Thermodynamics of lattice model of intercalation

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The thermodynamics of the lattice model of intercalation of ions in crystals is considered in the mean field approximation. Pseudospin formalism is used in describing the interaction of ions with electrons. The effective attractive interaction between ions is formed due to the pseudospin-electron interaction and the condition of the appearance of phase transition of the first order with jumps of the ion and electron concentration is established (in the regime of the fixed concentrations it corresponds to the phase separation). This interaction also leads to the shift of the electron band positions. It is found that the total capacity of the system increases near phase transition point. The influence of impurities on these transitions and electrostatic capacity of the system is investigated. The possibility of hopping of intercalated ions between different positions is taken into account. The existence of the phase with $\langle S^x \rangle \neq 0$ was revealed (this phase is an analog of superfluid phase in the systems of hard-core bosons). The possibility of phase transitions of the first and second order to the modulated phase is revealed. Phase diagrams in the plane the chemical potential of the ions-parameter of the ion transfer are built. It is shown that at high values of the parameter of ion transfer, the phase transitions with jumps of the ion and electron concentrations disappear.