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Charge Neutral Yukawa Lattice Gas on a FCC Lattice HE HUANG, S.D. MAHANTI, Michigan State University — Structural phase transitions associated with the ordering of Ag and Sb ions in the quaternary systems, $(AgSbTe_2)_x(PbTe)_{2(1-x)}$ (of current thermoelectric interest) has been investigated using an anti-ferromagnetic 3-state Ising model on a FCC lattice with screened Coulomb interaction (Yukawa lattice gas (YLG) model). We have carried out Monte Carlo simulations (MCs) to study phase transitions (PT) in YLG. The nature and the strength of PT depend on the screening parameter κ. The transition is 1^{st} order and the transition temperature T_c is a weak function of the concentration x (excepting when $x \sim 0$ or 1), in agreement with earlier work for $\kappa = 0$. We find $T_c(x, \kappa) = f(x)g(\kappa)$, where $g(\kappa) \to const$ when $\kappa \to 0$ and $g(\kappa) \to 0$ when $\kappa \to \infty$. For $x = 0.5$, there are two special structures, layered and tubular which have the same ground state energy, independent of κ. This is understood by looking at the connectivity and ordering of ions. Above but near T_c, the generation rates of different micro structures have been analyzed using a simple surface energy density picture. MCs results agree with this analysis and show that the energy barriers decide the generation rates of different micro structures.

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