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Phonon Driven BCC to Orthorhombic Transformation in U-Nb

Alloys AVADH SAXENA, TURAB LOOKMAN, Los Alamos National Lab — The martensitic transformation in uranium alloys is of great strategic importance. We study the crystallography and model the well characterized BCC to orthorhombic phase transformation in the shape memory alloy U-Nb for low Nb concentrations. Our predictions are consistent with the experimentally observed orientation relationship between the BCC and orthorhombic phases. We find that this temperature induced transformation is driven by a specific zone boundary phonon that couples to a particular shear mode. We also obtain a Landau free energy for this transformation. In addition, we compare our results with a similar shuffle based mechanism in a related martensitic alloy AuZn.

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