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First-Principles Modeling of Mechanical Properties for High-Entropy Alloys under Extreme Pressure LUKE MOORE, CHIA-MIN LIN, CHENG-CHIEN CHEN, University of Alabama at Birmingham — High-entropy alloys (HEAs) formed by five or more principal components have raised significant interests due to their superior mechanical properties and thermal stabilities for extreme-environment applications. Here, we utilize density functional theory (DFT) combined with special quasi-random structure (SQS) to study the mechanical properties of five-metal refractory HEAs in body-centered cubic (bcc) structures. We compute the volume and elastic moduli versus external pressure up to 300 GPa, and our DFT calculations with different size of SQS supercells show that the results can converge quickly with a few tens of atoms. We also study the strain-stress relations along different high-symmetry directions, which provide information for the ideal strengths of materials under consideration. Our results indicate the combined approaches of DFT and SQS are powerful methods for modeling mechanical properties of substitutionally random alloys under extreme conditions.

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