Understanding Intermetallic Intergrowths and Reactivity: Chemical Pressure-Driven Epitaxy Between Domain Interfaces

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The immense structural diversity of intermetallic phases offers promising avenues for accessing a wide range of materials with desirable properties. Although the development of design principles to guide the targeted synthesis of such materials is still needed, common themes arising in this class of materials show that even the most complicated structures can be understood in terms of intergrowth domains. Specifically, previous works have shown that the Ca3Cu7.8Al26.2 phase can be interpreted as a Chemical Pressure (CP) driven intergrowth between CaAl4 and CuAl2 units, which is further stabilized by electronegativity anchors. More recently, we have seen similar atomic packing considerations extended to a series of Frank-Kasper phases in the Mo-Fe-Cr system. Continuing this theme, we will present a new example in the Y-Ni system where the major packing issues present in the CaCu5-type parent structure serve as the major driving force for its intergrowth with YNi2 laves layers, with opportunities for stabilizing epitaxial interactions arising at the domain interfaces. It is through these examples that we aspire to illustrate a lens through which we can inform the design of new modular materials with multifunctional properties.