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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 *ab initio* electronic structure total energy method. Our calculation explains the unique weakness in FeAl under the $\langle 100 \rangle$ 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 $\langle 001 \rangle$ 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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