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Element Effects on High-Entropy Alloy Vacancy and Heterogeneous Lattice Distortion Subjected to Quasi-equilibrium Heating

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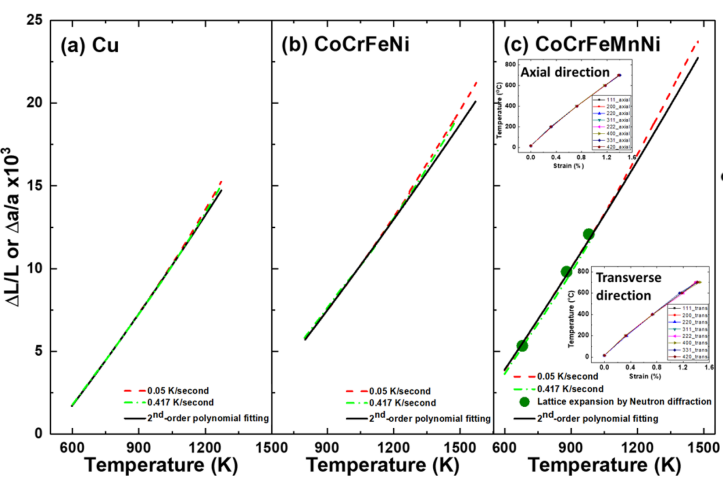
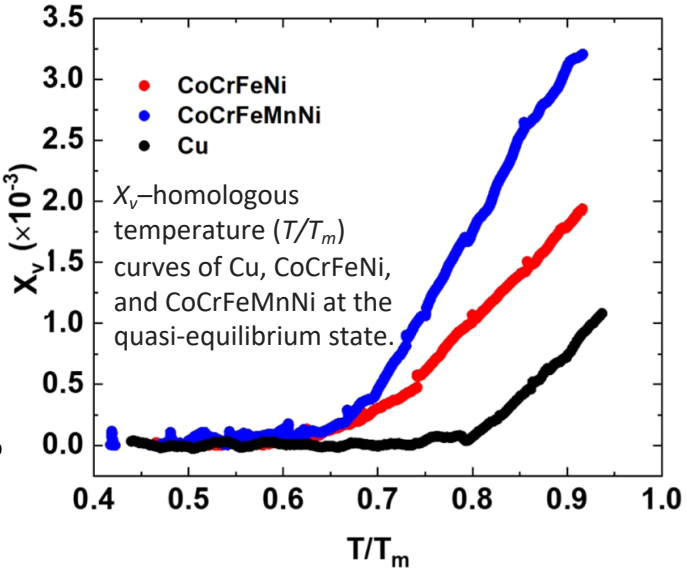
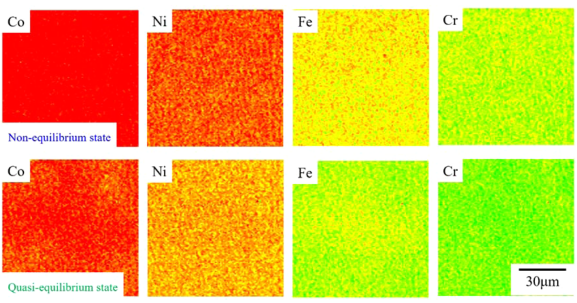
Abstract

We applied Simmons–Balluffi methods, positron measurements, and neutron diffraction to estimate the vacancy of CoCrFeNi and CoCrFeMnNi high-entropy alloys (HEAs) using Cu as a benchmark. The corresponding formation enthalpies and associated entropies of the HEAs and Cu were calculated. The vacancy-dependent effective free volumes in both CoCrFeNi and CoCrFeMnNi alloys are greater than those in Cu, implying the easier formation of vacancies by lattice structure relaxation of HEAs at elevated temperatures. Spatially resolved synchrotron X-ray measurements revealed different characteristics of CoCrFeNi and CoCrFeMnNi HEAs subjected to quasi-equilibrium conditions at high temperatures. Element-dependent behavior revealed by X-ray fluorescence (XRF) mapping indicates the effect of Mn on the Cantor Alloy.

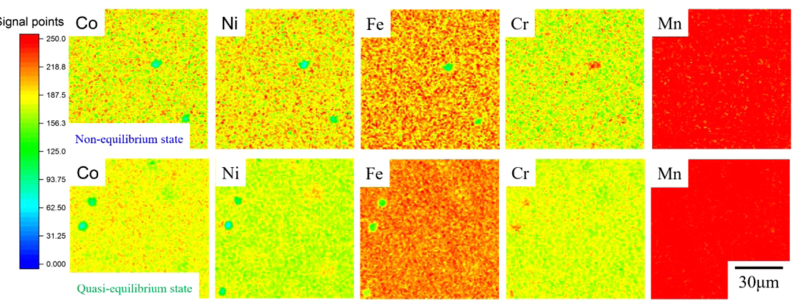


Measured strain *versus* temperature at the quasi-equilibrium and non-equilibrium states for (**a**) Cu, (**b**) CoCrFeNi, and (**c**) CoCrFeMnNi.



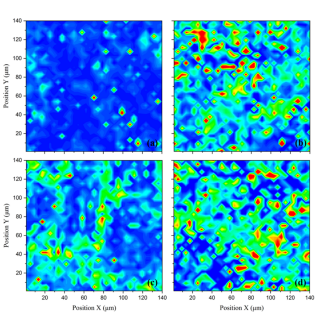


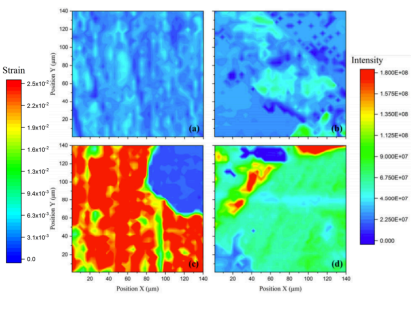
XRF maps of the CoCrFeNi HEA after non-equilibrium (upper) and quasi-equilibrium (bottom) heating.



XRF maps of the CoCrFeMnNi HEA after non-equilibrium (upper) and quasi-equilibrium (bottom) heating.

Lattice strain maps of the main diffraction peak (220) in (**a**) CoCrFeNi and (**b**) CoCrFeMnNi under non-equilibrium conditions, and the main diffraction peak (200) in (**c**) CoCrFeNi and (**d**) CoCrFeMnNi under quasi-equilibrium conditions.





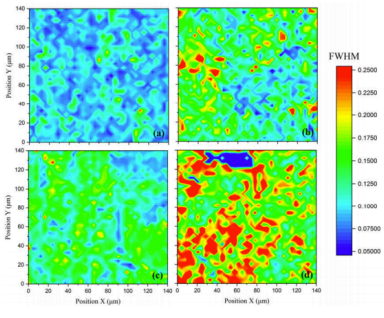


Fig. S2. Crystal orientation maps of the main diffraction peak (220) in (a) CoCrFeNi and (b) CoCrFeMnNi under non-equilibrium conditions, and the main diffraction peak (200) in (c) CoCrFeNi and (d) CoCrFeMnNi under quasi-equilibrium conditions.

Fig. S3. Full width maps of the main diffraction peak (220) for (a) CoCrFeNi and (b) CoCrFeMnNi under non-equilibrium conditions, and the main diffraction peak (200) in (c) CoCrFeNi and (d) CoCrFeMnNi under quasi-equilibrium conditions.

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