THE IMPORTANCE OF THE LATTICE DYNAMIC IN THE MAGNETIC PHASE TRANSITION IN FERH

Belov M.P.,[*1] ***Syzdykova A.B.,***[1] ***Ponomareva A.V.,***[1]
Smirnova E.A.,[1] ***Abrikosov I.A.***[1,2]

[1]*NUST "MISIS", Moscow, Russia,* [2]*LiU, Linköping, Sweden*
[*]*makspalych@gmail.com*

FeRh undergoes an unusual antiferromagnetic-to-ferromagnetic (AFM-FM) transition just above room temperature. This magnetic transition was discovered for the first time in the late 1930s [1] but the origin of this transition is still a source of active debate. There are basic questions about what drives this transition, and usually the driving force is discussed in terms of magnetic, lattice and electronic entropy differences between the phases. In this work we have carried out calculations in the framework of Temperature Dependent Effective Potential method (TDEP) [2] based on molecular dynamic simulations at different temperatures and obtained full phonon spectra and corresponding lattice entropies of AFM and FM FeRh at different temperatures. In this way we have demonstrated strong temperature dependence of phonon spectra for both phases and consequently the importance of temperature on lattice entropy difference which calculated value is 16 J/kg/K at 350 K.

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1. M. Fallot, Ann. Phys. Serie 11 18, 291 (1938).
2. O. Hellman, I.A. Abrikosov, S.I. Simak, Phys. Rev. B 84, 180301 (2011).