Use of numerical modelling for research and development of nickel-based superalloys and beyond

Prof. Dr. Roger Charles Reed
Departments of Engineering Science and Materials,
University of Oxford, United Kingdom

Abstract

Nickel-based superalloys are metallic materials, which are used in high temperature applications in the aerospace, defence and power generation sectors. In this presentation, some latest research on these materials is presented from Oxford. Included will be the development of new grades of alloy using modelling, testing of them using advanced analytical techniques and studies of their processing and manufacturing from components in real applications.

Integrated computational materials engineering for materials and process design

Chinnapat Panwisawas

BSc (Physics), PhD (Metallurgy and Materials), CEng, MInstP, MIMMM, MIMechE

School of Metallurgy and Materials, University of Birmingham

Edgbaston, Birmingham B15 2TT, United Kingdom

Abstract

Integrated computational materials engineering (ICME) modelling framework, nowadays, has been increasingly of use in many researches in metallurgy and materials for rapid design purpose. It plays a very important role in exploring materials behaviours in various applications across different length scales. Traditionally, empirical and phenomenological based model were adopted as a tool to serve this purpose. Constitutive law based upon observation from experiments was used to rationalise materials response. However, physics-based modelling under ICME approach probably provides more deep insight to obtain better understanding of any physical effects, which might be overlooked or underestimated. In addition, sophisticated experimental techniques, *e.g. in situ* experiment using high energy X-ray light source to investigate some kinetic behaviour, and high performance computing resources have now become available and have been more efficient to simulate physical phenomena ranging from atomistic interaction to manufacturing processes. In this talk, some examples of modelling of materials and processing have been discussed. These concern about modelling of metallic 3D printing (laser additive manufacturing) and laser fusion welding. Modelling of heat transfer and fluid flow during laser-material interaction is being discussed. The temperature history from this macro-model will transfer into simulating rapid solidification using cellular automata and phase field approaches to obtain better understanding of some defect formation during the process. Another example is modelling and prediction of recrystallisation during investment casting of single crystal superalloys. Use has been made of process modelling of the investment casting to predict localised plastic deformation incurred in a representative of jet engine turbine blade component. If the plastic stain is sufficiently high, recrystallisation can take place. This gives rise to rejection of the component owing to detrimental degradation of mechanical performance, *e.g.* creep and fatigue properties. The model can accurately predict the critical plastic strain for recrystallisation, compared with various experimental methods, including TEM investigation of dislocation structures, which are used to validate the model. Once the sound physics-based model is established and provides some predictive capability, it will be served as a physics-based tool for material and process design, especially in aerospace and power generation applications.

Keywords: 3D printing, ICME, aerospace materials, jet engine, modelling