 15 multi-component iron based alloys to generate the results shown for SAM40(3) and SAM7(1651) (1,3) to generate the multicomponent phase and Pourbaix diagrams shown in Figures 3-5 which were verified by Phase equilibria and Cyclic Potential measurements.

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REFERENCES

- 1.J.C.Farmer,J.Haslam,D.Day,D.J.Branigan,C.A.Blue,J.D.K.Brevard,L.F.Aprigliano, N.Yang,J.Perepezko and M.B.Beardsley. “Corrosion Characteristics of Iron-Based High-Performance Amorphous-Metal Thermal-Spray Coatings”Proceedings of the ASME PVP-Pressure Vessels and Piping Division,July 2005 Denver,Colorado,Paper PVP2005-71664
- 2.M.Palumbo,G.Ciacciamani,E.Bosco and M.Baricco “Thermodynamic Analysis of Glass Formation in the Fe-B System” CALPHAD 25(2001)625-37
- 3.J.H.Perepezko and K.Hildal “Analysis of Solidification Microstructure during Wedge Casting” Submitted to Philosophical Magazine March 2005 currently In Press.
- 4.V.Ponnambalam,S.J.Poon and G.Shiflet,“Fe-Based bulk metallic glasses with diameter thickness larger than one centimeter”J.Mater.Research 19(2004)1320

