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Modelling of Solid Solution Strengthening in Multicomponent Alloys

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Abstract

With increasing industrial interest in high alloyed multicomponent and High Entropy Alloy (HEA) systems the integration of solid solution strengthening in the ICME framework for efficient Materials Design becomes an important *translator* tool. A general model is proposed that performs as the framework for an extensive assessment of solid solution strengthening coefficients. The model assumes the concentration dependence of $x^{2/3}$ as proposed by Labusch but gives a non-linear composition dependence to the strengthening parameter yielding a better description for concentrated alloys. To calibrate the model, 895 alloy systems, including a wide range of elements, have been used giving a good agreement between calculated and experimental values. Additionally, a promising method is proposed to represent the temperature related softening in the investigated systems.

Keywords

Materials Design, Solid Solution Strengthening, ICME, Multicomponent alloys, Translator, HEA

1. Introduction

Increasing success of ICME (Integrated Computational Materials Engineering) and Materials Design and its implementation in a wide range of fields [1, 2, 3] emphasize the importance of novel and quite general models for materials engineering. Application of ICME and Materials Design will offer new possibilities to enhance the materials properties and to decrease the development time compared to the classical trial-and-error approach of materials development.

The Materials Genome initiative [4], launched by US President Obama in 2011, aims to decrease the development time and costs by relying on a combination of modelling, data management and experimental characterization. ICME is an important part in the general strategy and one may in fact regard the Materials Genome as the models and databases that enable ICME.

The models to be used need a sufficiently strong physical basis to allow accurate interpolation and extrapolation of data. The CALPHAD-type models and databases for thermochemical and diffusional data may be seen as a role model for materials genome databases [5]. The purpose of the present work is to provide a practical formalism and a database for the strengthening parameters that may be used to model the strength of multicomponent alloys.

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