Plasticity in Structurally Complex Crystals: Insights from and Beyond Fundamental Building Blocks

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Intermetallics, which encompass a wide range of compounds, often exhibit closely related crystal structures, resulting in systems with structurally derivative phases. However, the mechanisms governing plastic deformation in these structurally complex alloys remain poorly understood. We aim to elucidate the deformation mechanisms of these complex crystals by examining how plasticity can be inferred from their fundamental building blocks. Through nanomechanical testing, complemented by atomic-scale modeling, we demonstrate that the deformation behavior of fundamental building blocks, such as the Laves phase and $CaCu_5$ phase, can be extended to structurally related phases, such as the μ-phase and $PuNi_3$ phase. These findings highlight the critical roles of interplanar spacing, local chemical distribution, and bonding environments within and beyond fundamental building blocks in shaping the plasticity of structurally related phases. Ultimately, our work underscores the importance of fundamental building blocks in predicting and manipulating plasticity, opening new avenues for designing high-performance materials through atomic-scale modifications.