

NIST Data Resource for Curated Thermophysical Property Data of Metal Systems

Boris Wilthan^{C, S}

Physics Services@NIST, Boulder, CO, U.S.A.

boris.wilthan@nist.gov

Scott Townsend and Vladimir Diky

NIST, Boulder, CO, U.S.A.

Significant methodological improvements in novel metallic material development processes are at the core of the Materials Genome Initiative (MGI). MGI, a multi-agency effort, is creating a new era of policy, resources, and infrastructure to support U.S. institutions discovering, manufacturing, and deploying advanced materials faster, at a fraction of the cost. The Thermodynamics Research Center (TRC) within NIST has, for the last five years, actively engaged in addressing the challenges around availability of thermophysical property data for metal systems in an electronic format [1]. These data, in a well-structured machine-readable format, are one of the cornerstones of a robust Integrated Computational Materials Engineering (ICME) system. It promises substantially faster development and deployment of advanced materials at a fraction of today's cost. Equally important for a collection of well characterized experimental thermophysical property data is the provenance of the collection's data and a clear statement regarding their quality, quantified in statements of uncertainty. This talk covers our progress in the continuous development of the free, publicly available NIST/TRC online resource [2] for metals and alloy data. It includes the progress made in structuring the relevant information from open literature into well-vetted datasets and gives an overview of the data coverage provided. To access the data programmatically for larger scale applications we recently added a computer-oriented web-based Application Programming Interface (RESTful API) – this interface will be discussed in detail.

References:[

1] B. Wilthan, E.A. Pfeif, V.V. Diky, R.D. Chirico, U.R. Kattner, K. Kroenlein, Calphad 56 (2017) 126-138; doi: 10.1016/j.calphad.2016.12.004.[2] https://trc.nist.gov/metals_data