TITLE: **A Novel Low-Temperature Diffusion Aluminide Coating for Ultrasupercritical Coal-Fired Boiler Applications**

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OBJECTIVES

The main objective of the research project is to develop a low-temperature (≤ 700°C) diffusion aluminide coating with reduced brittleness and improved performance via pack cementation for protection of ultrasupercritical boiler internal tubing. Binary Al-containing alloys will be selected as the masteralloy for pack cementation based on thermodynamic calculations and physical metallurgy principles. These masteralloys will be utilized instead of pure Al to reduce the Al activity during the aluminizing process, which is expected to avoid the formation of liquid Al as well as Al-rich, extremely brittle intermetallic phases. The oxidation resistance to water-vapor environments of the low-temperature aluminide coatings will be evaluated and compared with model coatings synthesized by chemical vapor deposition (CVD). Furthermore, the effect of the developed coating on mechanical properties of the substrate alloys will be investigated via well-controlled laboratory testing. The ultimate goal is to develop a low-cost alumina-forming coating for higher-temperature steam conditions through integration of fundamental, technological and applicatory aspects.

ACCOMPLISHMENTS TO DATE

One concern with low-temperature aluminization by using binary masteralloys is whether sufficient vapor pressures of Al halides can be generated in the pack for coating formation. A knowledge of the thermodynamic properties of volatile halides in the pack system is essential, and the thermodynamic data for the formation of volatile halides can be used to determine suitable masteralloy compositions, the choice of the activator, and the desirable coating temperature.

The thermodynamic calculations were carried out by using a commercial software HSC 5.0.The calculation output by HSC was first verified via two approaches. One approach was to verify the equilibrium constant (K_{eq}) for a given equilibrium reaction which should be a constant at a given temperature. A more valid approach used in this study was to compare the calculation result for a pack system with that published in the literature using different thermodynamic software. This was done for a pack containing 4wt.% NH_4Cl, 73wt.% Al_2O_3, and 23wt.% (Al-Cr) masteralloys with various Al contents (5-20 wt.%). The equilibrium partial pressures at 1150°C were previously reported by Bianco et al. using ITSOL software. The partial pressures of the major gaseous species such as AlCl, $AlCl_2$, $AlCl_3$, Al_2Cl_6, and $CrCl_2$ calculated by HSC were nearly identical except that of $CrCl_3$. The difference in the $CrCl_3$ partial pressure is not clear. However, the value was extremely low, which would have negligible effect on the Al deposition.

The partial pressures of metal halide vapors formed inside the pack depend on both the composition of powder mixture and the coating temperature. The present thermodynamic calculations focused on using binary Al-Cr alloy as the masteralloy. For the Al-Cr system, the activities of Al and Cr were clearly a function of the alloy composition in the temperature range of 800-1000°C. The thermodynamic calculations were conducted for the packs containing 6wt.% NH_4Cl-74wt.% Al_2O_3-20wt.% (Al-Cr) masteralloy at 700°C. Six alloy compositions on the Al-Cr phase diagram were selected to cover three single-phase and three two-phase fields, ranging from 25 to 75wt.%Al. The partial pressures of Al subchlorides at 700°C were first increased from the Cr (Al) single phase to the $AlCr_2$+Al_8Cr_5 two-phase field. The increase in Al subchlorides became less when the Al content was greater than 50wt.%. These results suggest that it is thermodynamically feasible to tailor the Al activity in the pack cementation process by controlling the Al content in the masteralloy.

FUTURE WORK

Similar thermodynamic calculations will be carried out for the pack systems with Al-Fe as the masteralloy at 700°C.

Based on the thermodynamic results, binary alloys such as Al-Cr or Al-Fe which will result in suitable partial pressures of Al chlorides will be selected as the masteralloy candidates. Coating experiments will be designed and a group of Fe-9Cr-1Mo (P91) alloy specimens will be aluminized at temperatures ≤ 700°C. The pack coatings synthesized with the Al-Cr or Al-Fe masteralloy will be compared with the coatings fabricated with pure Al as the masteralloy.

LIST OF PAPER PUBLISHED, CONFERENCE PRESENTATIONS, STUDENTS SUPPORTED UNDER THIS GRANT

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Student(s) Supported Under This Grant

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