

GENERAL NATURE OF NON-CONGRUENT PHASE TRANSITIONS

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Non-congruence of phase transitions (NCPT) is general form of phase transitions in systems of two or more chemical elements. It means possibility of PT where coexisting phases have different chemical compositions ("stoichiometries") without violation of stoichiometry of whole system. NCPTs of fluid-fluid type are under discussion mainly. Two variants of such NCPT are possible in this case – simple mixtures, e.g. H₂+He, and NCPT in multicomponent products of high-temperature decomposition of chemical compounds, e.g. UO₂, NaCl, LiH etc. Main features of NCPT: (1) Two-dimensional (but not one-D) form of phase boundaries in intensive variables (P-T, μ -T etc); (2) More extensive domain of two-phase regions in extensive variables (P-V, V-T etc) and significantly more complicated form of iso-lines when crossing of this region; (3) Essential difference in properties and location of NCPT Critical Point (CP) in comparison with the ordinary CP in congruent PT. Present discussion based on investigations of NCPT in products of high-T boiling of uranium dioxide (UO₂) [1] and on results of NCPT modeling in simplified Coulomb model of ionic mixture [2].

In spite of general and fundamental nature of non-congruent form of phase decompositions NCPT do not have adequate understanding in high energy density matter investigations. This statement is illustrated on example of non-congruent evaporation in typical halide NaCl. Theoretical predictions of NCPT in this case [3] are in contradiction with the long time results of direct numerical simulations of this PT (e.g. [4][5] etc). The latter predict ordinary, congruent form of this phase transition in NaCl. Resolution of this contradiction needs providing special benchmarking experiments and/or decisive First Principle simulation of properties for gas-liquid transition in NaCl.

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