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【514】First-principles-based prediction of yield strength in the RhIrNiPdPtCu high entropy alloy

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High entropy alloys (HEAs) are random alloys with 5 or more components, of near-equi-composition. HEAs exhibit excellent mechanical properties, including high strength, ductility, and fracture toughness. Guiding the design of new HEAs across the composition space requires an ability to compute necessary underlying material parameters accurately. Here, we propose a methodology to compute, via density functional theory, the elemental misfit volumes and other alloy properties, in the fcc noble metal HEA RhIrNiPdPtCu. These properties are then used in a recently developed solute-strengthening model for yield strength, with the prediction 563 MPa in excellent agreement with the experimental value 527 MPa. This methodology links the alloy composition with the strength prediction, indicating a general methodology for exploring new potential high-strength HEAs.

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