The Evolution of Vibrational Modes of FeSe Under Uniaxial Strain

Jelena Pešić, Andrijana Šolajić, Ana Milosavljević, Sanja Đurđić Mijin, Borislav Vasić, Novica Paunović and Nenad Lazarević

Center for Solid State Physics and New Materials, Institute of Physics Belgrade, Serbia

Application of strain is one of the effective ways to engineer the various properties of materials. Iron-based superconductors are suitable materials to study the strain dependence of physical properties due to their high sensitivity to variations in the local crystal structure. Among the iron-based superconductor family, FeSe is a prominent example of the interplay between superconductivity, magnetism, and electronic nematicity, which can be tuned both by chemical substitution and by application of physical pressure and consequent lattice distortions [1].

Here we present a first principle study of evolution of vibrational modes of the strained FeSe. We performed a systematic computational study, using density functional theory formalism, on bulk FeSe crystals with applying the in-plane uniaxial strain in B_{1g} and B_{2g} symmetry channels, in the range -1.5% to 1.5%. For the calculation, we used the experimental parameters and the volume cell of the unit cell is conserved under applied uniaxial strain [2].

We focus on the effect of the modification of the lattice constant, and the consequent symmetry distortion, on characteristic A_{1g} and B_{1g} modes of FeSe. These findings are compared with experimental data from Raman measurements, studying the trend of changes of A_{1g} and B_{1g} modes with applied strain using a piezoelectric strain device. The sample was mounted in such a way that the strain was applied in the *ab*-crystallographic plane and that the direction of incident light propagation is along the crystallographic *c*-axes. The sample orientations were set so that [110] (B_{2g}) and [100] (B_{1g}) crystallographic directions were orthogonal to a gap between the holder plates.

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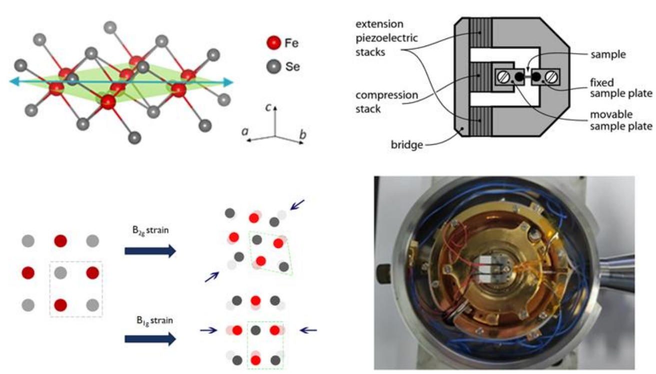

Left: Schematic representation of applied strain, Right: piezoelectric strain device, schematic and photography

[1] M. Ghini et al. Strain tuning of nematicity and superconductivity in single crystals of FeSe, Physical Review B,103, 205139 (2021)

[2] Willa, R. et al. Strain tuning and anisotropic spin correlations in iron-based systems. Physical Review B, 100(8) (2019).

[3] http://strainedfesc.ipb.ac.rs/