Statistical theory of crystals phases: the bound of thermodynamic stability

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Phase transformations in the solid state represent an interesting physical problem. Besides, they can have important meaning for practical applications. Accurate estimates of the thermodynamic limits of different crystal phases as equilibrium structures can play the decisive role when selecting the materials as candidates for use in real devices. Recently, it was established experimentally [1] that the fcc phase of Xe undergoes a transition of martensitic type into some intermediate phase having the sings of the hcp modification. In the present communication it is shown that the equations of the statistical theory of crystals [2,3] admit the existence of the equilibrium space-periodic solutions typical for the fcc phase of the noble gas crystals only in some definite domain of pressures and temperatures. The boundary of these domain is a line at which the fundamental thermodynamic condition of the positivity of the isothermal compressibility of the system is broken. The theoretical estimate of the limiting pressure of the loss of the thermodynamic stability of the fcc phase under discussion leads for Xe at the room temperature to the value ≈ 1.5 GPa. This value is rather close to the pressure at which the above said martensitic transition is fixed in Xe [1]. It seems useful to extend the range of the experimental study of the polymorphic transitions in order to stimulate further theoretical investigations of the effect of the thermodynamic instability in crystals.

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