CREEP BEHAVIORS AND MICROSTRUCTURAL STABILITIES OF CO-AL-W-TA-TI-BASED SUPERALLOYS

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In last decade, the discovery of high-temperature stable γ'-Co3(Al, W) phase in Co-Al-W-base alloys motivated plentiful interests in designing the next generation γ'-strengthened Co-based superalloys. Continued efforts have been focused on increasing the γ' solvus temperature and enhancing the γ/γ' microstructural stability as well as improving the creep resistance at elevated temperatures in this class of superalloys.

In the present work, the effects of Ti and Ta additions on the creep properties and the microstructural stabilities of Co-Al-W-Ta-Ti-based superalloys are investigated by means of integrated the experimental and computational approaches. The chemistry design of Co-Al-W-Ta-Ti alloys was supported by the thermodynamic calculations of phase stability using the Co-base alloys database in Pandat^{TM} developed by the CALPHAD method. The atomic and the electronic structures for solute-strengthened (001) anti-phase boundaries (APB) of Co_3(Al, TM) are investigated by first-principles calculations based on the density functional theory (DFT), where TM denotes transition metals.

It is observed that at 1000^{o}C, the creep property of a Co-based single-crystal superalloy containing Ti and Ta is superior in comparison with the other reported Co-Al-W-base single crystal alloys and the 1st generation commercial Ni-base single-crystal superalloys. The different creep behaviors between Co-based and Ni-based superalloys indicate that the creep deformation mechanism of Co-based superalloys is mainly associated with the stacking faults and anti-phase boundaries. Moreover, Co-Al-W-Ta-Ti model alloys have been developed with the variation of alloying additions, recently. Our designed alloys show better microstructural stability at higher temperature as well as high γ' solvus temperature. DFT-based first principles calculations further reveal the complex electron structures induced by the variation of the lattice distortion around the fault layers in the solute-containing (001) APB. It is observed that the formation of the (001) APB in Co_3Al changes the Co-centered deformation electron density isosurface from the typical tetrahedral shape in the FCC lattice into the "S" shape. With the segregation of solute atoms at (001) APB, the bond strength around the fault layers are increased by the electron redistribution by forming chemical bonds with Co, providing fundamental insights on interactions among alloying elements and their effects on APB and creep properties. The current study is helpful for continuous efforts on alloy design and development to improve temperature capability of γ'-strengthened Co-base superalloys.