8th International Conference on Physical and Numerical Simulation of Materials Processing (ICPNS)

14–17 October 2016

Seattle, Washington | Hosted by Purdue University

SESSION 1: MODELS AND METHODS, SALON A

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SATURDAY, OCTOBER 15, 2016

CALPHAD-based materials genome and its applications to additive manufacturing

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ABSTRACT

Based on multiscale physical models and materials genomic databases, the technique of Materials Design enables an accelerated development of cybermaterials by constructing a hierarchical architecture of Integrated Computational Materials Design (ICMD). The major design toolkit of materials genome is composed of the CALPHAD (Calculation of Phase Diagrams)-centered methods, which are indispensable to supply fundamental informatics of materials thermodynamics and diffusion kinetics by coupling both theoretical calculations and experimental measurements. In this talk, an ICMD infrastructure based on CALPHAD materials genome will be introduced. A combined approach of first-principles calculations, CALPHAD, and advanced characterization experiments is adopted to study process–structure relations in order to achieve optimal microstructure, and thus improve additive-manufactured Ti-alloy properties for high performance. Afterwards, opportunities and future research directions will be discussed particularly through the present ICMD research activities in additive manufacturing. Microstructure characterization of additive-manufactured alloys indicates that laser processing generates considerable portion of columnar structure causing undesired anisotropic properties. However, a comprehensive composition design based on the CALPHAD materials genome database can generate an adaptive microstructure, which is suitable for additive manufacturing. Preliminary mechanical tests clearly show that yield strength and elongation along all three dimensions exceed the Ti–6Al–4V casting alloys despite the notable anisotropy. The current research indicates that a successful materials design in additive manufacturing requires synergistic efforts made by engineers in both mechanical engineering and materials science.

KEYWORDS: Ti, additive manufacturing, materials genome, materials design, ICME