Effect of iron content and potassium substitution in $A_{0.8}Fe_{1.6}Se_2$ (A=Tl, K, Rb) superconductors studied by Raman scattering

A. M. Zhang, K. Liu, J. H. Xiao, J. B. He, D. M. Wang, G. F. Chen, B. Normand, and Q. M. Zhang

Department of Physics,Renmin University of China, Beijing 100872, P. R. China

We have performed Raman-scattering measurements on high-quality superconducting $K_{0.8}Fe_{1.6}Se_2$(Tc $\sim$ 32K), $Tl_{0.5}K_{0.3}Fe_{1.6}Se_2$(Tc $\sim$31K) and $Tl_{0.49}Rb_{0.31}Fe_{1.6}Se_2$(Tc $\sim$29K) crystals and parent compound $KFe_{1.5}Se_2$ at various temperatures. We carried out first-principles nonmagnetic calculations on vibration modes at zone center in $K_{0.8}Fe_{1.6}Se_2$. The observed modes in $K_{0.8}Fe_{1.6}Se_2$ can be well assigned with symmetry analysis and the calculations. Over ten modes are observed for each crystal, far more than expected for a normal 122 syste. This suggests that vacancy ordering is an intrinsic feature in AFeSe system. On basis of the assignment, we compare Raman modes in AFeSe compounds. For most phonon modes, a clear frequency difference between superconducting and non-superconducting potassium intercalated crystals is revealed. Potassium substitution by Tl or Rb makes no substantial frequency shift on Raman modes above 60 cm^{-1}. It demonstrates that the substitution of Tl or Rb for K has little effect on microstructures of FeSe layer. The results suggest that superconductivity is linked with particular microstructures of FeSe layer in $A_{0.8}Fe_{1.6}Se_2$ system. However in the Tl- and Rb-substituted samples, several additional modes appear below 60 cm^{-1}, which can be attributed to vibrations of Tl or Rb atoms. Anomalously the modes become very weak with decreasing temperatures, similar to 66 cm^{-1} Se modes. This may reveal an ordering process of (Tl, K/Rb)-layer at low temperatures.