Physical origins of the dependence of Tc on the As-Fe-As angle in iron superconductors : the 1111 and 21311 cases

Garbarino, G.,[1] Weht, R.,[2] Sow, A.,[3] Lacroix, C.,[3] Sulpice, A.,[3] Zhu, X.,[4] Han, F.,[4] Wen, H-H.,[4] and Núñez-Regueiro, M.[3]

[1] *European Synchrotron Radiation Facility (ESRF), 6 Rue Jules Horowitz 38043 BP 220 Grenoble*
[2] *Gerencia de Investigación y Aplicaciones, Comisión Nacional de Energía Atómica (CNEA), Avda. General Paz y Constituyentes, 1650 - San Martín, Argentina and Instituto Sabato, Universidad Nacional de San Martín - CNEA, 1650 - San Martín, Argentina*
[3] *Institut Néel, Centre National de la Recherche Scientifique (CNRS) Université Joseph Fourier (UJF), 25 Avenue des Martyrs, F-38042 BP166 Grenoble Cedex 9 France*
[4] *National Laboratory for Superconductivity, Institute of Physics and Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, P. O. Box 603, Beijing 100190, China*

Early in the study of high temperature superconducting compounds it was established that the superconducting transition temperature Tc was strongly dependent with the As-Fe-As angle of the FeAs4 tetrahedron: Tc was maximal for regular values (109°47') of the angle. Several theories were put forward to explain this behavior, all based on particular details of the band structure, that were supposed to be universal, i.e. applicable to all systems, as the empirical Tc vs angle relationship was based on recollections of data from different samples or measurements of different groups. To verify this relationship, we have started a systematic study of the behavior of different compounds under pressure. We are able to follow under pressure both the superconducting Tc by electrical resistivity measurements, and the evolution of the structure through synchrotron radiation measurements. We can then calculate the electronic band structure on the measured atomic positions at each pressure to follow the electronic properties. This method allows us to determine in each particular case the physical cause behind the relationship, that does not seem to be universal. For superconducting Sm-1111 it turns out to be a charge transfer issue, that is optimized under pressure. While for superconducting Sr2VO3FeAs it is associated to the disappearance of multiple nesting features when the tetrahedron becomes irregular under pressure and the degeneracy of the bands is broken. Our results call for more general symmetry related reasons to explain the relationship, that would then appear through different ways in different compounds.