Experimental and Simulation Analysis of Coefficient Thermal Expansion (CTE) in CoCrFeNi And CoCrFeMnNi High-Entropy Alloys

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Abstract

High-entropy alloys (HEAs), which are equiatomic alloys composed of four or five elements, possess excellent mechanical properties and corrosion resistance. In this study, we apply *in-situ* neutron diffraction experiments and Molecular Dynamics Simulator with LAMMPS to study the diffraction patterns of quaternary CoCrFeNi and quinary CoCrFeMnNi HEAs in both single crystal and polycrystal. Thermal expansion coefficients are determined for these two alloys within the temperature range from 60 K to 1173 K. The simulation models are available for quantifying fundamental aspects of solid solution strengthening and structural analysis/design. The addition of Mn may have a significant effect on the thermal expansion behavior.

Keywords: High-entropy alloys, thermal expansion, neutron scattering, LAMMPS