

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

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1. ABSTRACT

Objective: The objective of this research is to utilize modern computational tools, integrated with focused experiments, to design innovative ferritic superalloys strengthened mainly by the NiAl-type phase for fossil-energy applications at temperatures up to 1,033 K. Specifically, the computational alloy design aims toward (1) a steady-state creep rate of approximately $3 \times 10^{-11} \text{ s}^{-1}$ at a temperature of 1,033K and a stress level of 35 MPa, (2) a ductility of 10% at room temperature, and (3) good oxidation and corrosion resistance at 1,033K.

Accomplishments: The research yielded many outstanding research results, including (1) the development of a predictive first-principles framework for calculating impurity diffusion coefficients in ferritic alloys has been validated through comparisons with experimental data for W diffusion in α -Fe; (2) alloys with microstructures analogous to Ni-based alloys were successfully fabricated; (3) a secondary creep rate of 10^{-9} s^{-1} at 973 K and a compressive stress of 140 MPa was reached; (4) a bending strain of 5% was obtained at room temperature; and (5) an alloy system for further study was identified as Fe-6Al-10Ni-10Cr-3.4Mo-0.25Zr-0.005B in weight percent (wt.%).

First-principles calculations of impurity diffusion constants in the body centered cubic (bcc) Fe have been undertaken in order to augment existing kinetic databases. We employed periodic supercells containing 128 atoms to calculate the vacancy formation, migration, and binding energies, from which the diffusion activation energies of solutes were obtained. Transition matrix methods were carried out to compute correlation factors incorporating calculated vacancy-solute binding energies. The induced magnetization of the host atoms in the first and second coordination shells of the impurity were determined by first-principles, to compute the magnetization dependence of the diffusion activation energy, utilizing a previously published empirical relation. Harmonic vibrational contributions and electronic contributions were included to calculate relevant entropic terms for the computation of diffusion prefactors. These calculations employed a direct force-constant approach using 54-atom supercells. The self diffusivity in α -Fe and the solute diffusivity of W were obtained, which compare favorably with experimental data. The developed computational methodology will allow us to complete the impurity diffusion for other important solutes in the coming year, with the ultimate goal of identifying slow diffusing elements for the coarsening resistance.

Based on the prediction of slow diffusers by first-principles calculations, twelve Fe-based beta-beta' (FBB) alloys were successfully prepared by vacuum arc-remelting. Their microstructures were characterized by the transmission-electron microscopy (TEM) and analytical-electron microscopy (AEM). TEM showed that all prototype alloys exhibit the nucleation and growth of coherent *B2* precipitates. The partitioning of different alloying elements to the matrix and the NiAl-type precipitate were determined by AEM. Three-point-bending experiments were used as a preliminary measurement of the ductility. The results showed that the reduction in the Al concentration and hot deformation both helped improve the ductility. Short-term creep tests have been conducted under a constant compressive stress of 140 MPa at 973 K in air. FBB alloys with 5 ~ 6.5 wt.% Al exhibited superior low creep rates. A minimal secondary creep rate of 10^{-9} s^{-1} was reached.

Future work: To further improve the creep resistance at 1,033 K and the ductility at room temperature, an updated science-based systems engineering approach will be used. Large ingots with a composition of Fe-6Al-10Ni-10Cr-3.4Mo-0.25Zr-0.005B (wt.%) will be fabricated for the further detailed study. The coarsening kinetics of NiAl precipitates will be systematically investigated by the combination of TEM, AEM, and X-ray diffraction (XRD). The tensile tests at room temperature will be used to determine ductility. Creep-rupture tests instead of short-time compressive creep tests will be performed at different stress levels at 973 K and 1,033 K. First-principles calculations on the impurity diffusivity will be continued. A set of modern computational tools will be incorporated for the phase-stability modeling and microstructure design.

2. LIST OF PUBLISHED JOURNAL ARTICLES, COMPLETED PRESENTATIONS, AND STUDENTS RECEIVING SUPPORT FROM THE GRANT

Conference Presentations

- Calculation of Impurity Diffusivities in Ferrite from First-Principles, Daniel Worthington, TMS Annual Meeting, March 12th, 2008, New Orleans, Louisiana
- Computational Design and Prototype Evaluation of Aluminide-Strengthening bcc-Based Superalloys for Elevated-Temperature Applications, Zhenke Teng, TMS Annual Meeting, March 10th, 2008, New Orleans, Louisiana
- Diffusion of Substitutional Impurities in bcc Fe: First-Principles Modeling, Mark Asta, NIST Diffusion Workshop, May 12, 2008, Gaithersburg, Maryland

Students Supported Under this Grant

- Zhenke Teng and Shenyang Huang, Graduate Students in the Department of Materials Science and Engineering, The University of Tennessee, Knoxville