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Study of the ideal strength and electronic structure in B2 transition-metal aluminides TIANSHU LI, University of California, J.W. MORRIS, JR., University of California, Berkeley, D.C. CHrzAN, University of California, Berkeley and Lawrence Berkeley National Laboratory — The ideal tensile and shear strengths of the B2-type (CsCl) transition-metal aluminides FeAl, CoAl, and NiAl have been investigated systematically using an \textit{ab initio} electronic structure total energy method. Our calculation explains the unique weakness in FeAl under the \langle100\rangle uniaxial tension as compared to NiAl, in which the shear instability intrudes before it approaches the tensile instability at a large critical strain. The weakness of FeAl along \langle001\rangle direction is attributed to an instability introduced by the filling of antibonding $d$ states. The calculation thus provides a theoretical basis for the observed cleavage behavior of the three materials. This work is supported by Department of Energy, Basic Energy Sciences under the Office of Science under contract DE-AC03-76SF00098.

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