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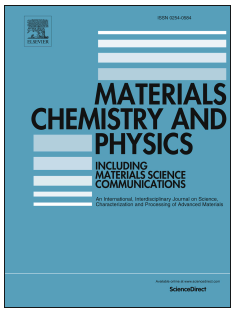

Elastic stability and lattice distortion of refractory high entropy alloys

Bojun Feng, Michael Widom

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Elastic stability and lattice distortion of refractory high entropy alloys

Bojun Feng and Michael Widom

Department of Physics, Carnegie Mellon University

Pittsburgh, PA 15213

Abstract

Refractory high entropy alloys containing elements from the Ti, V and Cr columns of the periodic table form body centered cubic (BCC) structures. Elements from the Ti column are noteworthy because they take the BCC structure at high temperature but undergo a shear instability and transform to the hexagonal (HCP) structure at low temperature. We show that the instability of these elements impacts the properties of the HEAs that contain them. In particular, the shear moduli are greatly reduced, causing increased dynamic contributions to lattice distortion. Relatively large size differences between elements of the BCC/HCP column compared with the regular BCC columns create additional static contributions to lattice distortion. These findings are supported by direct evaluation of elastic constants and lattice distortion in four representative HEAs. Comparing moduli of HEAs with those of compositionally averaged pure elements verifies the impact of BCC/HCP elements and allows us to estimate the compositions at which the BCC phases become elastically unstable, and these predictions could be useful in material design.

Keywords: High entropy alloy, shear instability, lattice distortion, elastic stability

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