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Possible metastable rhombohedral states of the bcc transition metals[1] MICHAEL MEHL, DANIEL FINKENSTADT, Center for Computational Materials Science, Naval Research Laboratory, Washington DC — The energy $E(c/a)$ for a bcc element stretched along its [001] axis (the Bain path) has a minimum at c/a = 1, a maximum at c/a = $\sqrt{2}$, and an elastically unstable[2] local minimum at c/a > $\sqrt{2}$. A rhombohedral strain is an alternative method of connecting the bcc and fcc structures. The primitive lattice keeps $R\overline{3}m$ symmetry, with the angle α changing from 109.4° (bcc), to 90° (simple cubic), to 60° (fcc). We studied this path for the non-magnetic bcc transition metals (V, Nb, Mo, Ta, and W) using both a full-potential LAPW and PAW VASP. Except for Ta, the energy $E(\alpha)$ has a local *maximum* at $\alpha = 60°$, with local minima near 55° and 70°, the later having lower energy. We studied the elastic stability of the 70° minimum structure. Only W is elastically stable in this structure, with the smallest eigenvalue of the elastic tensor at 4 GPa, while the other three elements are unstable. We discuss the possibility that Tungsten is actually metastable in this structure. We also consider the possible epitaxial growth of this structure.

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[2]M. J. Mehl, A. Aguayo, L. L. Boyer, and R. De Coss, *Phys. Rev. B* **70**, 014105 (2004).

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