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Verification and refinement of the Al-Mg-Zn Φ phase crystal structure model JEFF HOUZE, BOHUMIR JELINEK, SUNGHO KIM, SEONG-GON KIM, MARK HORSTEMEYER, Mississippi State University — Density Functional Theory calculations were performed to validate the crystal structure proposed by L. Bourgeis et al. for the Φ phase of the Al-Mg-Zn system. Their model has ambiguous site occupancies for Zn and Al and definite locations for Mg. The model's simulated electron diffraction patterns agreed very well with experimental patterns. Using DFT calculations we are able to determine optimal Zn and Al aluminum locations. We will also show that the energetically optimal structure's element concentrations are within the experimentally observed range.

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