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MODELING OF THREE-COMPONENT MULTI-PARTICLE DISCRETE CONGLOMERATIONS

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On the way to modeling composite structures consisting of discrete conglomerations containing special impurities in order to create materials with predictable properties, the study of the relationships between microscopic (structural) parameters and macroscopic properties plays a key role. For example, the compressibility of granular media (as well as molecular solutions) is one of the key characteristics that determine their mechanical and thermodynamic properties. In binary mixtures of solid balls described by the Kirkwood-Buff equations and the modified Carnahan-Starling-Mansouri (CSM) equations [1,4,5], specific states of bi-component systems are observed in which, due to the predominant concentration of particles with small or large sizes, the system as a whole demonstrates different types of behavior in terms of compressibility. The influence of the third component on the formation of states with maximum compaction and the compressibility behavior of the system remains an open question [2,3].

This work is devoted to the study of the properties of dense polydisperse mixtures of solid particles using models of the "solid spheres" type and is aimed at investigating the effect of the third component on the compressibility of a multi-particle mixture. The aim is to quantitatively analyze changes in the behavior of compressibility βT when a third component is added to a two-component system with a subsequent change in the relative sizes of all three components.

Particular attention is paid to identifying the conditions for the formation of maximally compacted states that correspond to the minimums of βT.In this way, criteria in terms of mole fractions and relative sizes of components of the formation of states with extreme packing and non-monotonic compressibility behavior are established.

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Primary authors: КУДАШКІН, Георгій; Prof. ГЕРАСИМОВ, Олег (Одеський університет ім. І.І.Мечнікова)

Presenter: КУДАШКІН, Георгій

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