

**P.N. Lebedev Physical Institute,
Russian Academy of Sciences**

Chemistry of superconducting pnictides

Kirill Pervakov

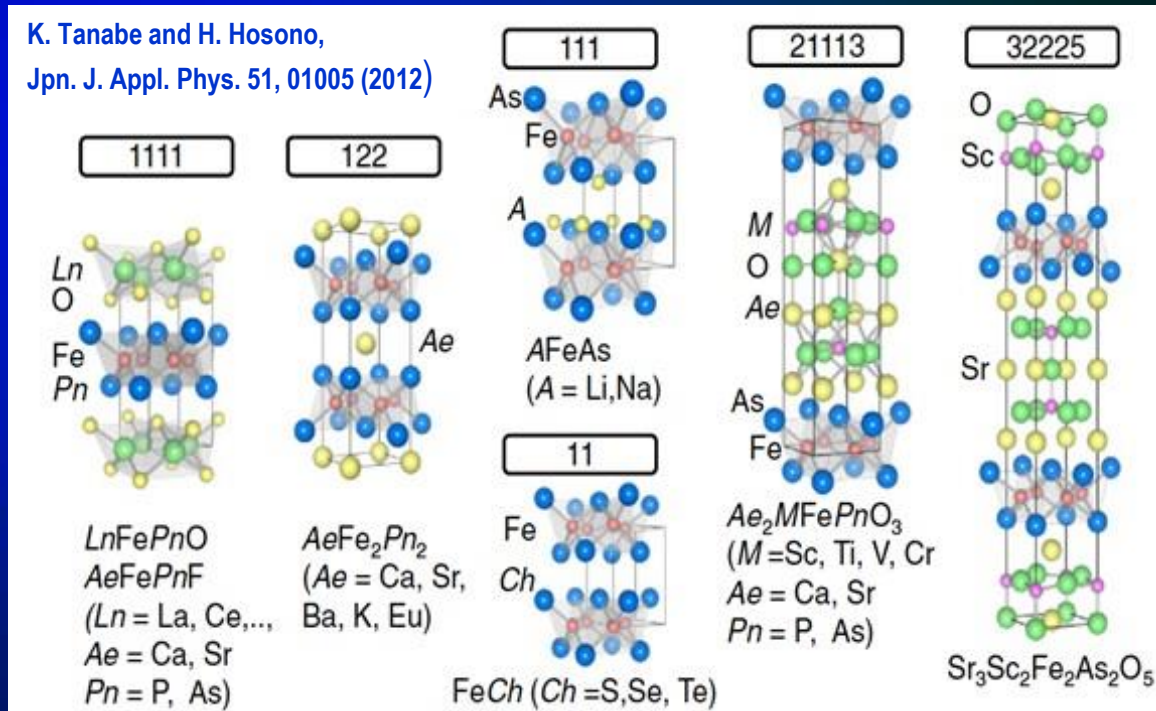
Zvenigorod, 2013

Outline

- Crystal symmetry
- 122 system
- Superconductor as a solid solution
- Self-flux method
- Contamination of single crystals
- Summary

Crystal symmetry

K. Tanabe and H. Hosono,
Jpn. J. Appl. Phys. 51, 01005 (2012)



Poor metals,
Low $E_F = 20\text{-}100$ meV,
Short $\xi = 1\text{-}2$ nm,
Huge $H_{c2} > 100$ T

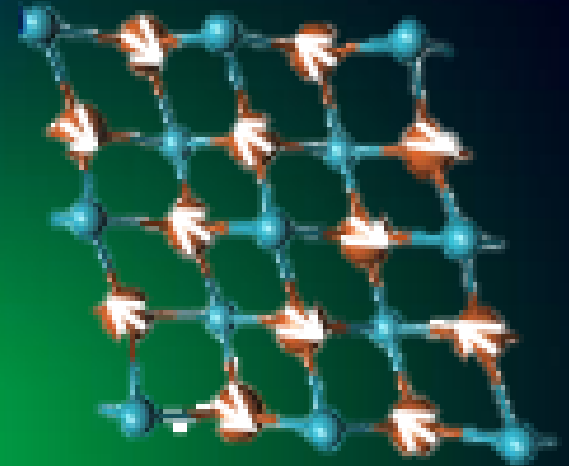
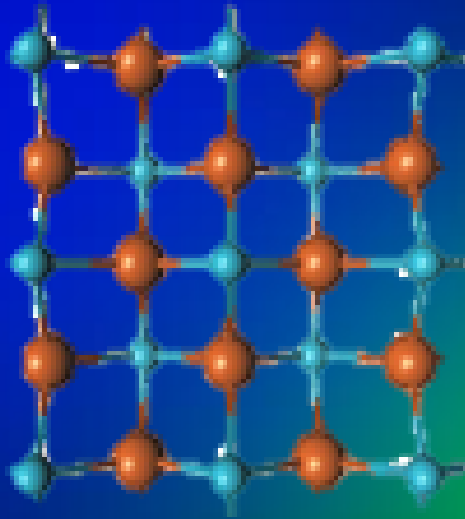
Superconductivity from magnetic Fe^{2+} ions

ReOFeAs based (1111) ($T_c = 55\text{K}$) ($\text{Re} = \text{Sm, Nd}$)

$\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ based (122) ($T_c = 38$ K)

$\text{FeSe}_x\text{Te}_{1-x}$ based (11) ($T_c = 18$ K)

Ba-122 system

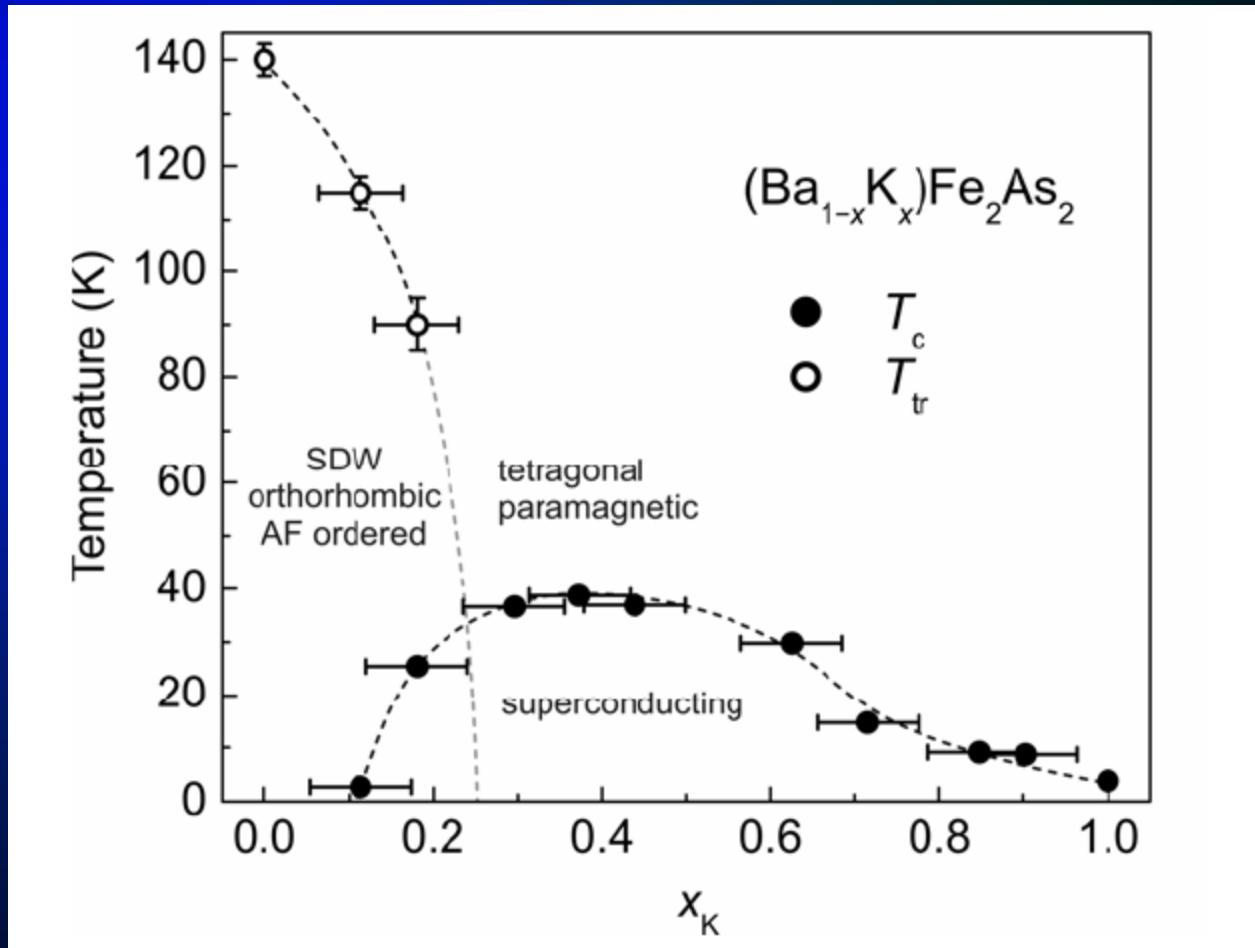


$I4/mmm$
Tetragonal
Paramagnetic

$Fmmm$
Orthorhombic
Antiferromagnetic

Doping suppresses this transition

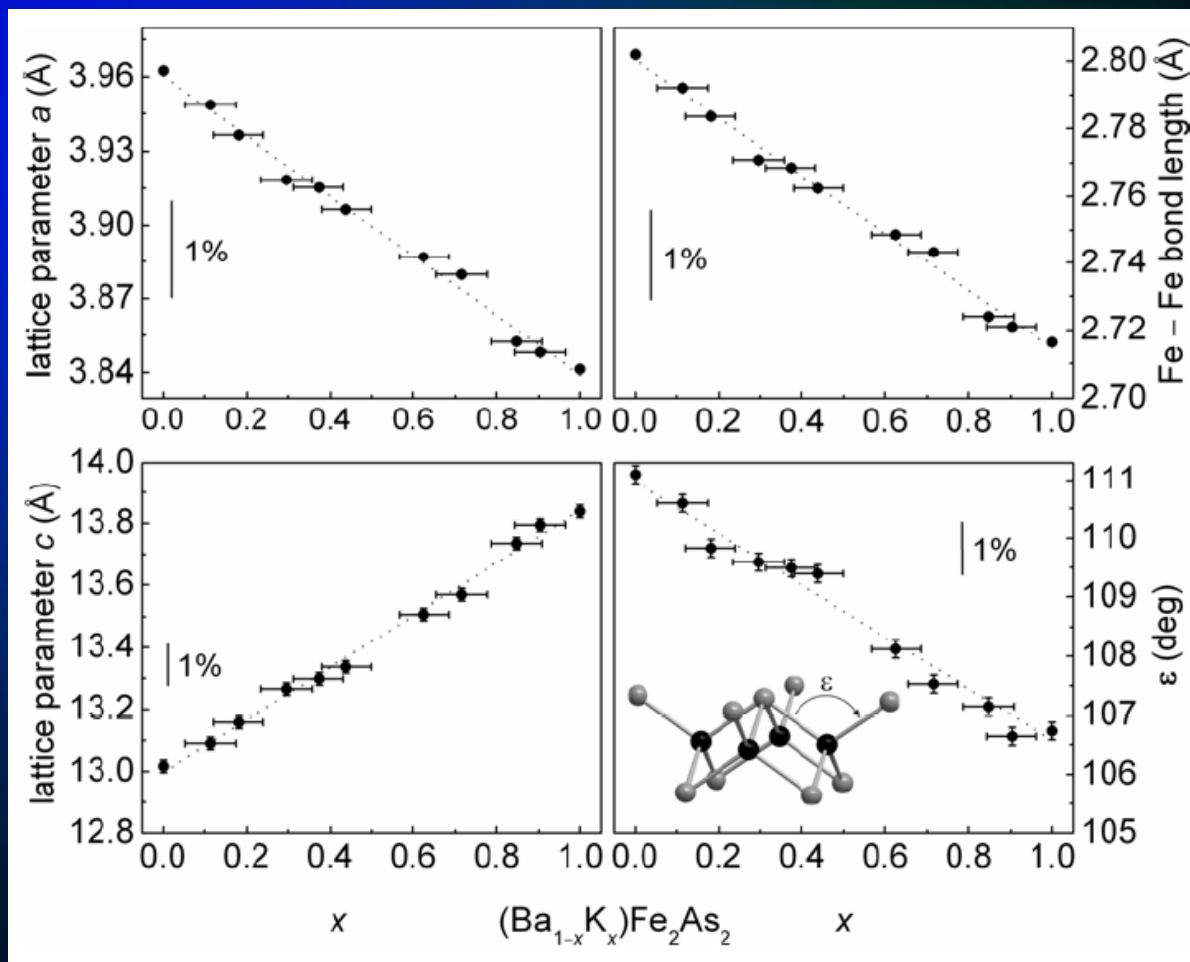
Ba-122 system



Magnetic phase diagram of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$

D. Johrendt and R. Poettgen, Physica C 469, 332-339 (2009)

Superconducting phase as a solid solution



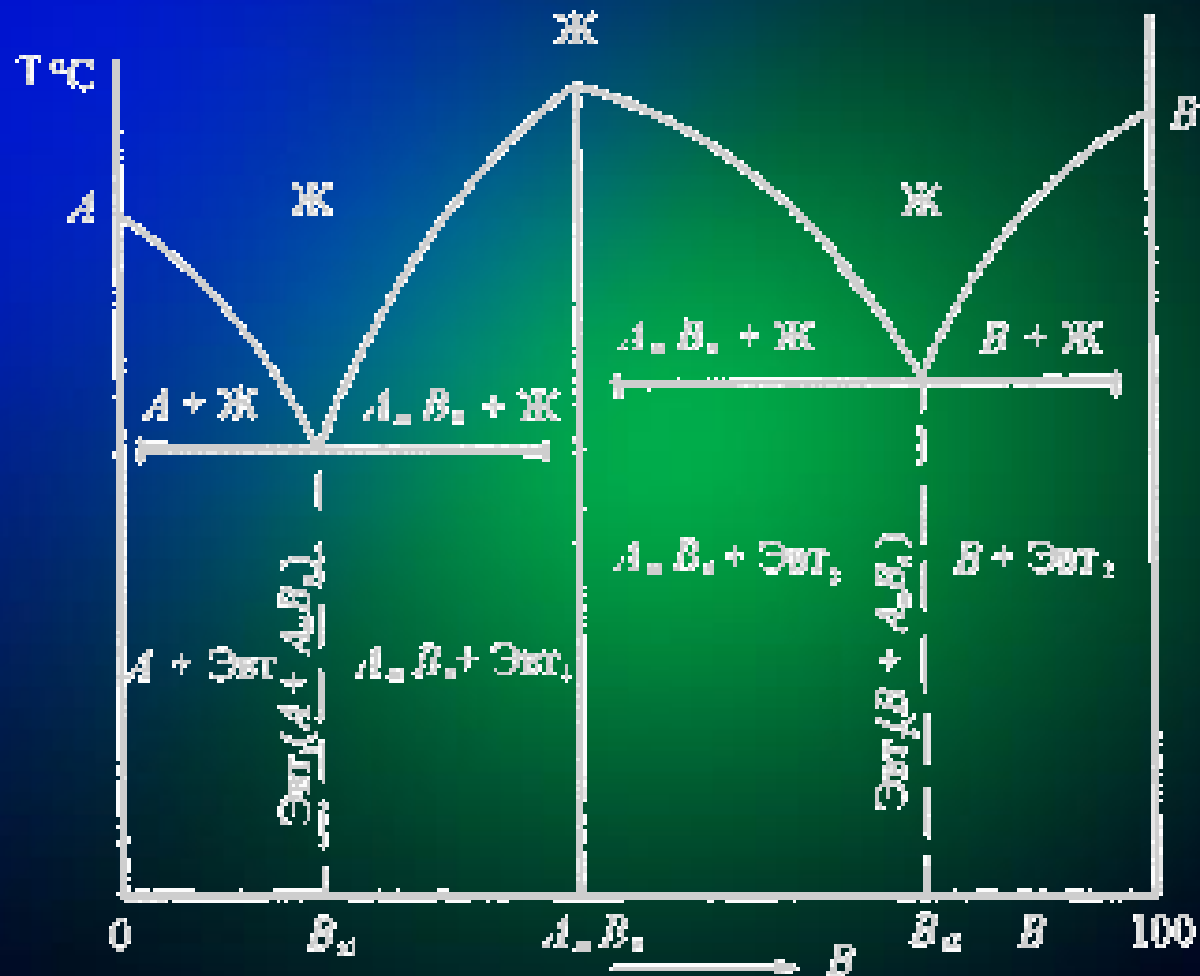
M. Rotter, M. Pangerl et al.

Angew. Chem. Int. Ed. 47 7949-52 (2008).

Superconducting phase as a solid solution

One should take into account that according to the phase diagram with congruently melting compound, after reaction between initial substances first crystallizes main phase with higher temperature of crystallization and then if it's a small difference between crystallization temperature of the main phase and the initial reagent, it forms the solid solution.

Superconducting phase as solid solution



Self-flux method

Our system is $\text{Ba(Fe,Ni)}_2\text{As}_2$

Various routes of synthesis:

1) From elements (pressure required):



2) From precursors:



3) From pure phases:



Self-flux method

Our system is $\text{Ba(Fe,Ni)}_2\text{As}_2$

Various routes of synthesis:

1) From elements (pressure required):



2) From precursors:



3) From pure phases:

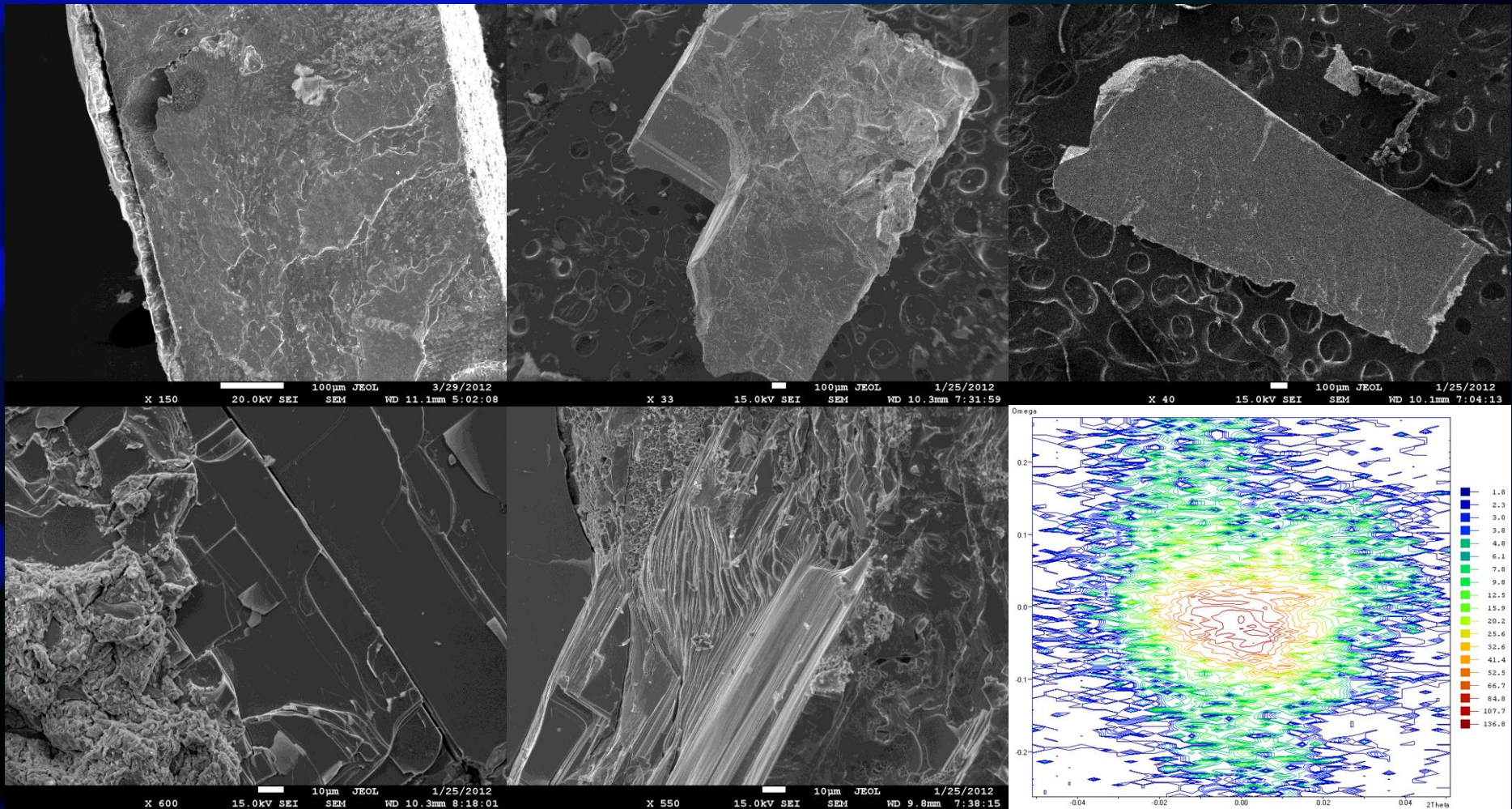


Contamination of single crystals

Possible contaminants:

- 1. Initial substances**
- 2. Crucible material**
- 3. Other outer contaminants**

Self-flux method



SEM images of BaFe₂As₂ single crystals with different dopants grown by self-flux method. Top panels (from left to right): BaFe_{1.94}Co_{0.06}As₂, BaFe_{1.9}Ni_{0.1}As₂, BaFe_{1.86}Ni_{0.14}As₂. Bottom panels (from left to right): BaFe_{1.88}Ni_{0.12}As₂, BaFe_{1.9}Ni_{0.1}As₂ and 2D view of the (006) reflex for BaFe_{1.9}Ni_{0.1}As₂.

Summary

- ✓ 122 compound is a solid solution
- ✓ There is no notable contamination of single crystals by reagents or flux
- ❖ Contamination of the single crystals may be induced by wrong speed of crystallization

**Thank you
for your
attention!**