When brittle crystals turn ductile – understanding the crystal plasticity of intermetallics from their fundamental building blocks

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Abstract

In materials design, understanding and manipulating the behaviour of dislocations - key drivers of plastic deformation - is a cornerstone. Yet while dislocations are well-explored in simple crystalline materials, their structure and mechanisms of motion remain largely enigmatic for complex crystals, such as topologically closed-packed phases. This vast class of materials contains many intermetallics ranging from high-temperature structural materials to functional crystals that can act as superconductors, magnets, or hydrogen storage materials. In all of these applications, structural integrity and therefore controlled plasticity is paramount. We aim to bridge our current knowledge gap in plasticity of complex crystals by delving into the most prevalent among them, the Laves phase, and other related phases that contain elements of the Laves phase as building blocks, such as the μ-phase. Small-scale mechanical testing is key to this research as the reduction in size suppresses cracking in favour of plastic deformation. By transmission electron microscopy, we then unveil previously unreported defect structures in the cubic Laves and the μ-phase. Complementing these observations, atomistic simulations elucidate the underpinning mechanisms, revealing novel deformation behaviours. We spotlight the role of full dislocations traversing multiple $\{1\ 1\ n\}$ slip planes, a departure from the conventional confinement to $\{1\ 1\ 1\}$ planes in the cubic Laves phase, and reveal changes in dislocation mechanism and critical stress induced by slight changes in composition that in turn give rise to sublattice order. Based on this better understanding on how the most fundamental building blocks of intermetallic crystals behave and change upon combination into larger unit cells, we propose a tangible pathway to understand the plasticity of brittle intermetallics. Ultimately, our goal is to provide characterisation and design strategies that will enable phase selection and materials engineering for intermetallics in advanced alloys, where much too often they are still considered as detrimental or at the very least unchangeably brittle, although first examples exist where this is not the case.

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