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Deformation Behaviour and Strengthening Mechanism of High-Entropy Alloys Using Model and Simulation

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ABSTRACT

The high-profile high-entropy alloy shows outstanding mechanical properties. However, the accurate and reasonable models for describing the mechanical behavior of HEAs are still scarce due to their distinctive characteristics such as serious lattice distortion, which limit the engineering application. We have developed a new general framework combining atomic simulation, discrete dislocation dynamics and crystal plasticity finite element method, to study the deformation behaviour and strengthening mechanism of HEAs, and realized the influence of complex cross-scale factors on material deformation [1-3]. Compared with the classic crystal plasticity finite element, the bottom-up hierarchical multiscale model could couple the underlying physical mechanisms from the nano-micron-meso scales and captures the inhomogeneous strain field induced by the serious lattice distortion and chemical short-range order, thus showing the high accuracy and ubiquitous availability for HEAs. The predicted results show that the strain-stress curve of HEAs is in good agreement with the experimental results, which verifies the accuracy of the proposed method. In addition to the dislocation evolution, the heterogeneous strain distribution combined with the significant change from the orientation of some grains could be an important reason for the enhanced strength at the micron scale. The present work not only gives an insight into the relationship between the multiscale microstructure and deformation behaviour considering the mechanistic linkages of the lattice distortion, dislocation behaviour, and grain structure, but also provides a general approach to physically predict the mesoscopic mechanical response in HEAs.

KEYWORDS

High-entropy alloys; deformation behaviour; strengthening mechanism; hierarchical multiscale model; lattice distortion

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References

1. Li, J., Chen, Y., He, Q., Xu, X., Wang, H., Jiang, C., Liu, B., Fang Q., Liu, Y., Yang, Y., Liaw P. K., Liu, C. T. (2022). Heterogeneous lattice strain strengthening in severely distorted crystalline solids. *Proceedings of the National Academy of Sciences, 119(25)*, e2200607119.
2. Fang, Q., Lu, W., Chen, Y., Feng, H., Liaw, P. K., Li, J. (2022). Hierarchical multiscale crystal plasticity

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framework for plasticity and strain hardening of multi-principal element alloys. *Journal of the Mechanics and Physics of Solids, 169,* 105067.

3. Fang, Q., Chen, Y., Li, J., Jiang, C., Liu, B., Liu, Y., Liaw, P. K. (2019). Probing the phase transformation and dislocation evolution in dual-phase high-entropy alloys. *International Journal of Plasticity, 114*, 161-173.