

Effects of Mn addition on High Entropy Alloys Vacancy and Subjected to Heating

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Abstract

In order to investigate the vacancy of CoCrFeNi and CoCrFeMnNi high entropy alloys, we apply Simmons-Balluffi's methods, positron measurements, neutron diffraction, and spatially-resolved synchrotron x-ray measurements and use Cu as benchmark. This study estimates the corresponding formation enthalpies and associated entropy of the high entropy alloys and Cu. Element dependent behavior is investigated by spatially-resolved x-ray fluorescence mapping which reveals the effect of Mn addition on the Cantor Alloy.

Keywords: High-entropy alloy, CoCrFeMnNi, CoCrFeNi, vacancy

Introduction

Due to the difference of atomic sizes (3), high entropy alloys (HEAs) are known for lattice distortion (1, 2). Particularly, Lei et al. (7) indicate that vacancies and interstitials are still lacking for high temperature applications of HEA (4-6). Lately, Chen et al.'s first-principles calculations indicate that CoCrFeNi has a higher vacancy formation entropy (8). Wang et al.'s thermodynamics analyses suggest that the equilibrium vacancy concentrations and their clusters in HEAs are substantially higher with the number of principle elements (9). However, Santodonato et al. show element dependent behavior, which is not solely attributed to configurational entropy effects (10).

To characterize the effective vacancy sizes, we applied Simmons-Balluffi methods (11), Seeger's approach (12), Bichile and Kulkarni's formula of thermal expansion calculation (13) to quantify vacancy as well as positron annihilation lifetime spectroscopy. We conducted spatially-resolved synchrotron x-ray diffraction and fluorescence mapping to characterize the vacancy effects on the local structure and chemical distribution for CoCrFeNi and CoCrFeMnNi HEAs, and compared with Cu as the reference sample.

Results

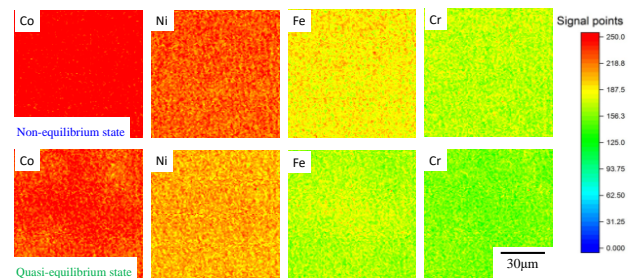


Fig. 1. XRF maps of CoCrFeNi HEAs after non-equilibrium (upper) and quasi-equilibrium (bottom) heating.

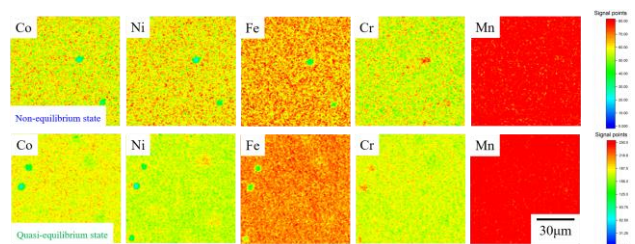


Fig. 2. XRF maps of CoCrFeMnNi HEAs after non-equilibrium (upper) and quasi-equilibrium (bottom) heating.

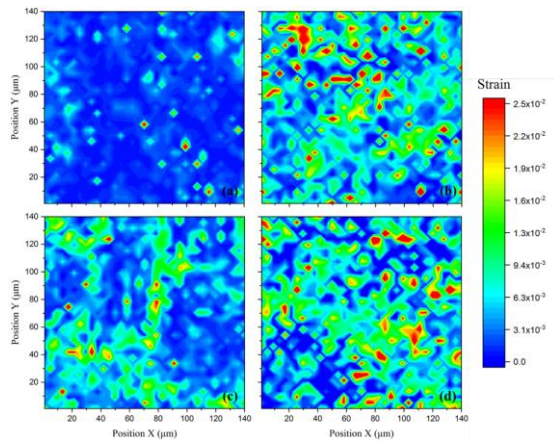


Fig. 3. The lattice strain mapping for (a) CoCrFeNi and (b) CoCrFeMnNi at non-equilibrium condition; (c) CoCrFeNi and (d) CoCrFeMnNi at quasi-equilibrium condition. The samples are comparable to measurements shown in red dash line of Figure 1(b) at 0.417 K/sec and red dash line of Figure 1(c) at 0.417 K/sec, respectively.

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