

Abstract Submitted
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Electronic origin of atomic-level stresses in High-Entropy Alloys KHORGOLKHUU ODBADRAKH, JICS at ORNL, University of Tennessee, TAKESHI EGAMI, MADHU OJHA, UTK, DON NICHOLSON, UNCA, MALCOLM STOCKS, ORNL — High-entropy alloys are multi-component solid solutions in which four or more elements occupy the same crystallographic lattice sites with roughly equal compositions. The underlying chemical disorder gives rise to small local lattice distortions and atomic-level stresses, which are also disorders on their own. These disorders lead to radiation resistance and mechanical strength in high temperature environment, making HEAs alloys attractive candidates as nuclear materials. We report electronic origin of the atomic-level stresses based upon first-principles calculations using Locally Self-consistent Multiple Scattering theory method. Strong atomic-level stresses are present in HEAs due not only to the differences in the intrinsic atomic sizes but due to charge transfer among the elements. We suggest that the improved properties of HEAs originate mainly from the high magnitudes of atomic-level stresses in these complex disordered alloys.

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