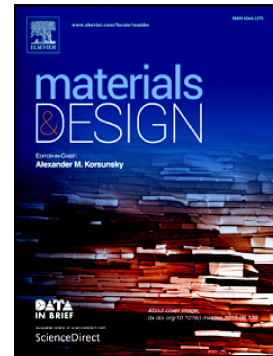


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## Phase Equilibria, Mechanical Properties and Design of Quaternary Refractory High Entropy Alloys

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### Abstract

Refractory high entropy alloys (RHEAs) are candidates for replacing conventional refractory alloys. In this work, twelve new RHEAs were selected and produced. The phases present in the as-cast and heat-treated conditions were characterized and compared with CALPHAD simulations and empirical parameters. Here we propose a new interpretation for the two widely used  $\delta$  and  $\Omega$  empirical parameters. In this work, they are shown to be inaccurate when applied to a large group of RHEAs, but can be a powerful alloy design tool if applied on specific subsystems of alloys. Experimentally, chromium-containing alloys are shown to form Laves phases, especially when the lattice distortion ( $\delta$ ) is high, while aluminum-containing alloys are shown to form the A15 phase upon heat-treatment, due to their highly negative enthalpy of mixing ( $\Delta H_{\text{mix}}$ ). In addition to microstructural characterization, mechanical properties of these alloys via hardness testing were assessed. A poor correlation was observed between the hardness and the atomic size and elastic modulus mismatch in these single-phase BCC RHEAs, suggesting that core structure of the screw dislocations is a crucial parameter in understanding the strength of these alloys.

**Keywords:** Refractory high entropy alloys, phase equilibria, CALPHAD, materials characterization, mechanical properties, solid solution strengthening.

### Introduction

High Entropy Alloys (HEAs) or Complex Concentrated Alloys (CCAs), are typically mixtures of 3 to 6 elemental constituents in near equimolar concentrations [1,2]. This creates a vastly unexplored composition and property landscape. Based on the hundreds of HEAs that have been studied to date [1], these alloys display interesting combinations of mechanical and functional properties in comparison to conventional alloys [1,3,4]. Different classes include: 3-d transition metal HEAs [5–10] (the most widely studied class), lightweight HEAs [11], lanthanide HEAs and refractory HEAs (RHEAs) [12–18], the focus of this work.

Recently, there has been much interest in RHEAs because of the continued demand to deliver increased mechanical performance at elevated temperatures. These alloys are primarily composed of mixtures of high melting point refractory elements, typically from groups 4-6 in the periodic table, to give the alloy increased temperature stability, along with other elements such as aluminum (Al) to deliver a balance of properties (oxidation resistance, ductility, low density) [19–23]. The microstructures of these alloys are usually composed of a body centered cubic (BCC) structure, sometimes present with other phases such as the B2 phase [15,24,25],

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