The Kob–Andersen model crystal structure: Genetic algorithms vs spontaneous crystallization

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The crystal structure of the Kob–Andersen mixture has been probed by genetic algorithm calculations. The stable structures of the system with different molar fractions of the components have been identified, and their stability at finite temperatures has been verified. It has been found that the structures of composition AB_n, where n = 2, 3, or 4, can be formed in the system. Metastable structures with compositions $AB_{0.4}$ and $AB_{0.58}$ have also been identified. Molecular dynamics simulations of spontaneous crystallization from liquid have been performed. We find several stable crystal phases which correspond to the concentrations of the components $c_B = 0, 1/2, 2/3, 3/4$ and 1. At the same time these structures are not observed upon spontaneous crystallization of a liquid with given concentration. For this reason these structures are difficult to obtain in a simple molecular dynamics simulation, which prevented their discovery before. At the same time there are some indirect evidences of existence of the different crystal structures at $c_B > 0.5$, for instance, the kinks on the isothermal dependence of viscosity on the concentration of the components [1].

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