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Competition of Bergman-type approximants with other packing motifs in the Cu-Zr system FENG ZHANG, MIN JIN, X.W. WANG, CAI-ZHUANG WANG, M.J. KRAMER, M.I. MENDELEV, KAI-MING HO, Ames Laboratory, US DOE, and Iowa State University — Knowledge about the topological and chemical ordering in metallic liquids and glasses is essential in predicting phase selection and understanding glass formation dynamics. Taking the Cu-Zr system as an example, previous studies have established Bergman-type medium-range ordering (MRO) from a structural analysis with cluster alignment methods [1]. In this study, we examine the thermodynamic stability of a crystalline approximant of Bergman-type quasicrystals [2] against packing geometries existing in other intermetallic compounds for a wide range of Cu compositions. The most stable structures for each structural motif at each Cu composition are obtained using an efficient genetic-algorithm search. Our results show that the Bergman-type approximant structure is thermodynamically favored over other packing geometries at the glass-forming region with Cu compositions around 65%, reaffirming the Bergman-type MRO is the lowest energy in Cu-Zr glasses.

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