Formation of clusters in the suspension containing three types of charged colloidal particles studied by Monte Carlo simulations

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We present a numerical study of formation of assemblies of charged colloidal particles in aqueous suspensions. According to our experiments different types of clusters form at different experimental conditions in the aqueous suspension for Pb(Mg1/3Nb2/3)O3 synthesis. With the control of pH in the suspension we control the particle-particle interactions and consequently the formation of the clusters. We believe that cluster formation in the suspensions is crucial for the solid-state synthesis of perovskite Pb(Mg1/3Nb2/3)O3 phase. The aim of the work was to verify this hypothesis with the use of numerical simulations. Three types of charged colloidal particles were used for simulation of aqueous suspension containing particles of PbO – lead oxide, MHC – magnesium hydroxy carbonate, and Nb2O5 – niobium oxide. Particle-particle potential of DLVO form with parameters from experiment and literature was used. This type of potential is suitable for systems with charged colloidal particles. The results from Monte Carlo simulations reveal that at pH 11.4, which is inherent pH of the suspension, clusters with close contacts between PbO and Nb2O5 particles form, which is not beneficial for the synthesis of the pure perovskite phase according to the literature. In contrast at pH 12.5 clusters form where close contacts between PbO and Nb2O5 are prevented by MHC particles. These conditions are more favorable for the perovskite formation. The results are in agreement with the experiment, where only from pH 12.5 suspension pure perovskite powder is formed, whereas after heating pH 11.4 sample contains secondary pyrochlore phase.