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**Metastable states along the Bain path in AgZr with AFLOW**[1]
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AgZr crystallizes in the B11 structure, which is bcc-like with stacking AABB along [001]. Using AFLOW[2] we find another low energy structure, "Z2" ,[3] an fcc-like variant of B11. The B11 to Z2 transition follows the Bain path, with c/a changing from 1.9 (B11) to 2.6 (Z2). This seems similar to results for elemental bcc solids,[4] where we find a secondary Bain path minimum which is elastically unstable. Here there is no simple path from the Z2 structure back to the B11 structure, and the Z2 structure is metastable. Using first- principles DFT we demonstrate the possibility of a pressure induced phase transition from B11 to Z2 at 35 GPa. We also examine the $L1_0$ structure, which is higher in energy than Z2 at zero pressure. We find that a transition from B11 to $L1_0$ at 32 GPa, so that $L1_0$ is the true high-pressure phase of AgZr. We discuss the stability of all three of these phases at both zero and high pressure, and the possibility of similar transitions in more useful materials.

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[2]S. Curtarolo *et al.*, http://materials.duke.edu/aflow.html
[3]Z.W. Lu *et al.*, *Phys. Rev. B* **44**, 512 (1991)
[4]M. J. Mehl *et al.*, *Phys. Rev. B* **70**, 014105 (2004)

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