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Inherited (In)stabilities in Transition Metal Superlattices SVEN RUDIN, Los Alamos National Lab — Many transition metals exhibit a solid phase with a body-centered cubic (bcc) crystal structure. For some elements, e.g., tungsten (W), bcc is the only solid phase; for others, e.g., titanium (Ti), the bcc phase only appears at high temperatures. Titanium's high-temperature bcc phase exhibits soft phonon modes. These reflect the atomic movements upon transformation into the low-temperature phases. One such mode shows atomic displacements that also appear in the top few layers of tungsten's surface reconstruction. Superlattices constructed from alternating nanometer-thick layers of W and Ti would allow the two displacement patterns to interact. The work presented here uses density functional theory calculations to predict how the structure and mechanical response of such superlattices depends on the choice of transition metal elements and the layer thicknesses.

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