Theoretical justification of the second-order phase transition in the LuLiF4 compound

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The ferroelastic phase transition in the LuLiF4 compound from the tetragonal phase with I41/a symmetry to the fergusonite type phase with C12/c1 symmetry has been found experimentally at the pressure of 10.7 GPa [1], but the type of this transition has not been studied.

We performed ab initio calculations by means of Density Functional Theory [2] with using VASP 5.2 [3] (Vienna Ab Initio Simulation Package), the part of the MedeA® interface. The paper states that the phase transition occurs at the pressure of 10.5 GPa [4]. Conclusion was made that the LuLiF4 compound most likely underwent to a second-order phase transition according to the Landau criteria [5].

Another criterion of a second-order phase transition presence is vanishing of the coefficient at squared order parameter in the expansion of the free energy at the phase transition point. To confirm the second-order phase transition presence in the LuLiF4, we introduced the 2-dimensional order parameter with components $e(B_g^1)=(e_{xx}-e_{yy})/2$ and $e(B_g^2)=exy$ (here e_{ab} are the deformation tensor components) transforming accordingly to the B_g irreducible representation of the factor group in the high-symmetry phase, and the expansion of the free energy in powers of the order parameter was carried out.

The dependence of the elastic constants combination D(P) on pressure P was then built. D(P) has a pronounced minimum at the pressure of 10.5 GPa which indicates the structural instability of the LuLiF4 compound. The direction of the atom displacements at an angle to the crystallographic a-axis in the basis ab-plane at the second-order phase transition was also determined.

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