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Influence of controlled point disorder on normal state and superconducting properties of iron pnictides

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International workshop on
Recent developments in Fe-based high-temperature superconductors

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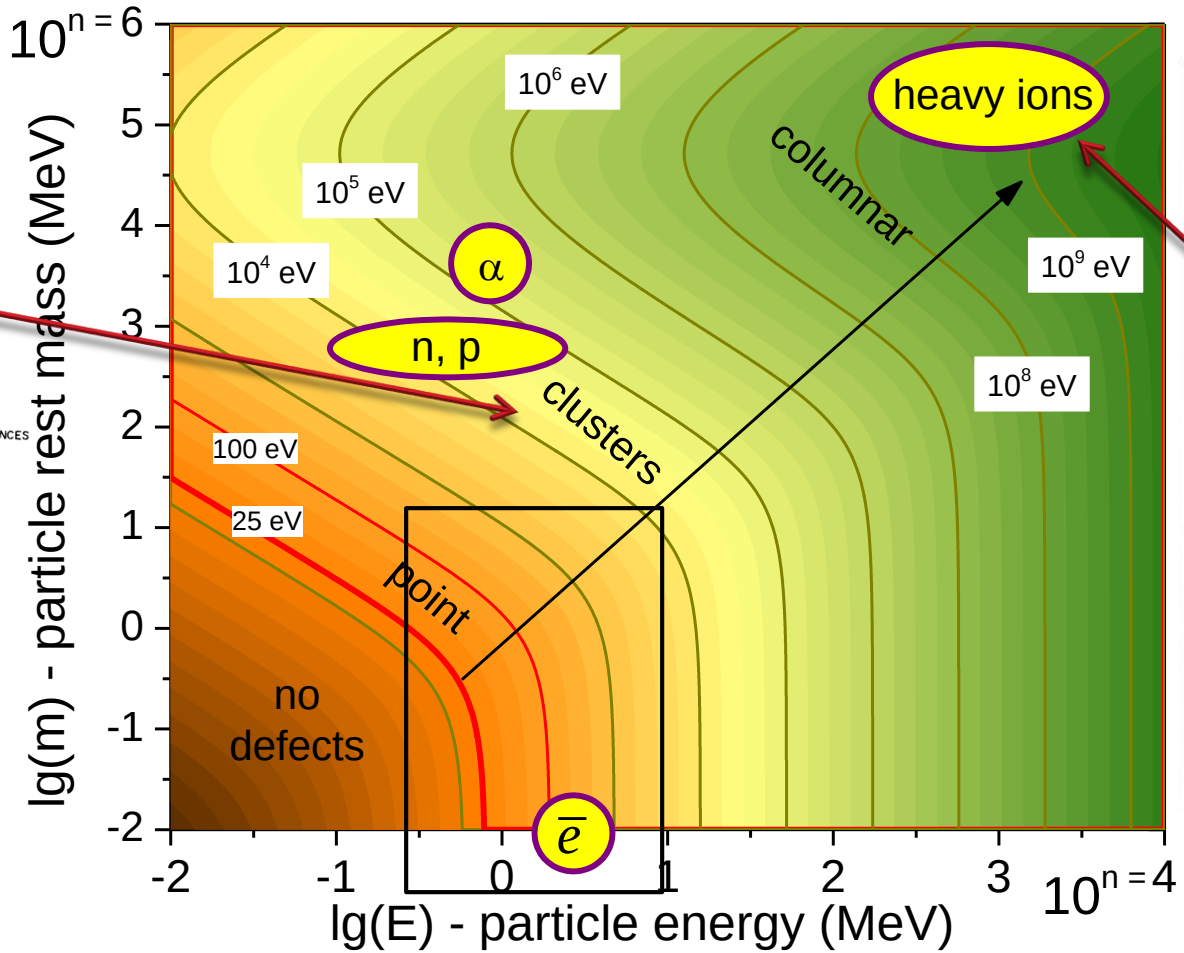
3 September 2013

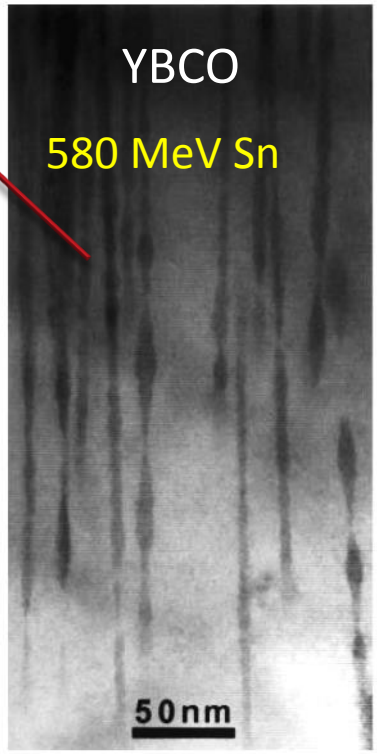
different types of irradiation – we need point defects

$$E_{p,\max} = \frac{2E\left(E+2mc^2\right)Mc^2}{\left(\left(m+M\right)c^2\right)^2 + 2EMc^2}$$

- maximum energy transfer to Fe upon head – on collision

A. C. Damask and G. J. Dienes, *"Point Defects in Metals"* (1963)





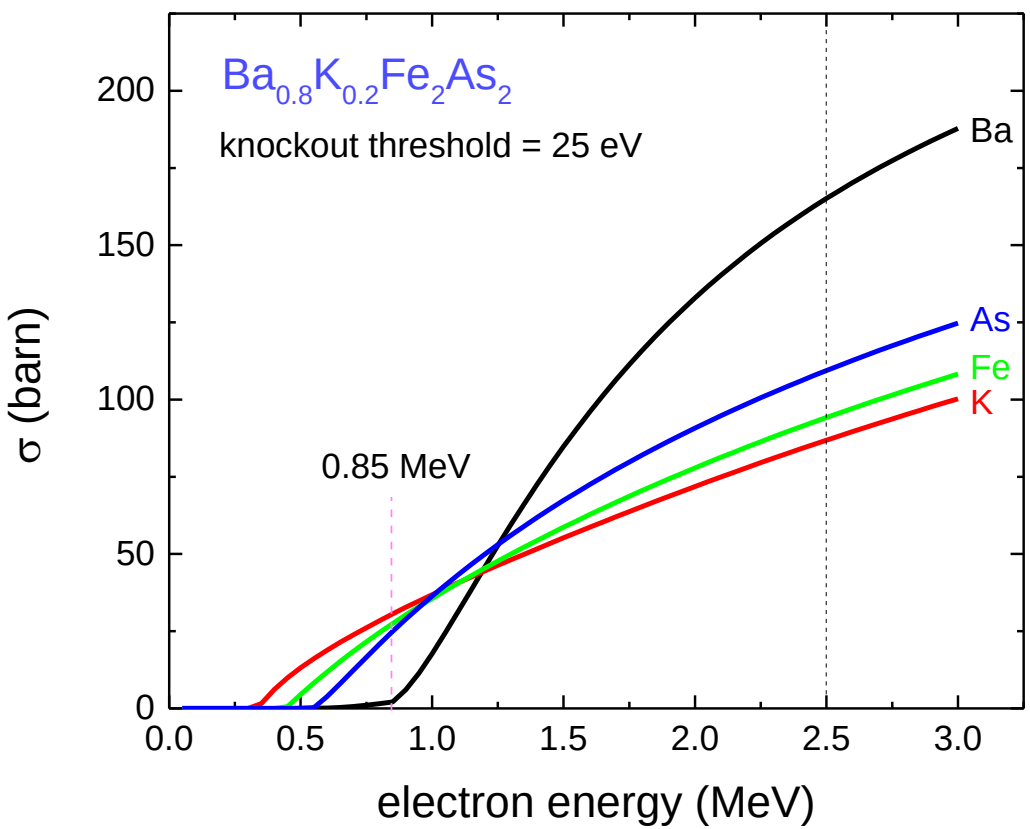
electron irradiation. Dose is measured in C/cm^2

(we omit cm^2 and just write C)

$$|e| = 1.60217733 \times 10^{-19}\ \mathrm{C}$$

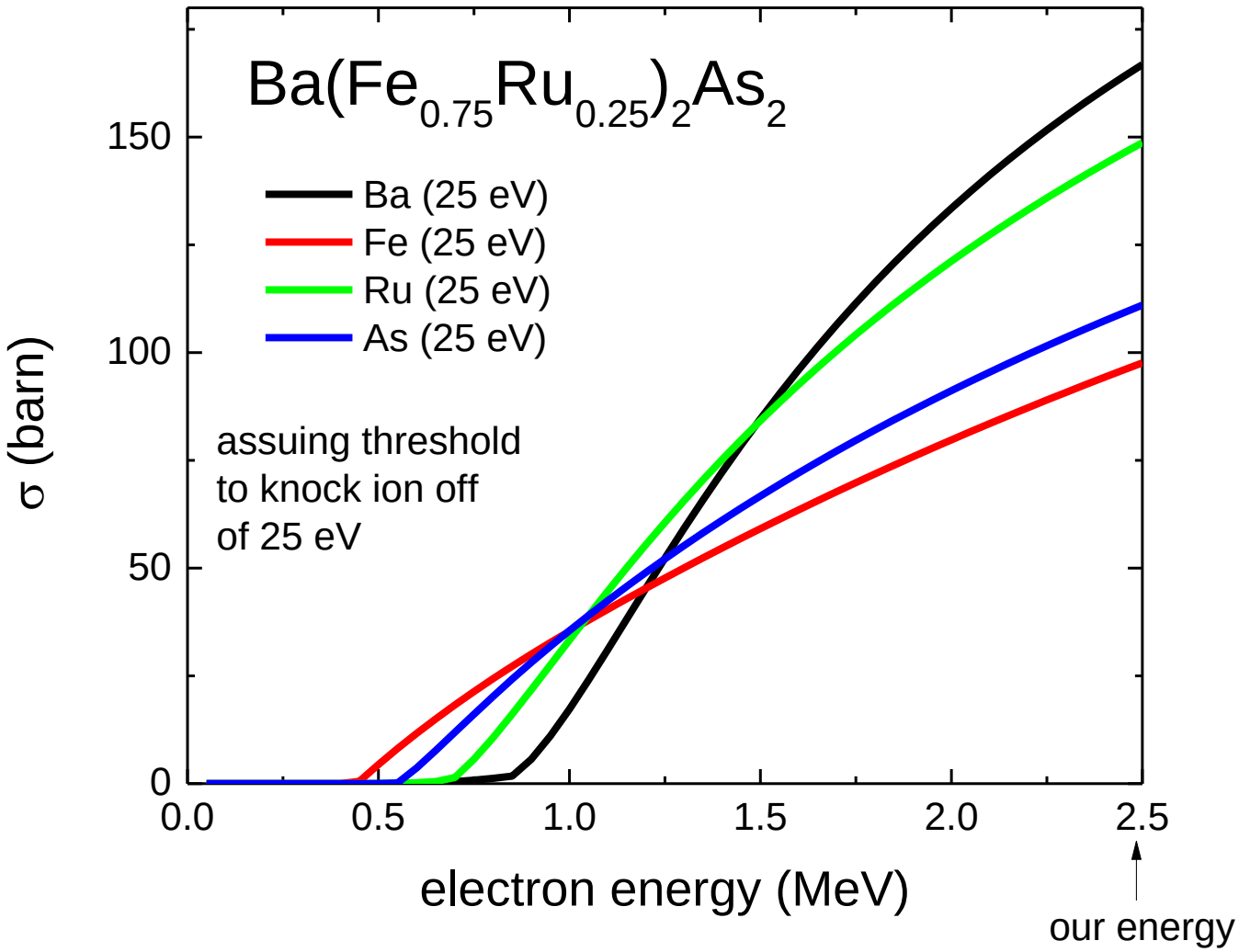
$$1\,\mathrm{C} = 6.2415 \times 10^{18}\ \text{electrons}$$

Knockout cross-section assuming 25 eV threshold energy

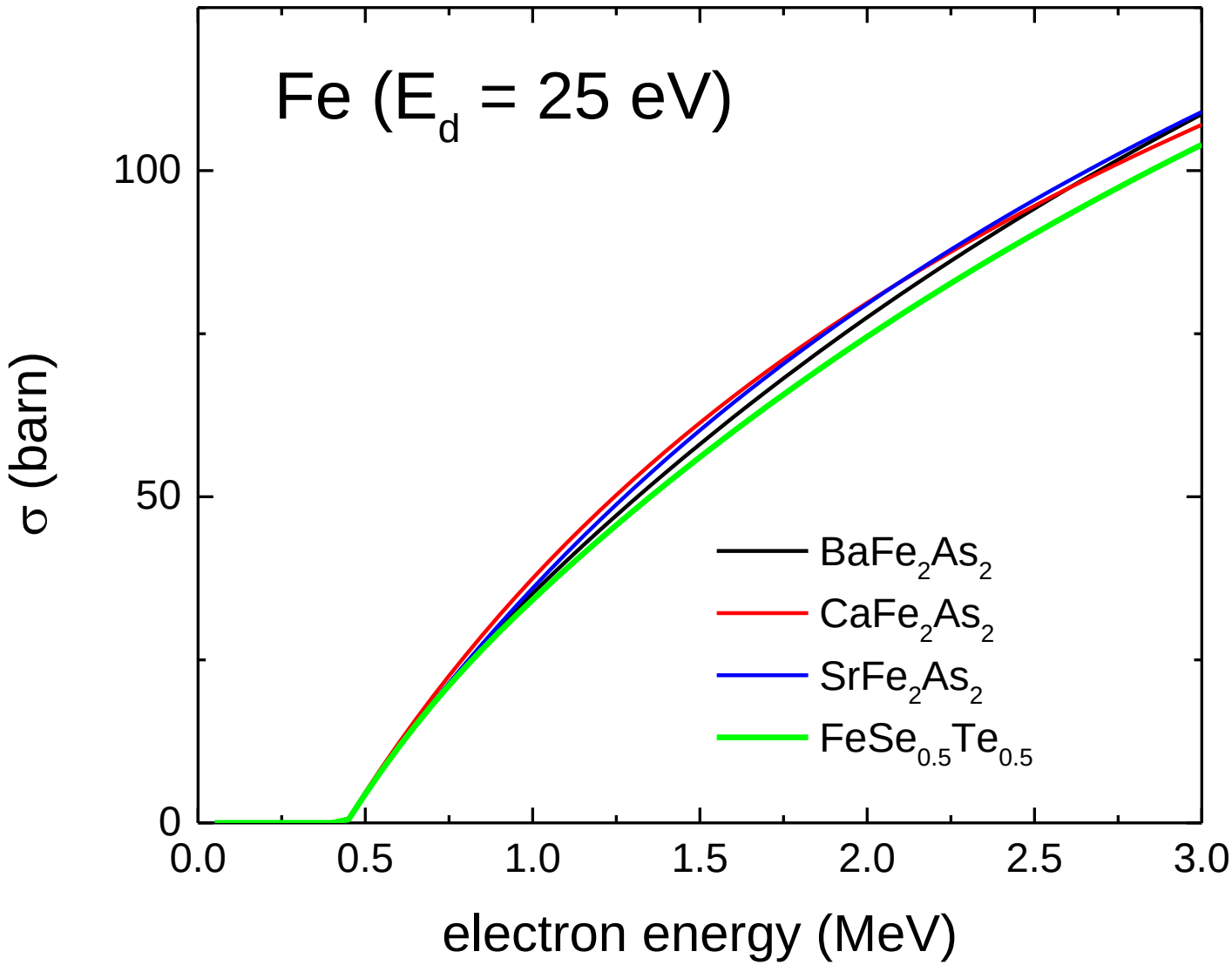


It would be nice to calculate actual threshold energies for different ions and the resulting magnetic state of defects.
I can re-calculate the cross-sections if I knew the thresholds.
Now I assumed 25 eV

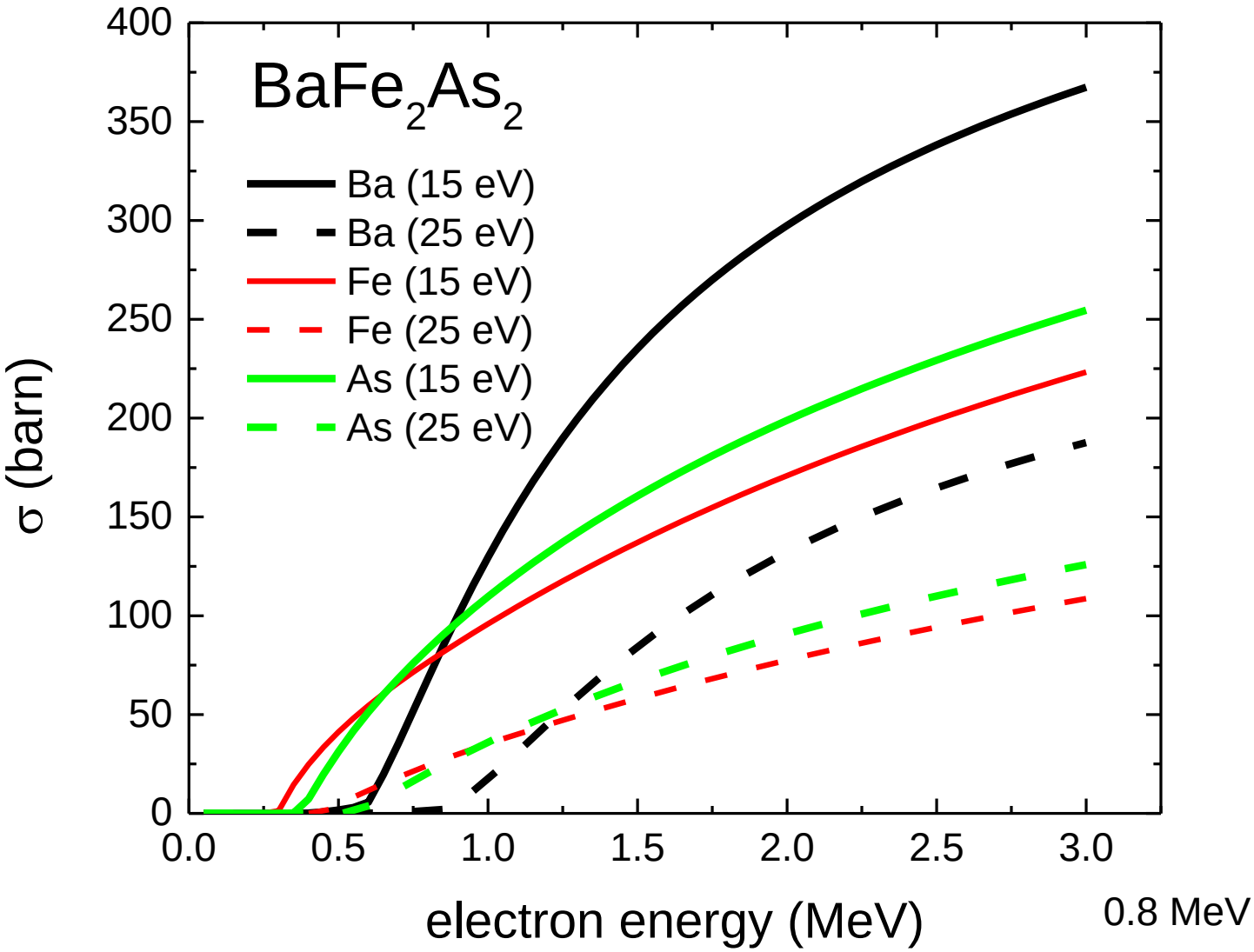
cross - section for producing primary knock-outs by electron irradiation



Fe knock – out – different compounds



different threshold energies

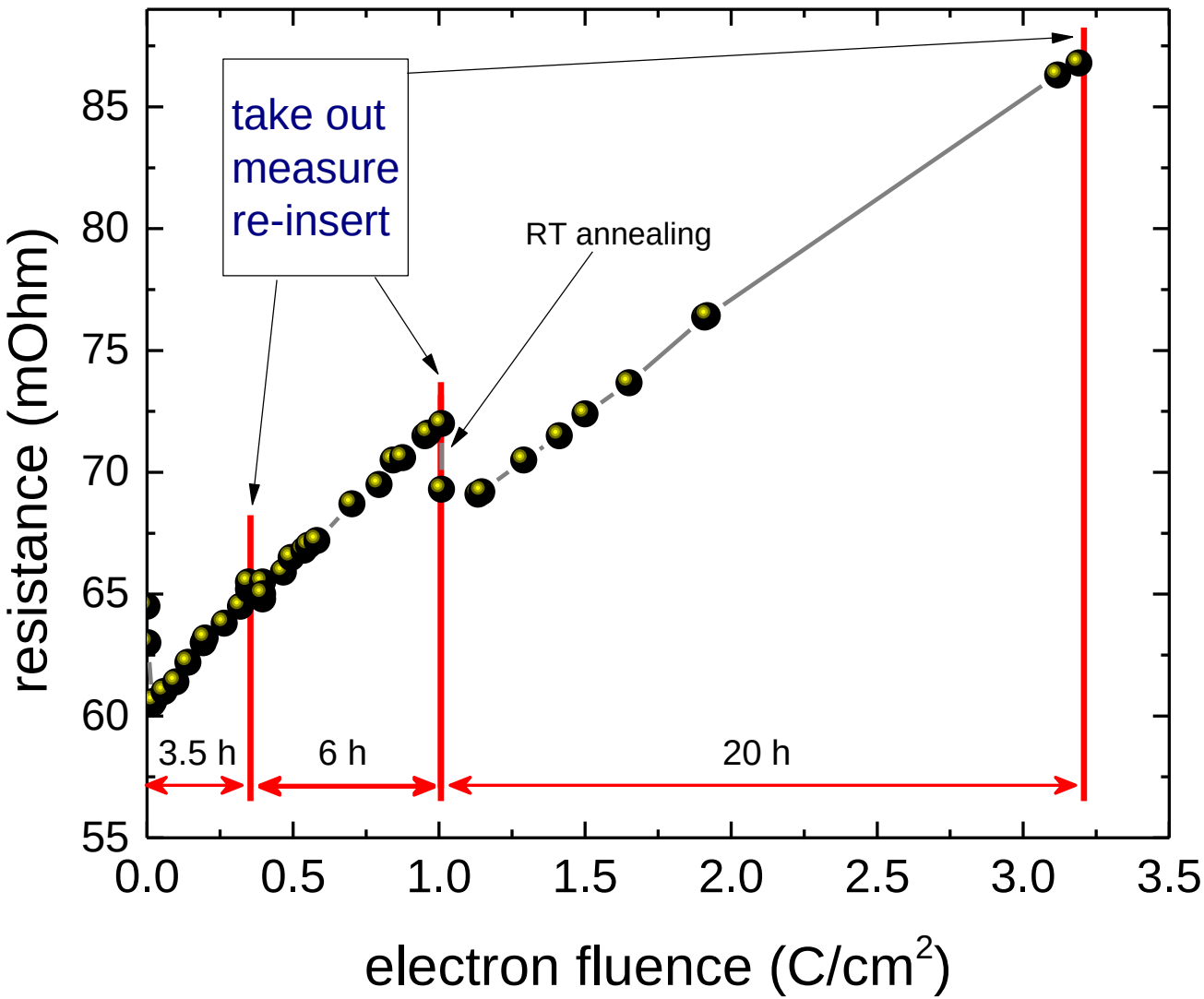


0.8 MeV

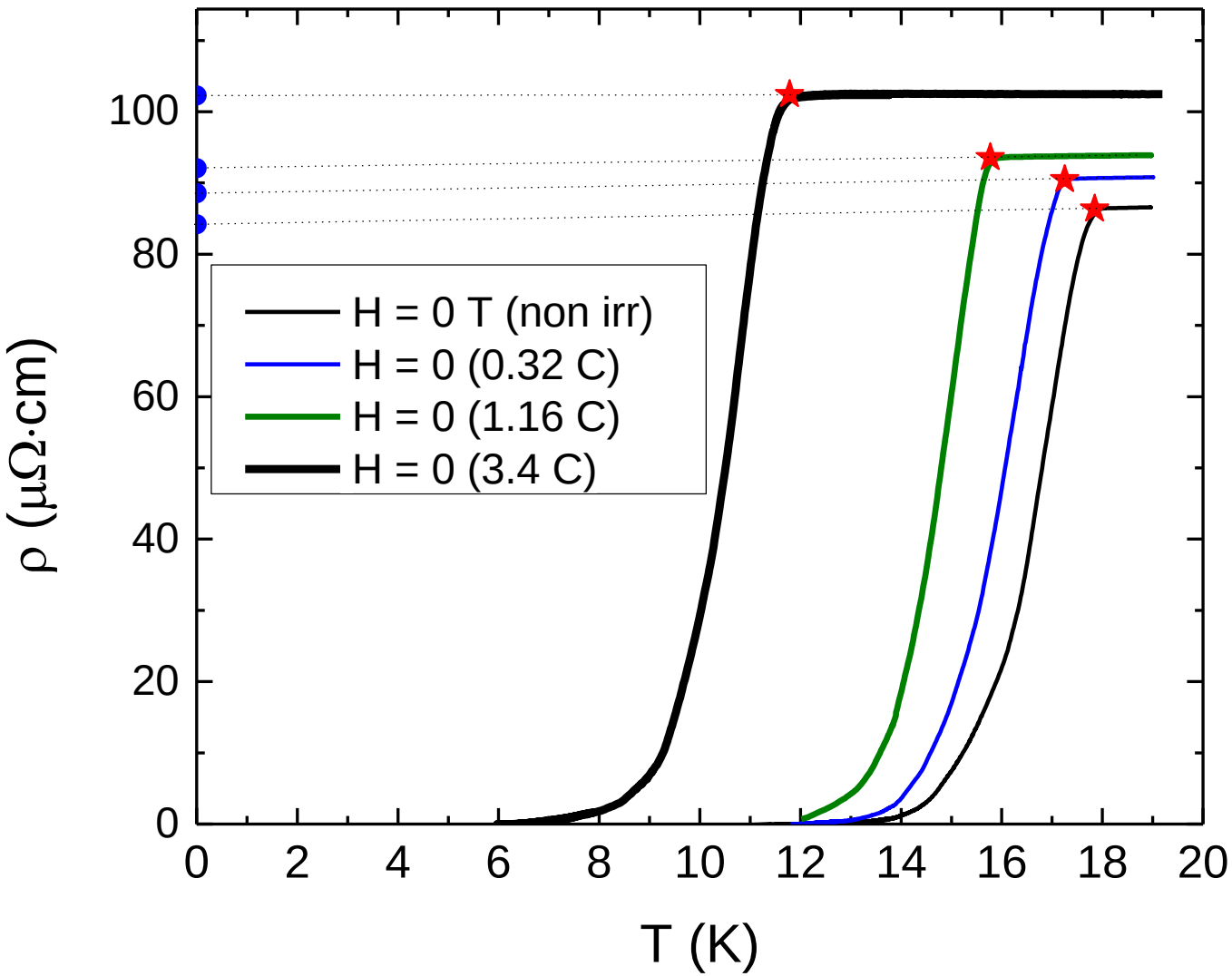
$Ba(Fe_{1-x}Ru_x)_2As_2$

May 2012

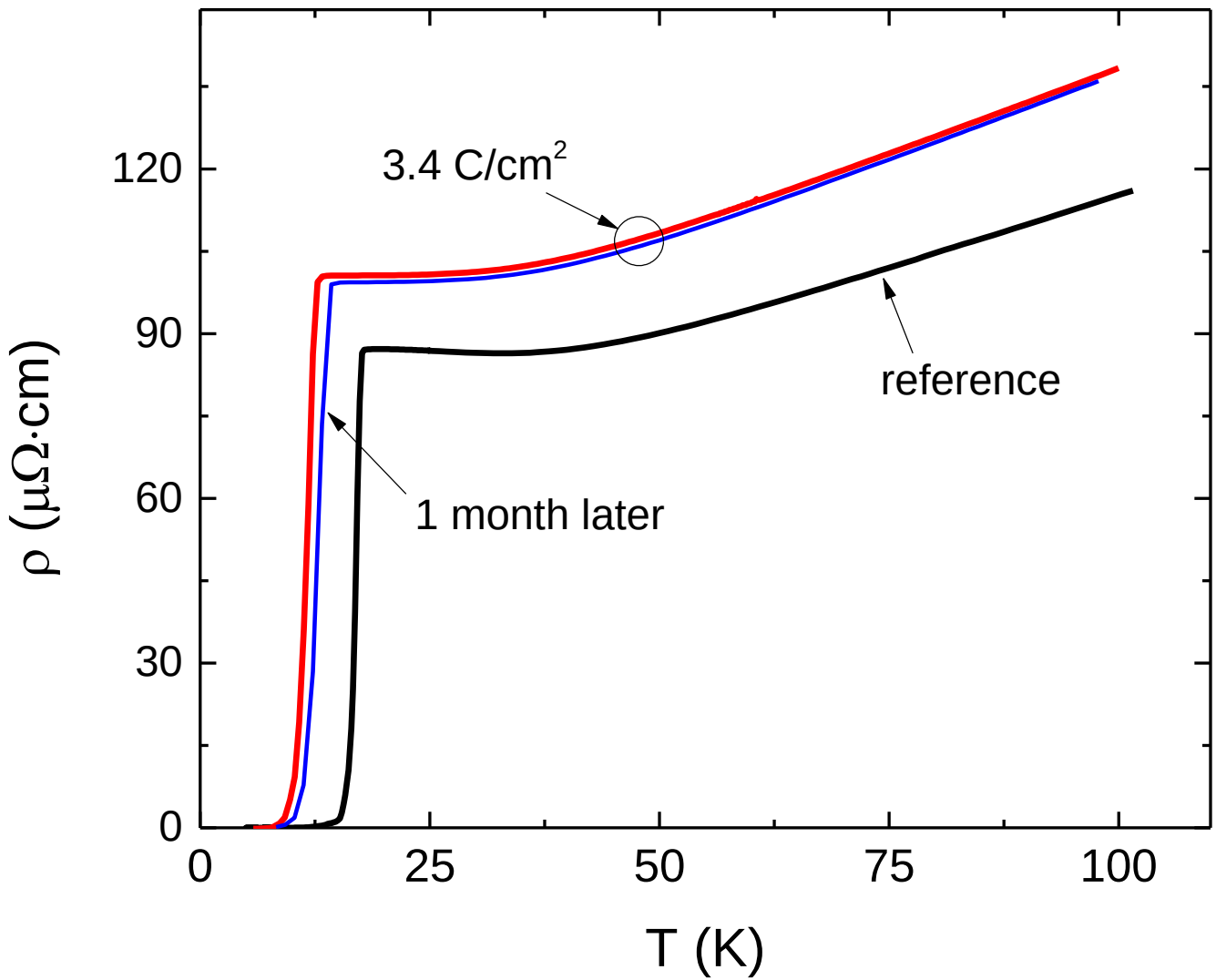
$Ba(Fe_{1-x}Ru_x)_2As_2$: in situ measurements of ρ(T)



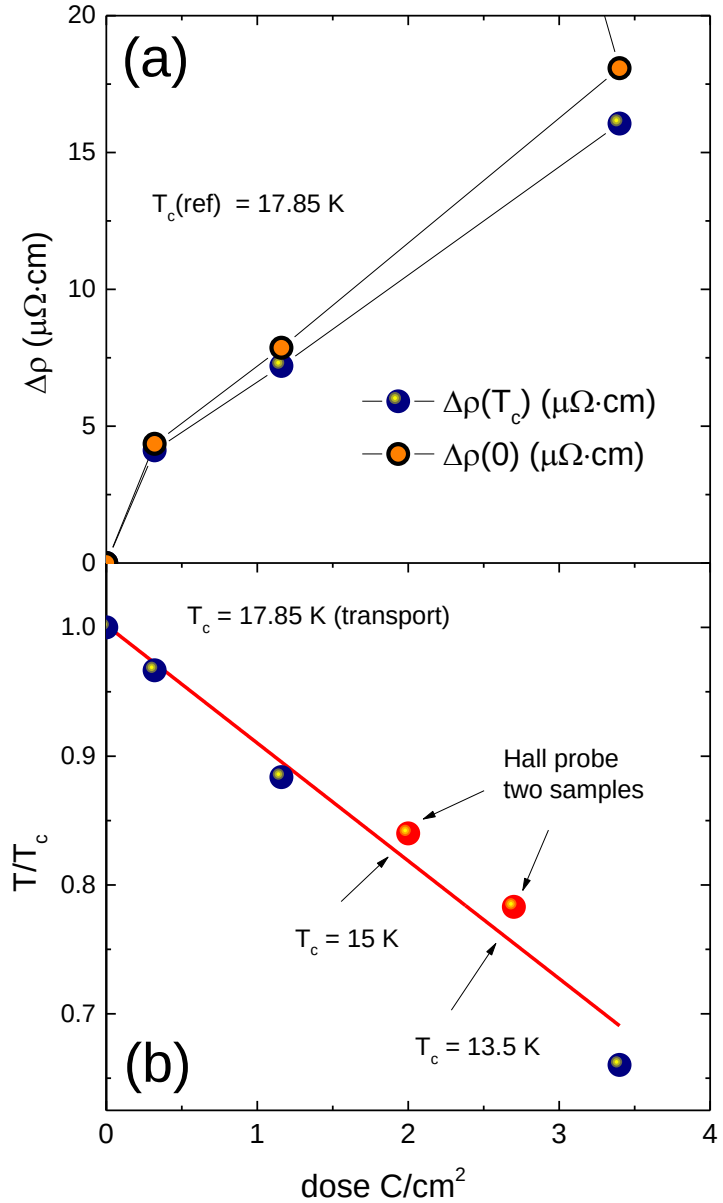
$Ba(Fe_{1-x}Ru_x)_2As_2$: take out and measure



after initial annealing defects stay



T_c decreases, ρ increases, - not isotropic s_{++}!



the main question:

how to calculate the scattering rate?

Spherical cow (AG + Drude) model:

$$\rho = \frac{\hbar}{2\pi k_B T_c \tau} = \frac{\hbar}{2\pi k_B T_{c0} \tau}\frac{T_{c0}}{T_c} = g\frac{T_{c0}}{T_c}$$

so, we need τ^{-1}. From Drude: $\rho = \frac{m^*}{ne^2\tau} \Rightarrow \frac{1}{\tau} = \frac{\rho n e^2}{m^*}$

Δρ or ρ - Peter says Δρ . . .

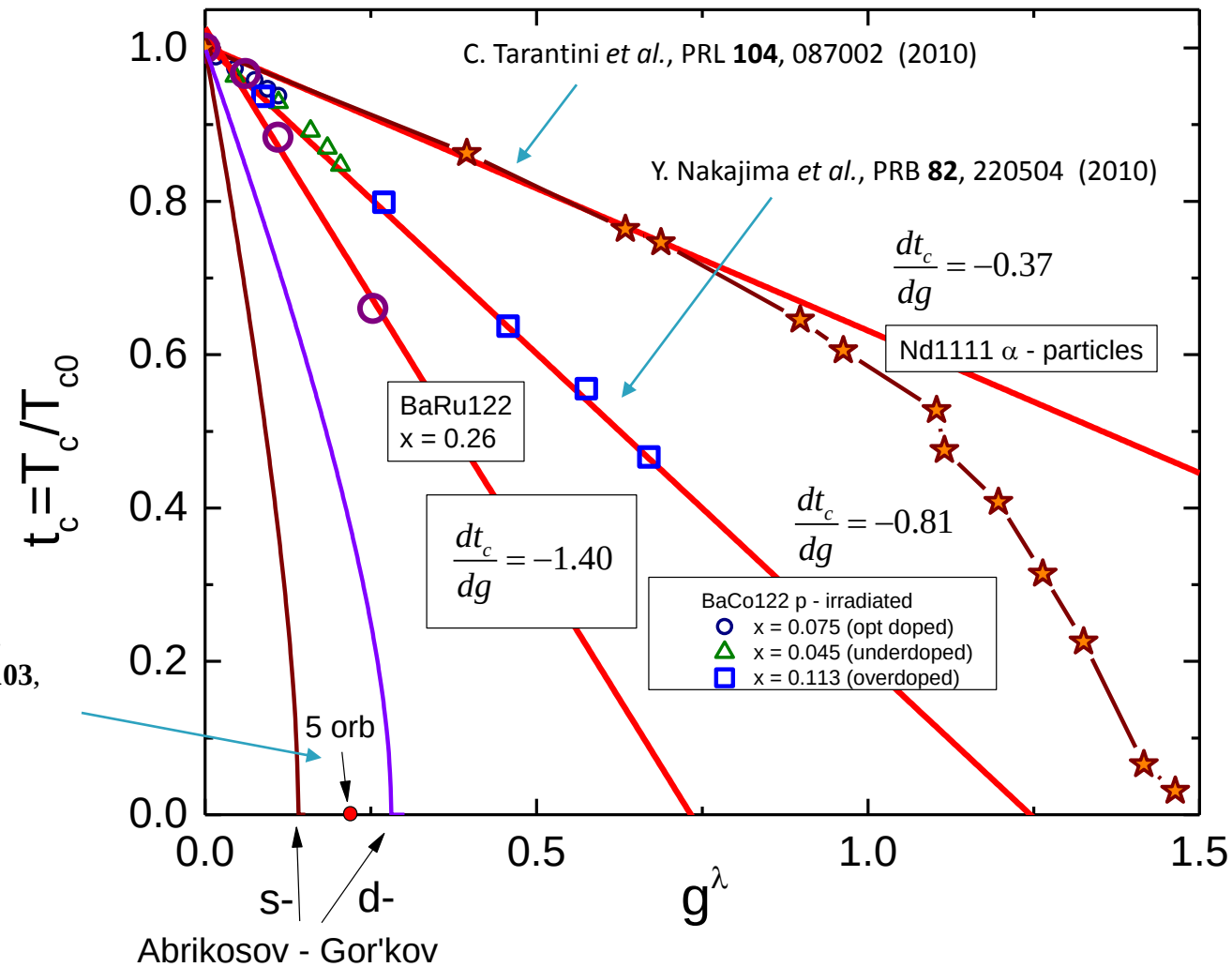
with Hall: $R_H = \frac{1}{ne}, \tau^{-1} = \frac{\rho e}{R_H m^*}$

using penetration depth is the best choice as it avoids the question of the effective mass

With London pen. depth: $\lambda^2 = \frac{m^*}{\mu_0 n e^2} \Rightarrow \tau^{-1} = \frac{\rho}{\lambda^2 \mu_0}$

$$g^\lambda = \frac{\hbar}{4\pi k_B \mu_0}\frac{\Delta\rho}{T_{c0}\lambda^2} \approx 9674\frac{\Delta\rho\ [\mu\Omega\cdot\mathrm{cm}]}{T_{c0}\ [\mathrm{K}](\lambda\ [\mathrm{nm}])^2}$$

summary of T_c suppression data (using g^λ)



S. Onari and H. Kontani, PRL **103**, 177001 (2009)

A. A. Abrikosov and L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **39**,1781 (1960). [Sov. Phys. JETP **12**, 1243 (1961)].

L. A. Openov, Phys. Rev. B **58**, 9468 (1998) ; V. G. Kogan, Phys. Rev. B **80**, 214532 (2009).

Generalized Abrikosov – Gor'kov theory

Classical Abrikosov – Gor'kov:

A. A. Abrikosov and L. P. Gor'kov, Zh. Eksp. Teor. Fiz. 39,1781 (1960). [Sov. Phys. JETP 12, 1243 (1961)].

$$t_c = T_c / T_{c0}\,,\; g_m = t_c \rho_m = \frac{\hbar}{2\pi k_B T_c \tau_m}$$

$$\ln(t_c) = \psi\left(\frac{1}{2}\right) - \psi\left(\frac{g_m}{t_c} + \frac{1}{2}\right),\; g_m^{crit} = 0.1403$$

Generalized AG – arbitrary FS and gap. Both magnetic and non – magnetic scattering:

L. A. Openov, Phys. Rev. B **58**, 9468 (1998) ; V. G. Kogan, Phys. Rev. B **80**, 214532 (2009).

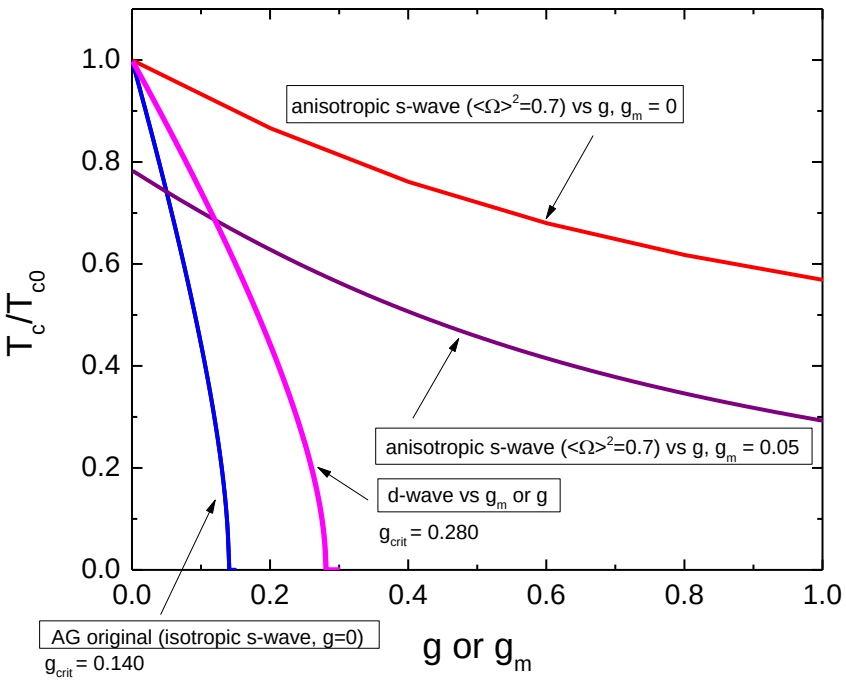
$$\ln(t_c) = \psi\left(\frac{1}{2}\right) - \psi\left(\frac{g+g_m}{2t_c} + \frac{1}{2}\right) + \langle\Omega\rangle^2 \left[\psi\left(\frac{g+g_m}{2t_c} + \frac{1}{2}\right) - \psi\left(\frac{g_m}{t_c} + \frac{1}{2}\right)\right]$$

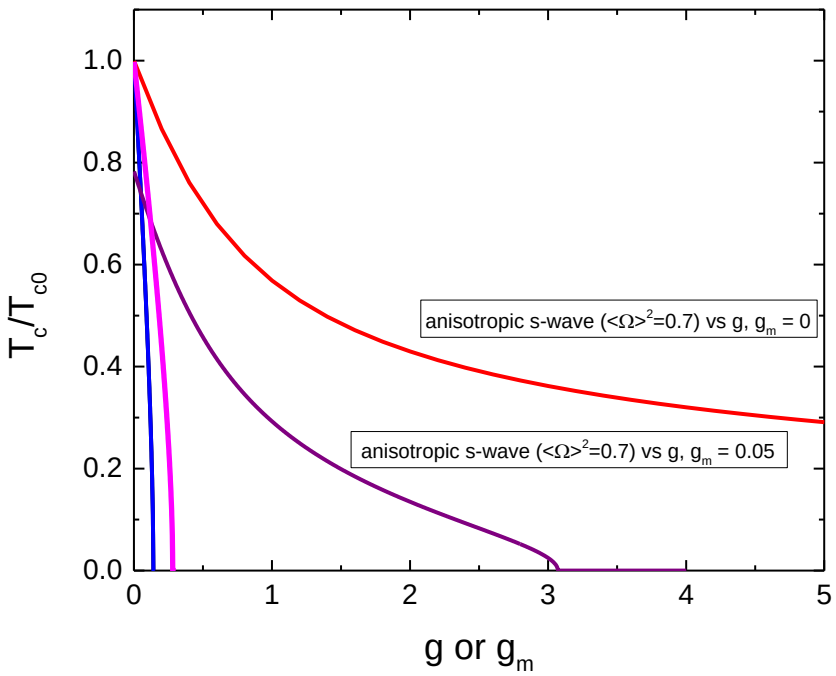
$$\frac{1}{\tau_\pm} = \frac{1}{\tau} \pm \frac{1}{\tau_m} \qquad \langle X \rangle = \oint\!\!\oint_{FS} \frac{X(\mathbf{k_F})}{(2\pi)^3 \hbar N(0) |\mathbf{v_F}|} d^2\mathbf{k_F}, \qquad \langle \Omega^2 \rangle = 1$$

- angular part of the order parameter

Still the scattering potential strength and two – band effects are not considered

even in this simple picture dt_c/dg varies





$$g^{crit} = \frac{\Delta(0)}{4\pi T_{c0}} = 0.140$$

If the gap is anisotropic, dt_c/dg can have any values

arbitrary strength, interband scattering

D. V. Efremov *et al.*, PRB **84**, 180512 (2011)

$$\tilde{\Gamma}_{ab} = \Gamma_{a(b)} \frac{1-\tilde{\sigma}}{\tilde{\sigma}(1-\tilde{\sigma})\eta \frac{(N_a+N_b)^2}{N_a N_b} + (\tilde{\sigma}\eta - 1)^2}$$

- effective inter-band scattering rate

η defines intraband (v) and interband (u) scattering: $v^2 = \eta u^2$

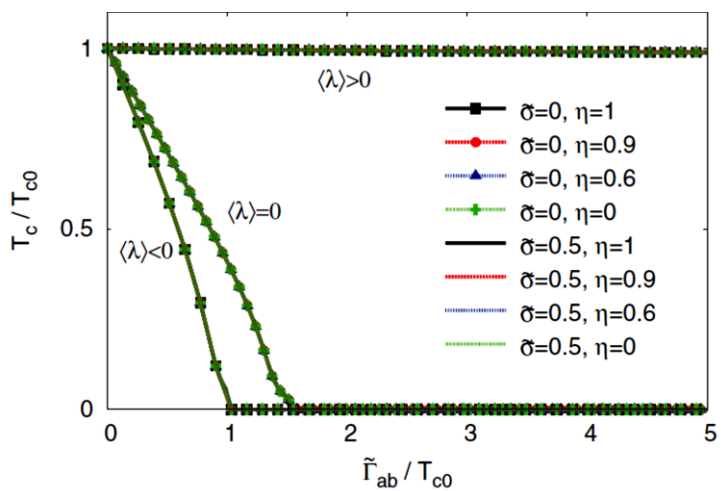
$$\mathbf{U}_{\alpha\beta} = (v-u)\delta_{\alpha\beta} + u$$

$$\tilde{\sigma} = \frac{\pi^2 N_a N_b u^2}{1+\pi^2 N_a N_b u^2}$$

- scattering cross - section

$$\Gamma_{a(b)} = n_{imp}\pi N_{b(a)} u^2 (1-\tilde{\sigma})$$

- generalized normal state scattering rate parameter used in a γ-model



$$\boldsymbol{\lambda} = \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{pmatrix}, \lambda_{ij} = \frac{N_i}{N(0)} \lambda_{ij}^{\gamma} = N_i V_{ij}$$

matrix of interactions

$$\langle\lambda\rangle = (\lambda_{11}+\lambda_{12})\frac{N_1}{N(0)} + (\lambda_{22}+\lambda_{21})\frac{N_2}{N(0)} = \lambda_{11}^{\gamma} + \lambda_{22}^{\gamma} + 2\lambda_{12}^{\gamma}$$

for pnictides we typically find:

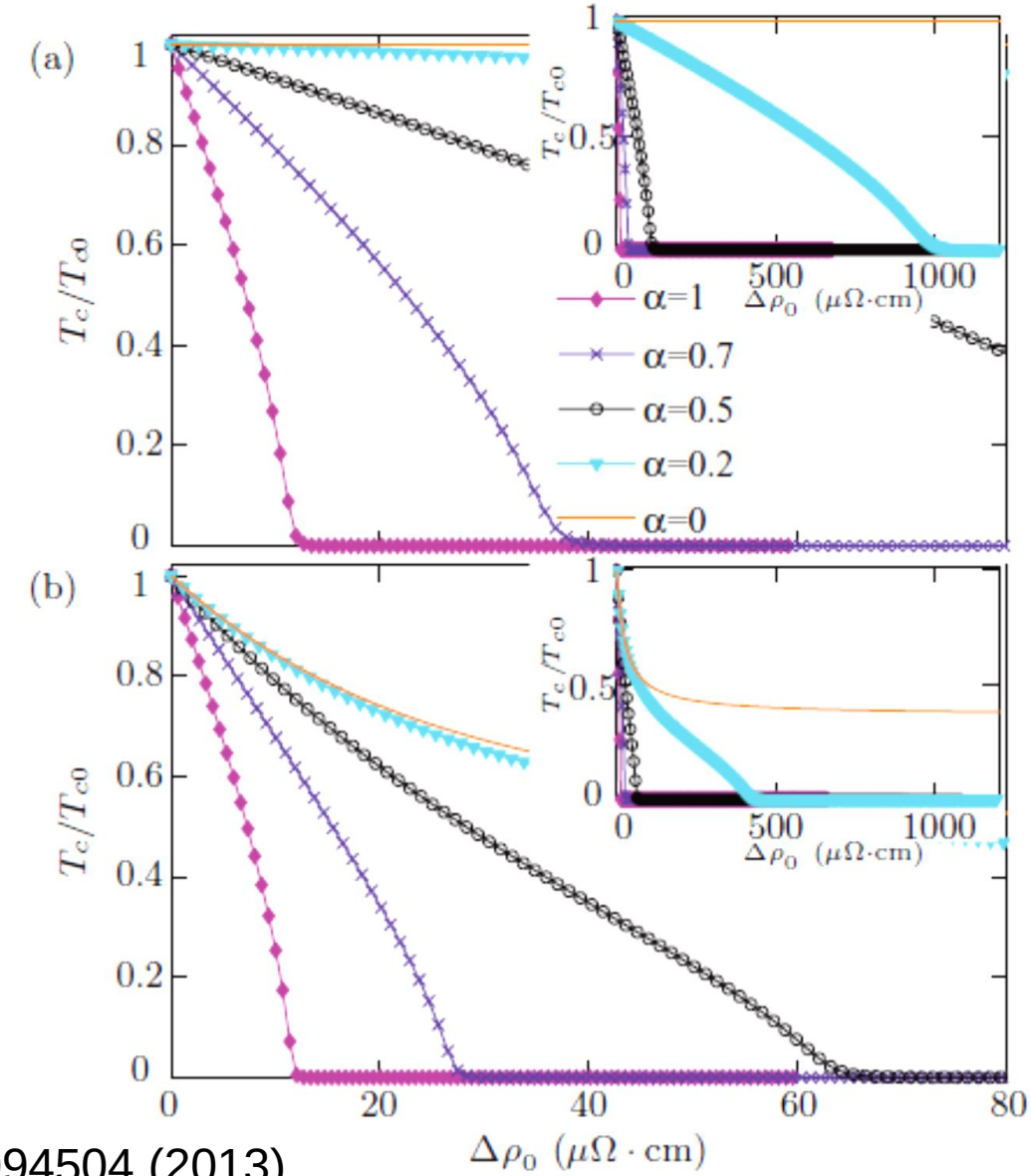
$$\boldsymbol{\lambda}^{\gamma} = \begin{pmatrix} 0.8 & -0.05 \\ -0.05 & 0.4 \end{pmatrix} \Rightarrow \langle\lambda\rangle = 0.11 > 0\,!$$

so, if we include gap anisotropy, it may explain the observed rates of T_c suppression

and with a realistic change of resistivity

Inter to **Intra** – band scattering ratio

$$\alpha = u/v$$

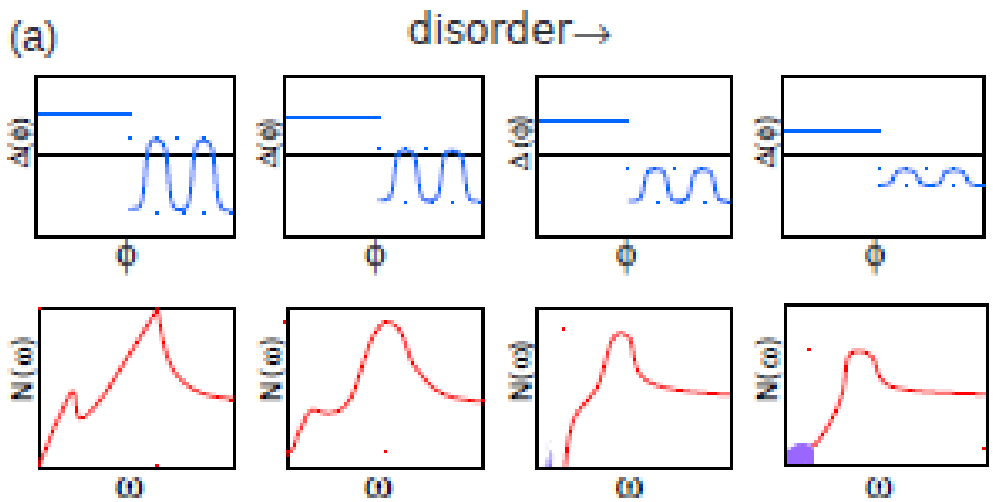


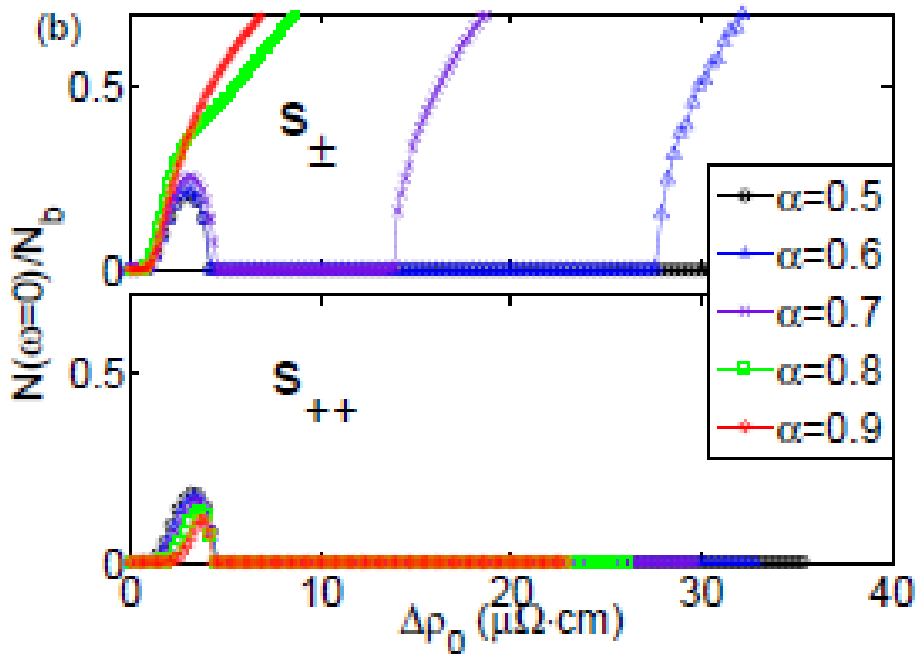
isotropic $s_{\pm}$

nodal $s_{\pm}$

Y. Wang et al, PRB **87**, 094504 (2013)

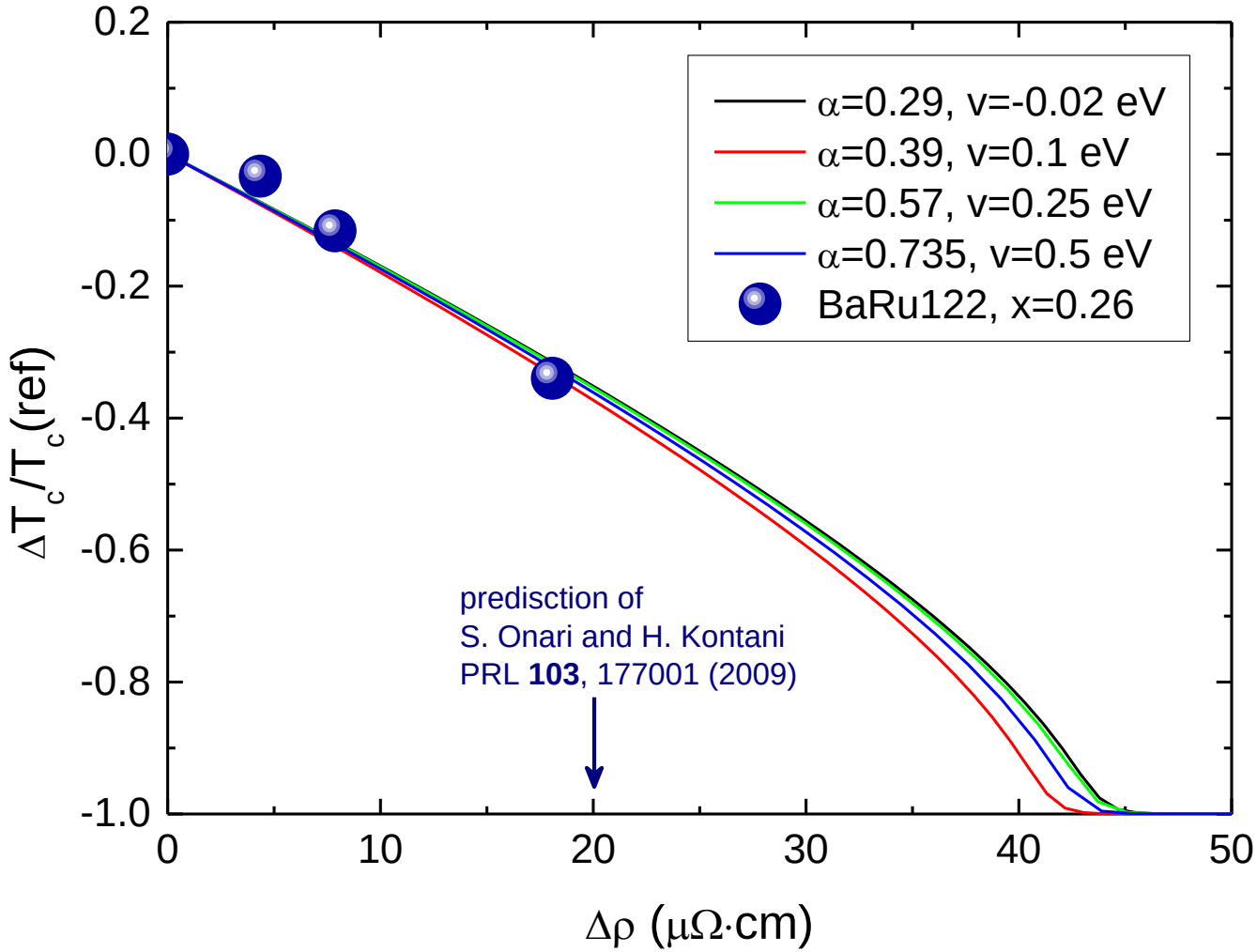
evolution of the order parameter



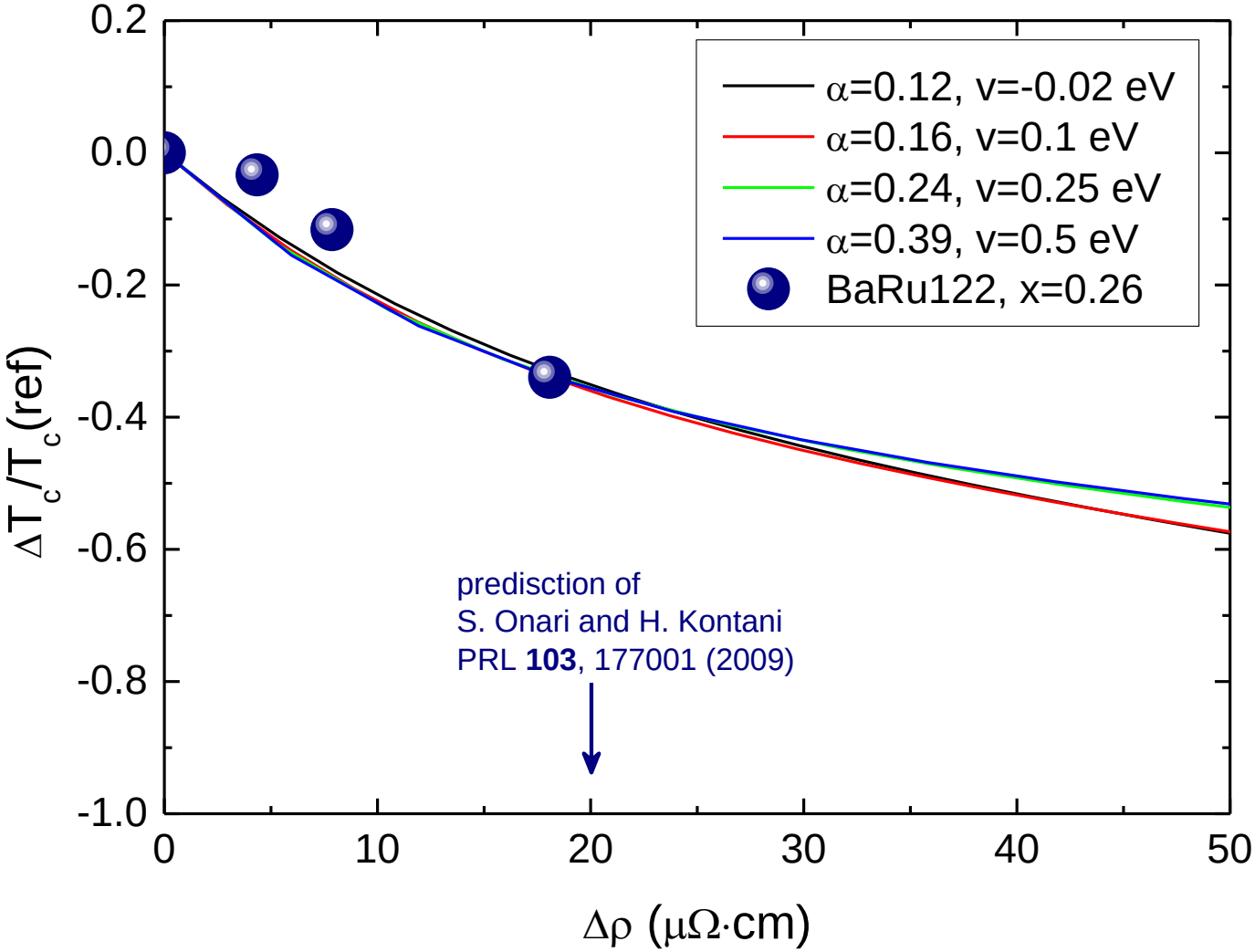


fitting the data with $s_{\pm}$

$\alpha = u/v$ - **Inter** to **Intra** – band scattering ratio

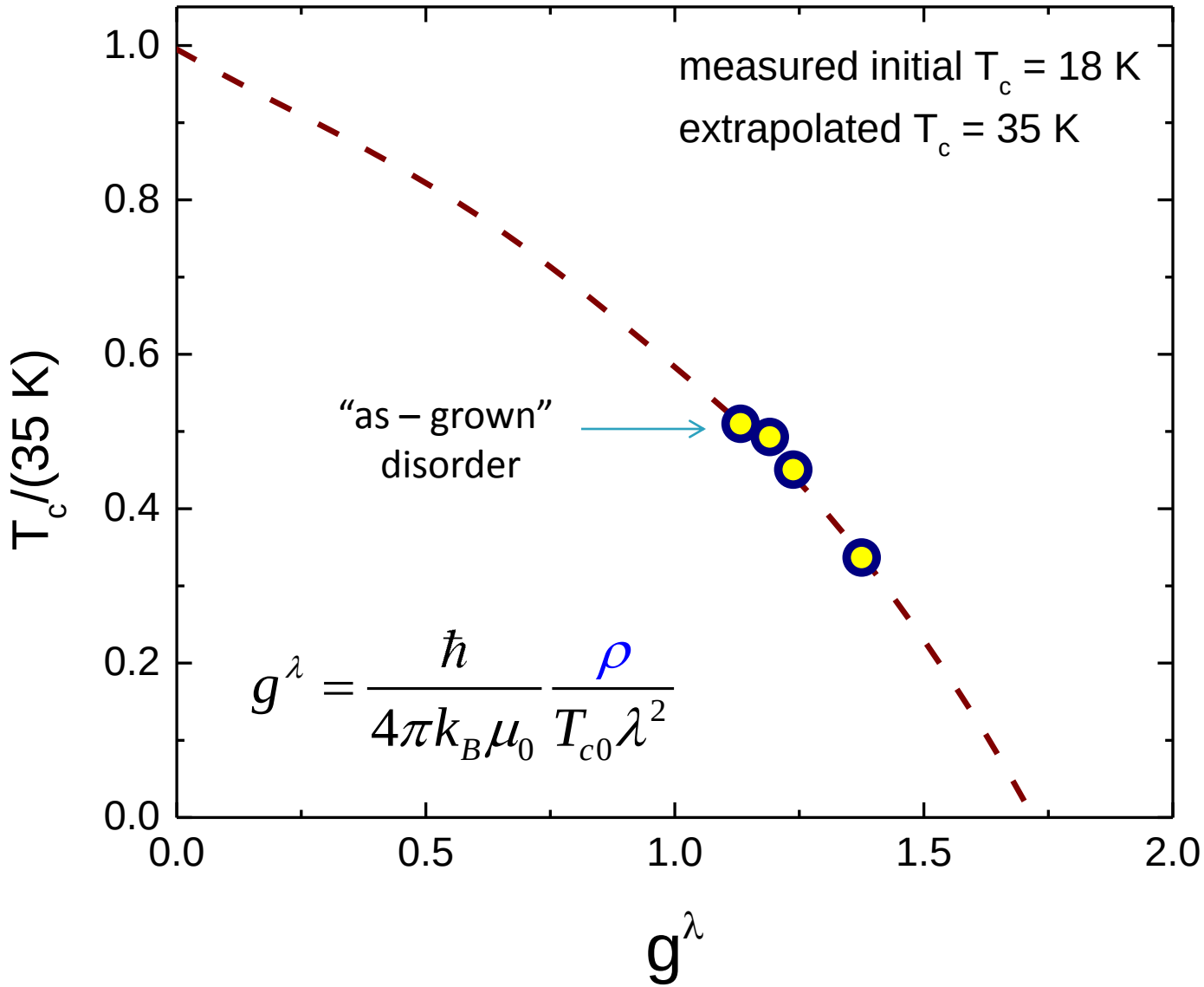


$s_{\pm}$ is definitely compatible with the experiment



but we need more measurements to restrict the phase space

using full resistivity, ρ not Δρ

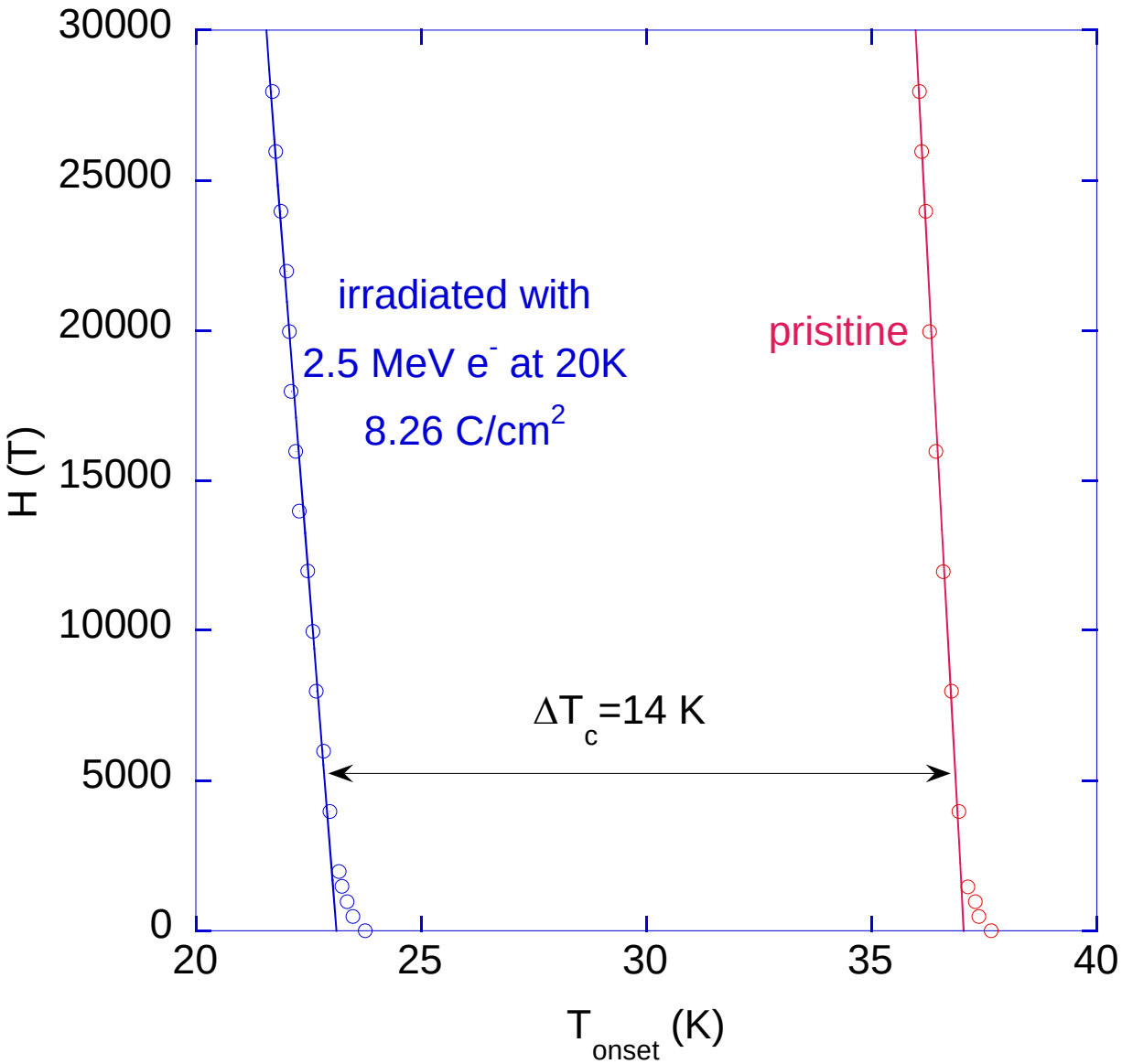


$$g^\lambda = \frac{\hbar}{4\pi k_B \mu_0} \frac{\rho}{T_{c0}\lambda^2}$$

Optimally doped $(Ba_{0.6}K_{0.4})Fe_2As_2$

April 2013

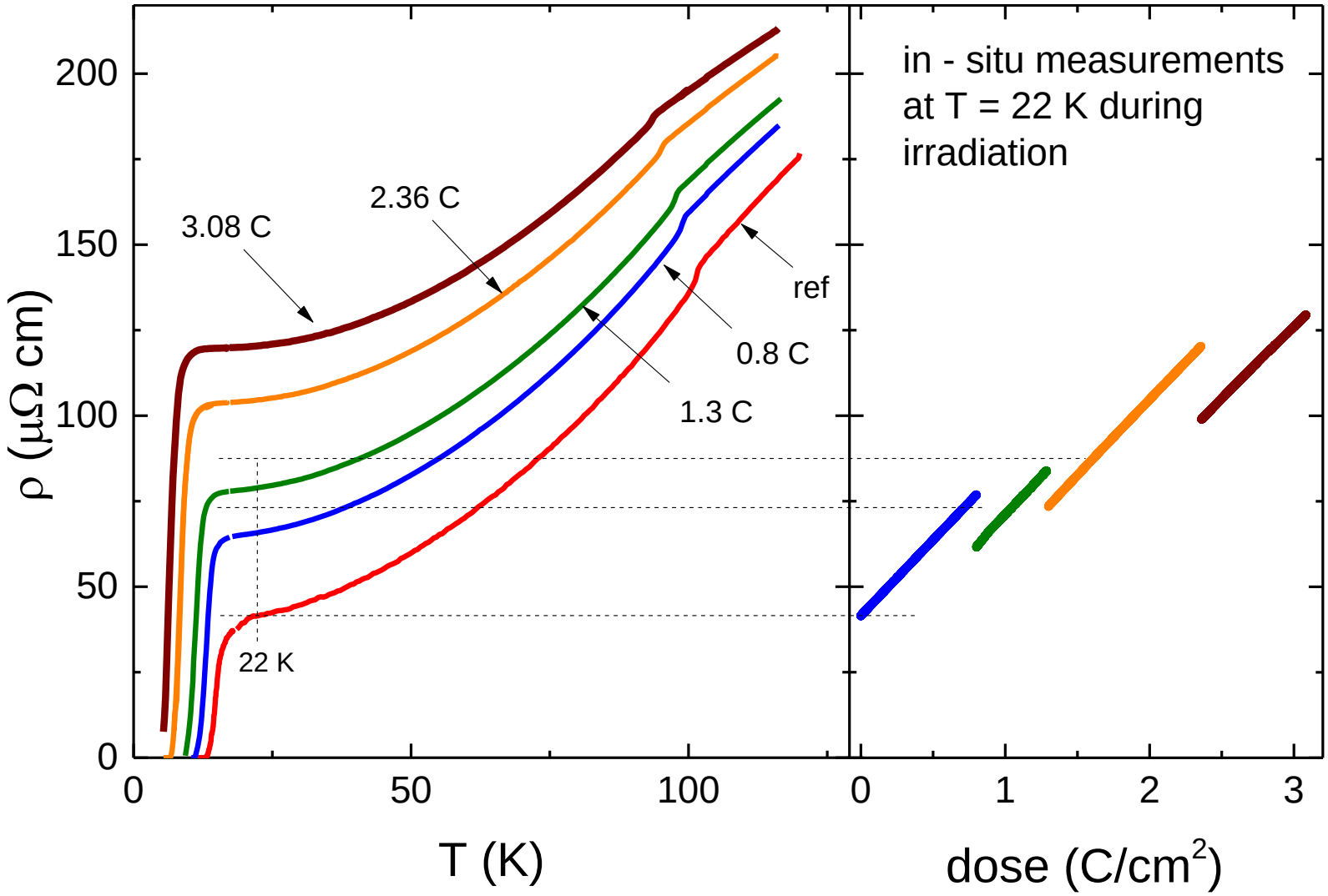
$(Ba_{0.6}K_{0.4})Fe_2As_2$ - definitely not s_{++} !



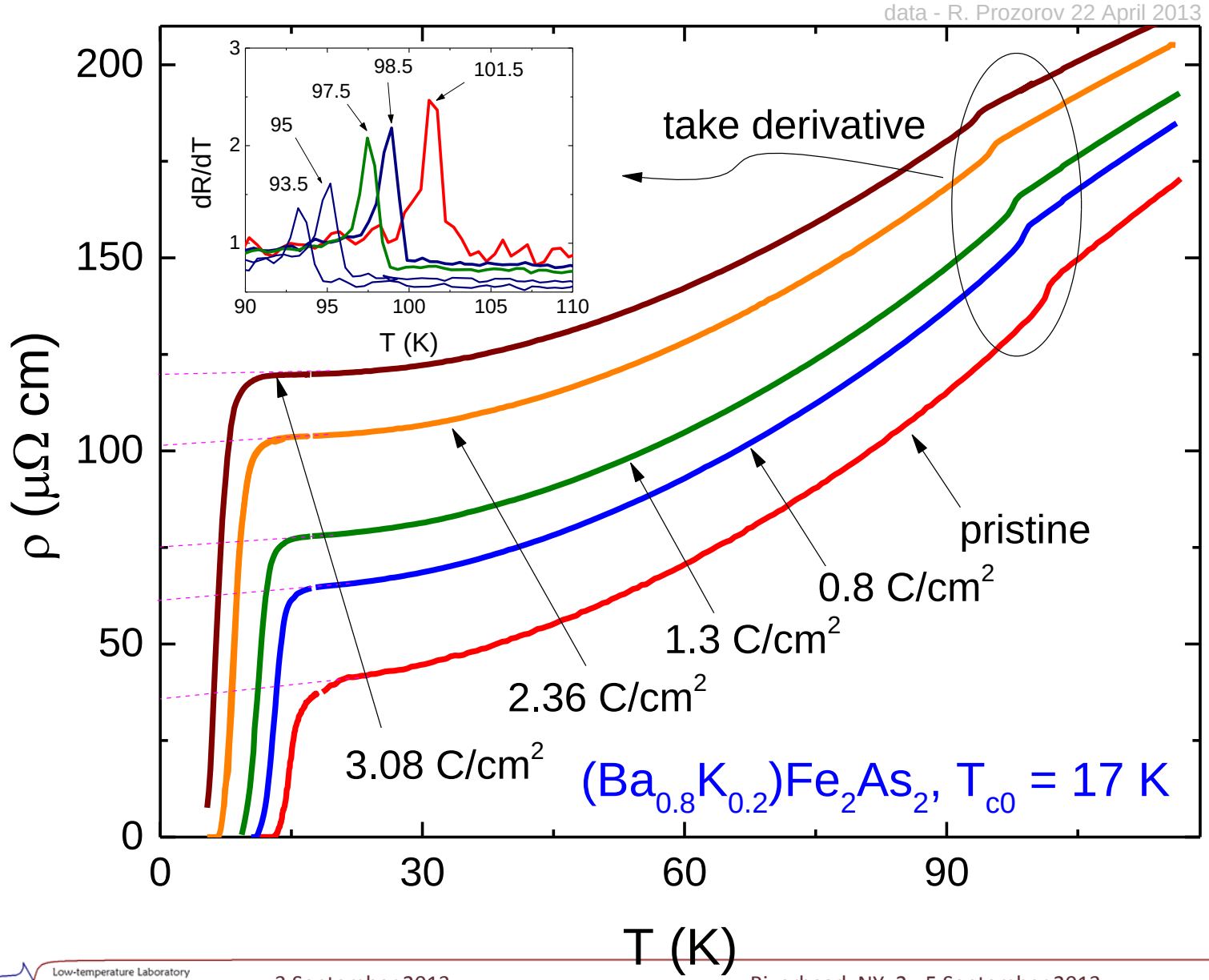
Underdoped (T_{c0} = 17 K), $(Ba_{0.8}K_{0.2})Fe_2As_2$

April 2013

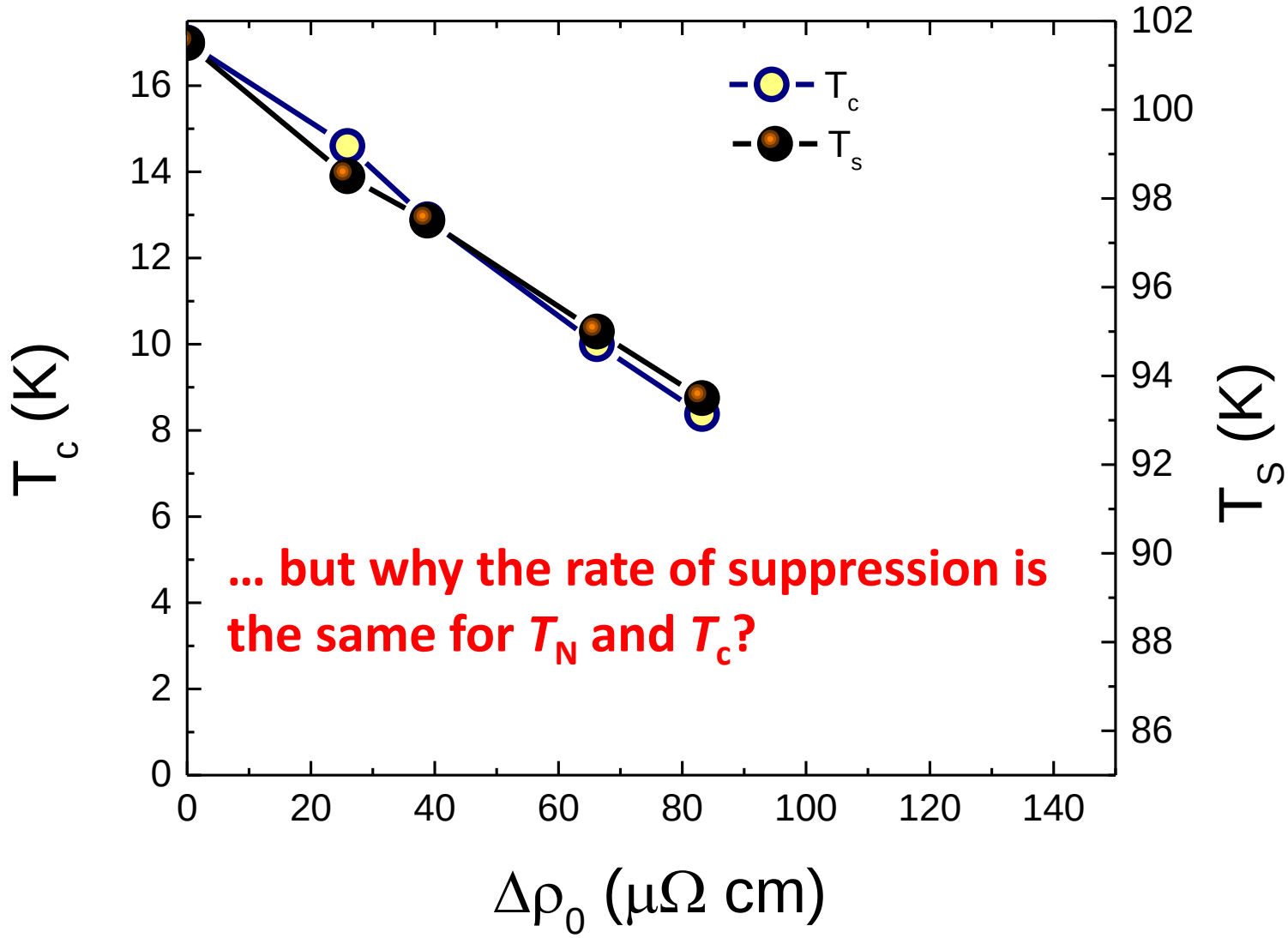
resistivity vs T during irradiation and in between runs



determination of T_S and T_c



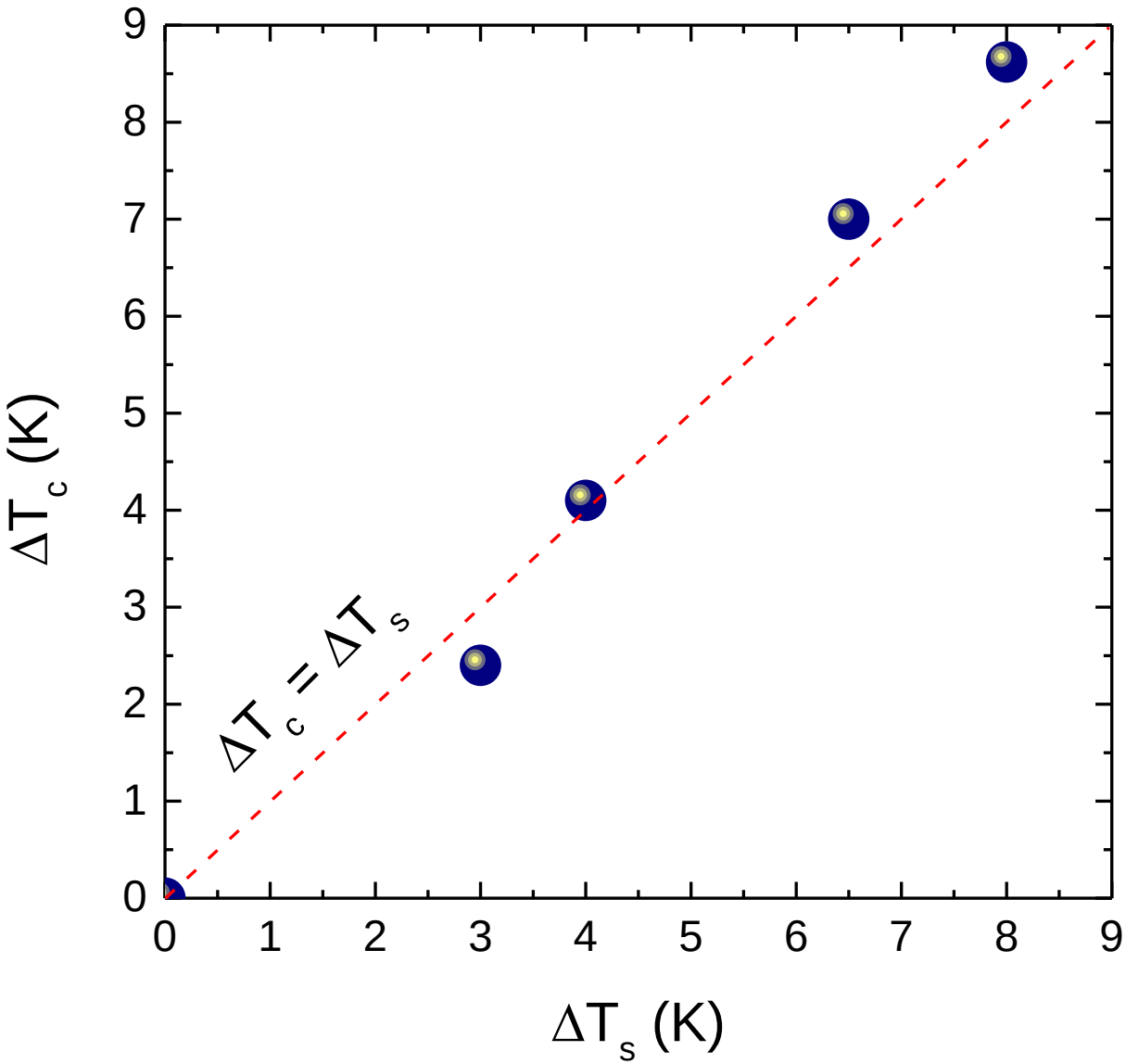
variation of T_s and T_c with induced residual resistivity



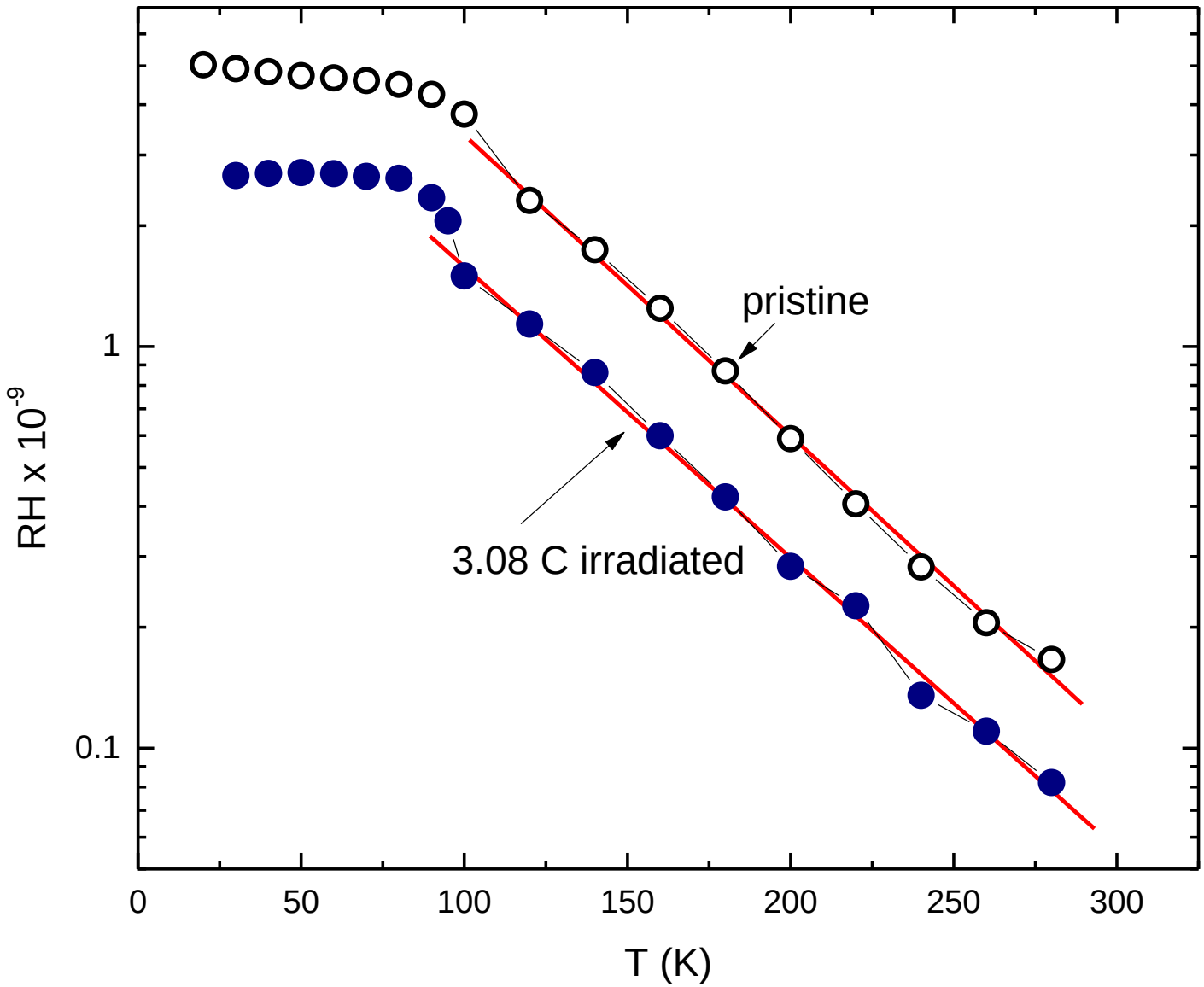
Disorder suppresses itinerant magnetism

R. M. Fernandes, M. G. Vavilov, and A. V. Chubukov, PRB 85, 140512 (2012)

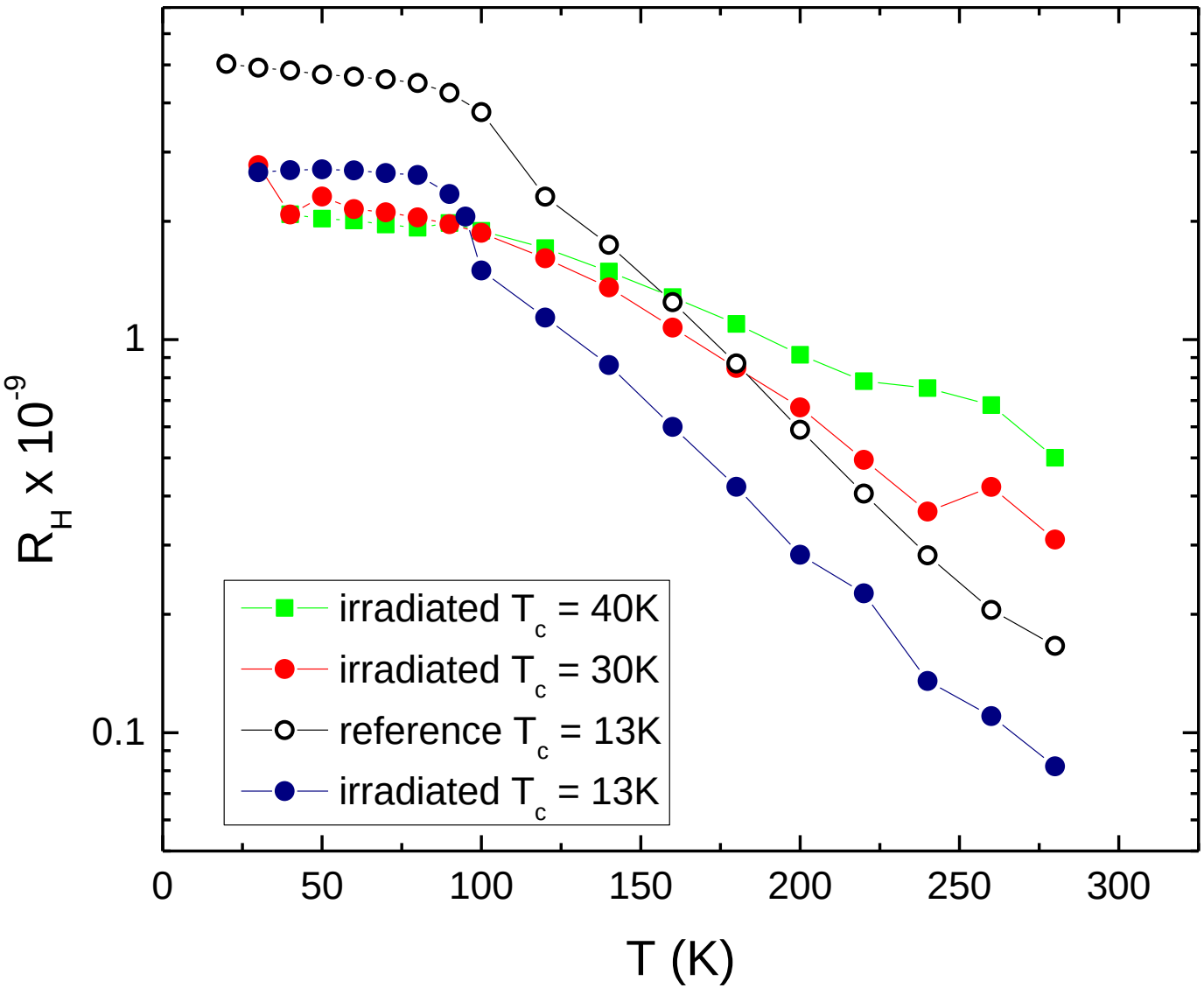
what energy scales are at play?



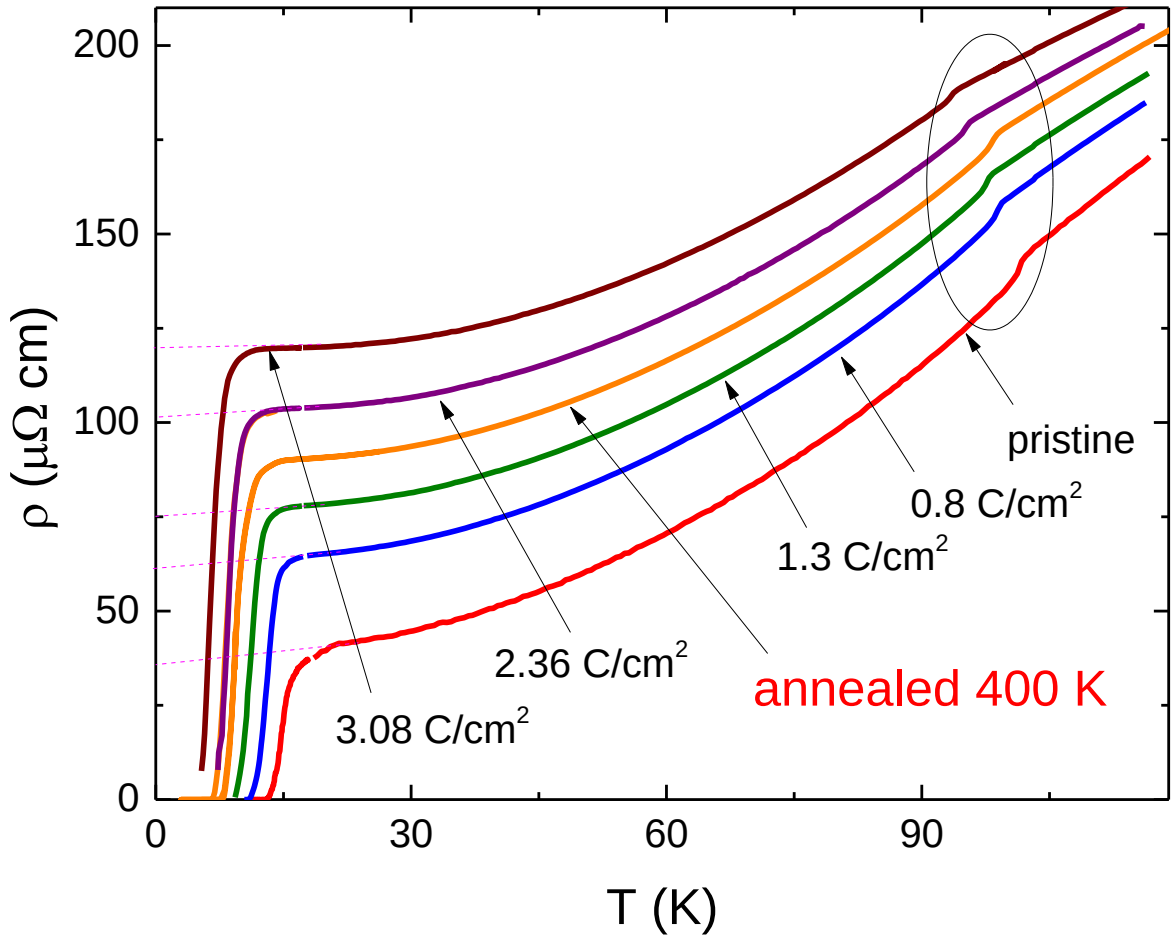
compare Hall coefficient vs T



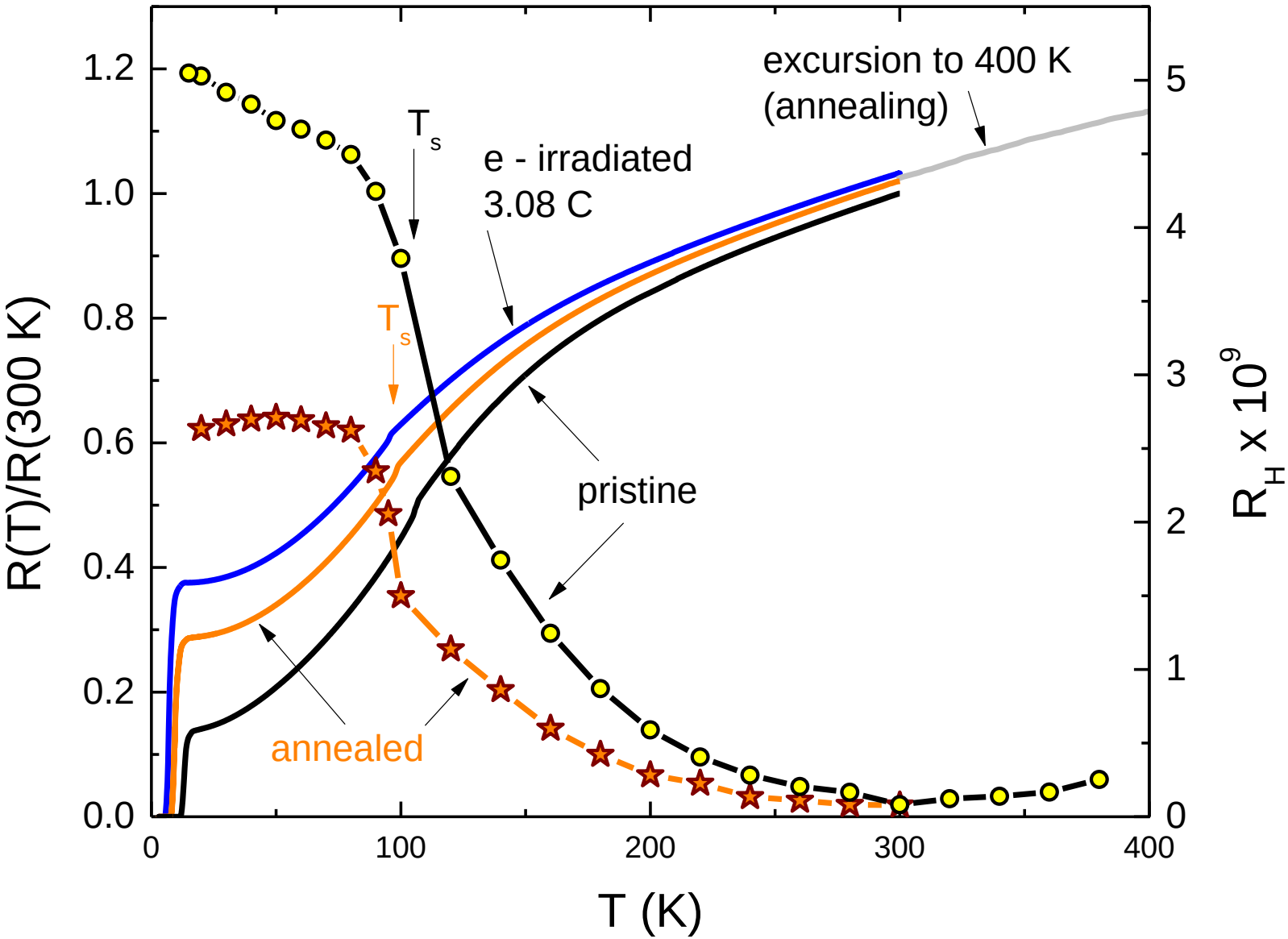
compare Hall coefficient vs T with higher – T_c samples



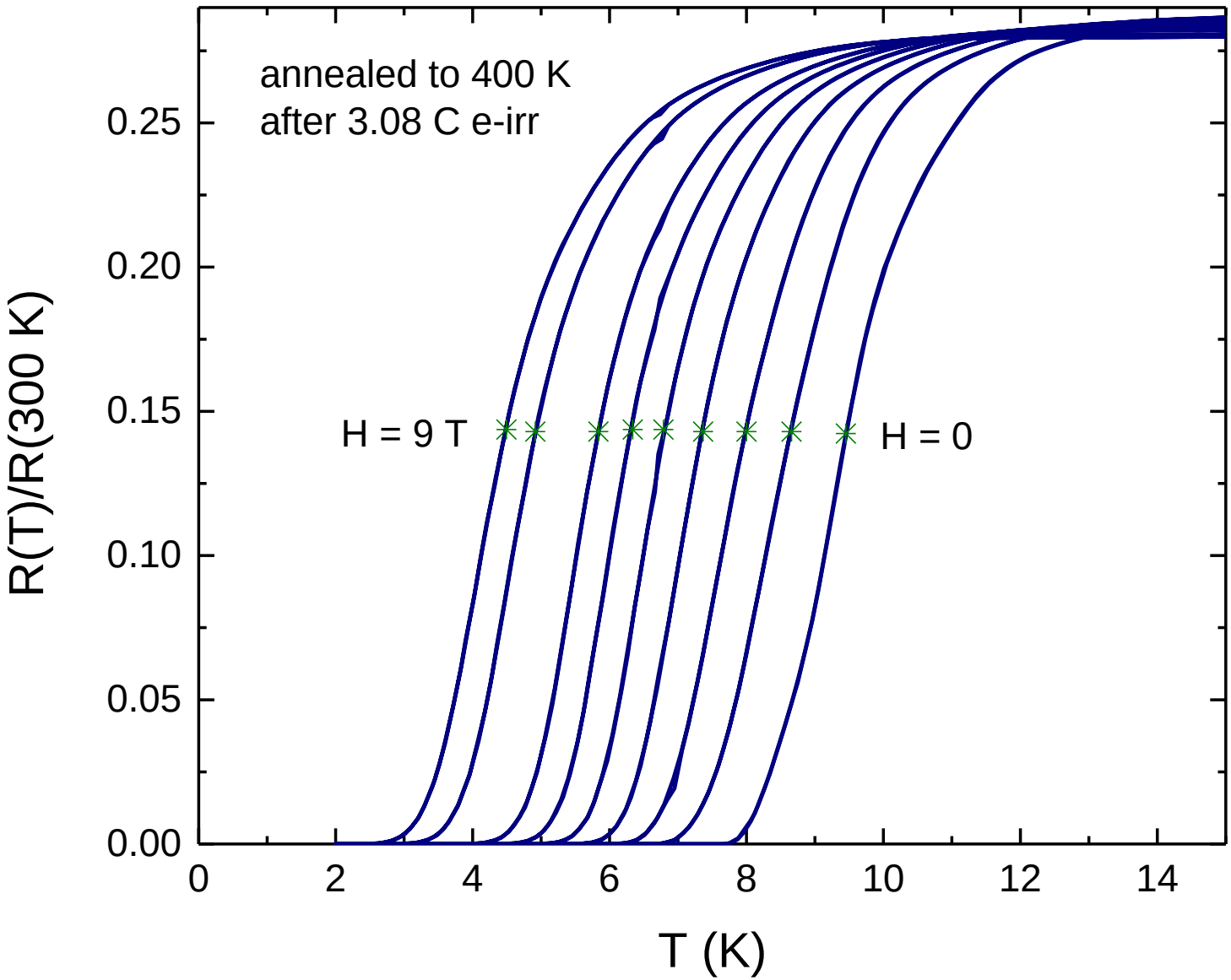
R(T) after annealing (slow excursion to 400 K and back)



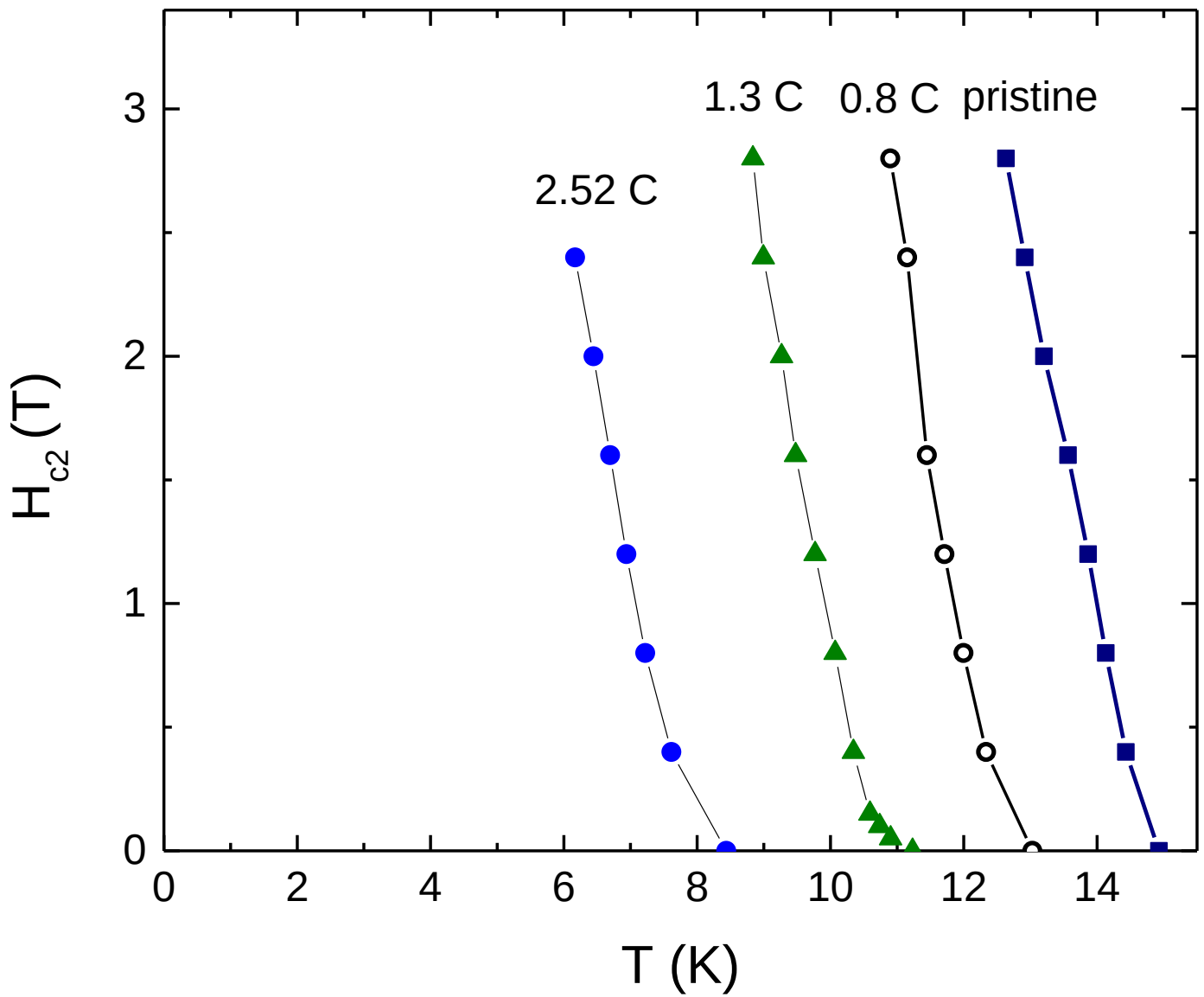
R(T) and R_H(T) after annealing



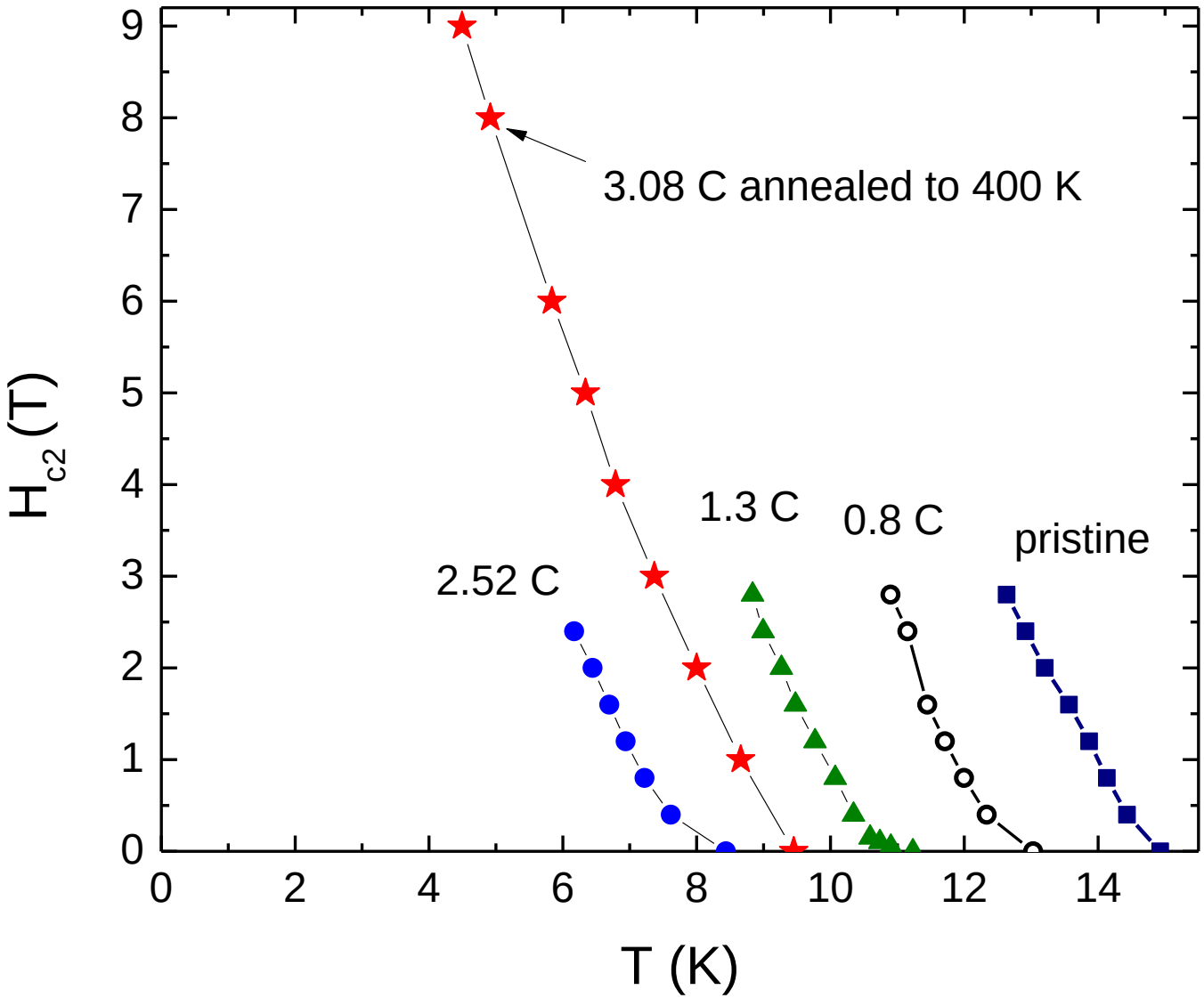
R(T,H) after annealing



H_{c2} (determined at 50% of the transition)



H_{c2}: effect of annealing



constant slope of H_{c2}?

$$\left.\frac{dH_{c2}}{dT}\right|_{T\to T_c} = 0.727\frac{H_{c2}(0)}{T_c} = 0.727\frac{\phi_0}{2\pi\xi^2 T_c} \propto \frac{\Delta^2}{T_c} \propto T_c$$

observations, conclusions, questions

- Observed suppression of T_c is compatible with $s_\pm$ pairing
- complete violation of Matthiessen's rule

- Highly temperature – dependent Hall
  (thermally activated carriers over the bands?)
- $R_H(T)$ does not change (much) with irradiation
- $R_H(T)$ decreases approaching optimal doping

- Huge change in both T_c and T_s after irradiation – by the same amount
- both transitions remain sharp after irradiation

- $dH_{c2}(T)/dT$ does not change