Perspectives on Using the Integrated Computational Materials Engineering (ICME) Research Methodology to Accelerate Discovery to Transition in Light Metals in Aerospace

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Abstract

Alloys based on Ti and Al have been pivotal in structures for lightweighting in aircraft and space. The main strengthening mechanisms are vastly different; one (Ti alloys) is, by and large, via solid solution and second-phase strengthening and the other (Al alloys) precipitation strengthening. However, the path from scientific discovery to application mostly takes way too long for advanced alloys and processes to be timely and feasible.

Integrated computational materials engineering (ICME) is a new R&D methodology that has been making important advances in materials science and engineering. Combining the theoretical models, experimental tools and digital data, it could not only make the R&D progress and results more robust, but also accelerate the critically needed transition. The two most important factors of low risk tolerance and long product cycles have a profound impact to make aerospace a most difficult industry to find benefit in ICME. This challenge is exacerbated by a large product scale and a correspondingly large component scale, which lead to substantial kinetic differences between the laboratory and production. However, considerable needs persist for cost and weight reduction, and more critically, for accelerating the introduction of materials that enable such improvements. In this presentation, I will try to deconstruct the life cycle of aircraft materials and identify where ICME can offer substantial value. Several examples of the application of computational methods to aerospace materials problems will be presented, from exploratory material design, to scale-up simulations, to the estimation of damage tolerance properties, and for polymer and metallic systems. Specific areas where ICME development is required will be highlighted. These tools will be relevant and pointed to general and specific aerospace materials and the R&D. Modeling and microstructural development during processing and machining of Ti and Mg alloys will also be discussed.

I will also present some highlights of the *KUMADAI* Mg alloy system. It is the ultrahigh strength and heat resistant Mg alloy system that has been developed at the Magnesium Research Center of the Kumamoto University. The microstructure of the alloy system, Mg-Zn-Y, is consisted of alpha-Mg and LPSO phases and it is highly strengthened by the LPSO phase and kinking mechanism.

A most promising alloy system, based on Mg-Al-Ca, for multifunctional applications has the concurrent properties of high thermal conductivity, high tensile strength and non-flammability. The Mg-4.5Al-2.5Ca, Mg-5Al-3Ca, Mg-6Al-4Ca, and Mg-4Al-2Ca-0.03Be (at%) alloys were produced by hot extrusion of the heat-treated cast alloys. These alloys have a microstructure consisting of alpha-Mg, and C36, C14 and C15 compounds, and exhibit a high thermal conductivity of 111-119 W/m/K, a high ignition temperature of 1343-1408K, and a high tensile yield strength of 318-363 MPa.

In addition, some key aspects of cellular metallics and hydrogen behavior and hydrogen embrittlement mechanisms in Ti alloys will be briefly discussed.