Computational Design and Prototype Evaluation of Aluminide-Strengthened Ferritic Superalloys for Power-Generating Turbine Applications up to 1,033 K

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ABSTRACT

Objective: The objective of this research is to design a creep and corrosion-resistant ferritic Fe-based alloy useful up to 1,033K in a superheated steam environment. The research will employ (i) first-principles calculations for the modeling of the phase-stability and for the computer-aided microstructure design, (ii) nanoscale characterizations of microstructures, and (iii) creep and corrosion tests. The alloy/microstructure design aims at achieving a steady-state creep rate of approximately 10^{-11} s^{-1} at a temperature of 1,033K and a stress level of 35 MPa.

Accomplishments: A total of eight FBB alloys (Fe-based β-β' alloys) were fabricated, and the compositions are listed in Table.1. Microhardness was measured for each sample at room temperature. The alloys show a high hardness of 460 - 485 diamond-pyramid hardness (DPH) in the solution-treated condition. FBB-5 exhibits the highest hardness after a 100-hour anneal, due to the hardening effect associated with the inclusion of 3.5% W. Bend tests were used for screening the mechanical properties of the alloys. The scanning-electron-microscopy (SEM) characterization of the bend-fractured specimens showed an almost fully brittle cleavage

fracture for all of the alloys. This tendency is believed to be associated with the relatively high Al concentrations in the alloys. We note that even though the Al concentration of FBB-8 was reduced from 10% to 6.5%, this alloy still showed brittle fracture, indicating that further reductions in the Al concentration may be needed to increase appreciably the ductility.

Table 1. FBB Alloy compositions (in weight%)

Alloy	Fe	Al	Cr	Ni	Mo	Hf	Zr	B	Nb	V	C	W
FBB-1	70	10	10	10	-	-	-	-	-	-	-	-
FBB-2	66.3	10	10	10	3.4	0.25	-	0.005	-	-	-	-
FBB-3	66.3	10	10	10	3.4	-	0.25	0.005	-	-		-
FBB-4	66.1	10	10	10	3.4	-	0.25	0.005	0.1	0.1	0.05	-
FBB-5	63.2	10	10	10	3.3	-	-	0.005	-	-	-	3.5
FBB-6	65.6	10	10	10	1.7	-	0.25	0.02	-	-	-	2.5
FBB-7	68.3	8	10	10	3.4	-	0.25	0.005	-	-	-	-
FBB-8	69.8	6.5	10	10	3.4	-	0.25	0.005	-	-	-	-

The microstructures of FBB-1 to 8 alloys were characterized by the transmission-electron microscopy (TEM). All alloys exhibit the nucleation and growth of B2 (β'-NiAl-Type) precipitates in the as-quenched state, and they undergo coarsening during the subsequent aging at 700˚C. All the alloys show fully coherent precipitates except FBB-2, which contains semi-coherent B2 precipitates. In FBB-7 and FBB-8, the B2 domains exhibit an additional internal phase separation. From an analysis of B2 precipitate sizes, Hf is found to be more effective than Zr in improving the coarsening resistance. Initial creep tests have been carried out on FBB-1, 2, 3, and 4 alloys under a constant compressive stress of 100 MPa in a vacuum chamber at 700˚C for an hour. Alloy FBB-1 shows a typical creep curve with primary and secondary creep stages but alloys FBB-2, 3, and 4 exhibit no obvious primary creep stage. The steady-state-creep rates decrease in the order of FBB-4 > FBB-2 > FBB-3 > FBB-1. Further creep tests were performed for the FBB-3 alloy with stresses of 50 MPa and 80 MPa in air at 700°C for 100 hours. The samples exhibit very small strains (< 0.15%) at 50 MPa and 80 MPa after 100 hours.

First-principles calculations have focused primarily on the computation of solute-impurity-diffusion constants as a framework for augmenting mobility databases required in the computer-aided optimization of coarsening-resistant microstructures. Extensive convergence tests were undertaken to determine the calculational settings and supercell sizes required to compute well-converged values of the saddle point, vacancy-formation and solute-vacancy binding energies. Work to date has focused primarily on W solutes for which the experimental data are available to validate the calculations. Related calculations for Mo, Ta, Hf, and Zr solutes are also in progress. A central finding of the calculations performed to date is that vacancies and solute atoms interact strongly at first and second neighbors. We have recently developed a general kinetic-Monte-Carlo code that will use the results from the first-principles calculations to derive the correlation factors required to compute impurity-diffusion coefficients.

Future work: To gain further insight into the intrinsic factors affecting the pronounced brittleness of the FBB alloys, we will investigate independently the effects of alloy chemistry and microstructure. New samples with a lower Al concentration will be fabricated and solution treated at 1,200 and 1,000 ℃. The different solution treatments will give rise to different volume fractions and average sizes of the strengthening precipitates. For each of the new samples, microstructures will be characterized, and the bend ductility will be evaluated. Ni or/and Co solutes will be added to the alloys, as these solutes have been reported to increase ductility in steels. We will also aim to derive a scientific understanding of the relation between precipitate microstructures and creep; a central issue is to understand the optimal precipitate size and volume fraction for the creep resistance. In this work, the state-of-the-art TEM will be employed to characterize chemical compositions of different phases, and X-ray diffraction (XRD) will be used to measure the lattice misfits between the precipitates and matrix. The calculations of impurity-diffusion coefficients will be completed to augment the available kinetic databases for ferritic alloys.