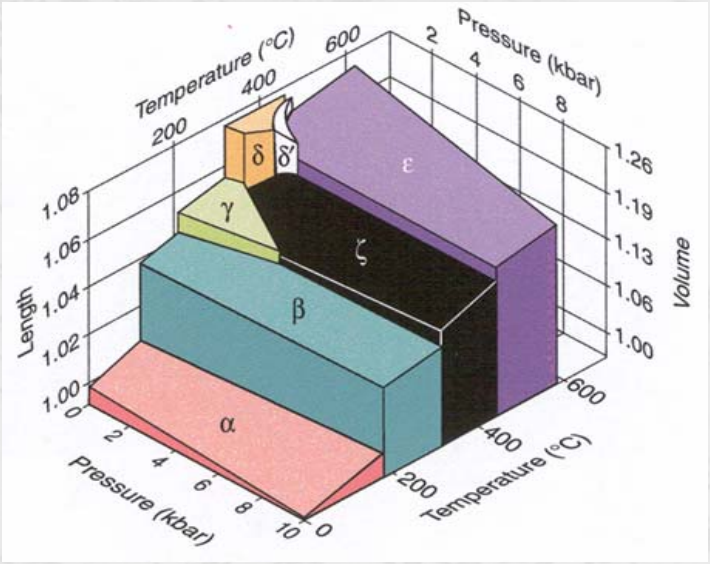
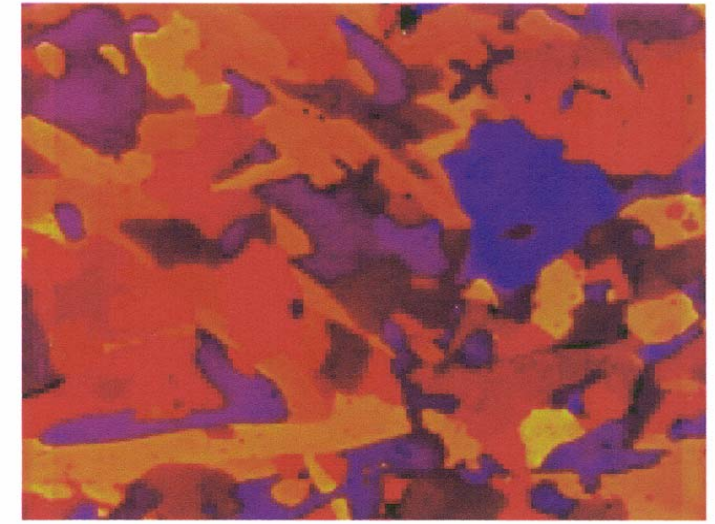
Phonon dispersion of fcc δ-Plutonium

J. Wong et al. Science 301, 1078 (2003); Phys. Rev. B 72, 064115 (2005)

Pu is one of the most fascinating and exotic element known

- Multitude of unusual properties
- Central role of 5f electrons
- Radioactive and highly toxic



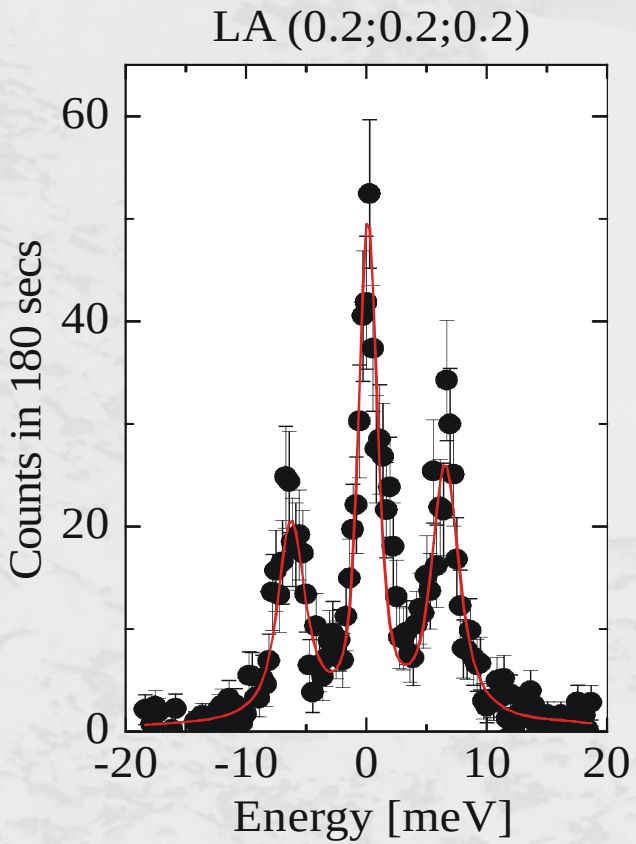


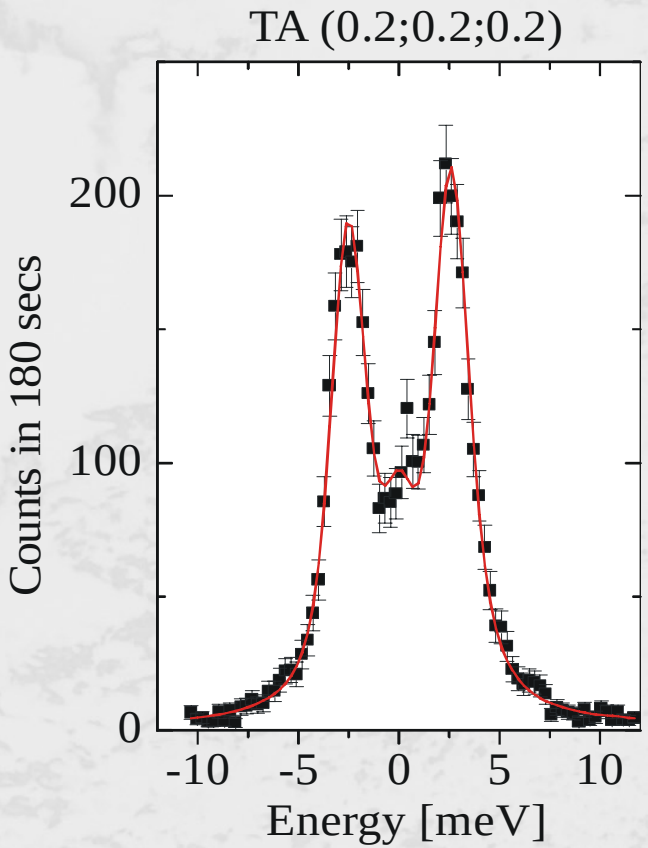
strain enhanced recrystallisation of fcc Pu-Ga (0.6 wt%) alloy

typical grain size: **90 μm**
foil thickness: **10 μm**

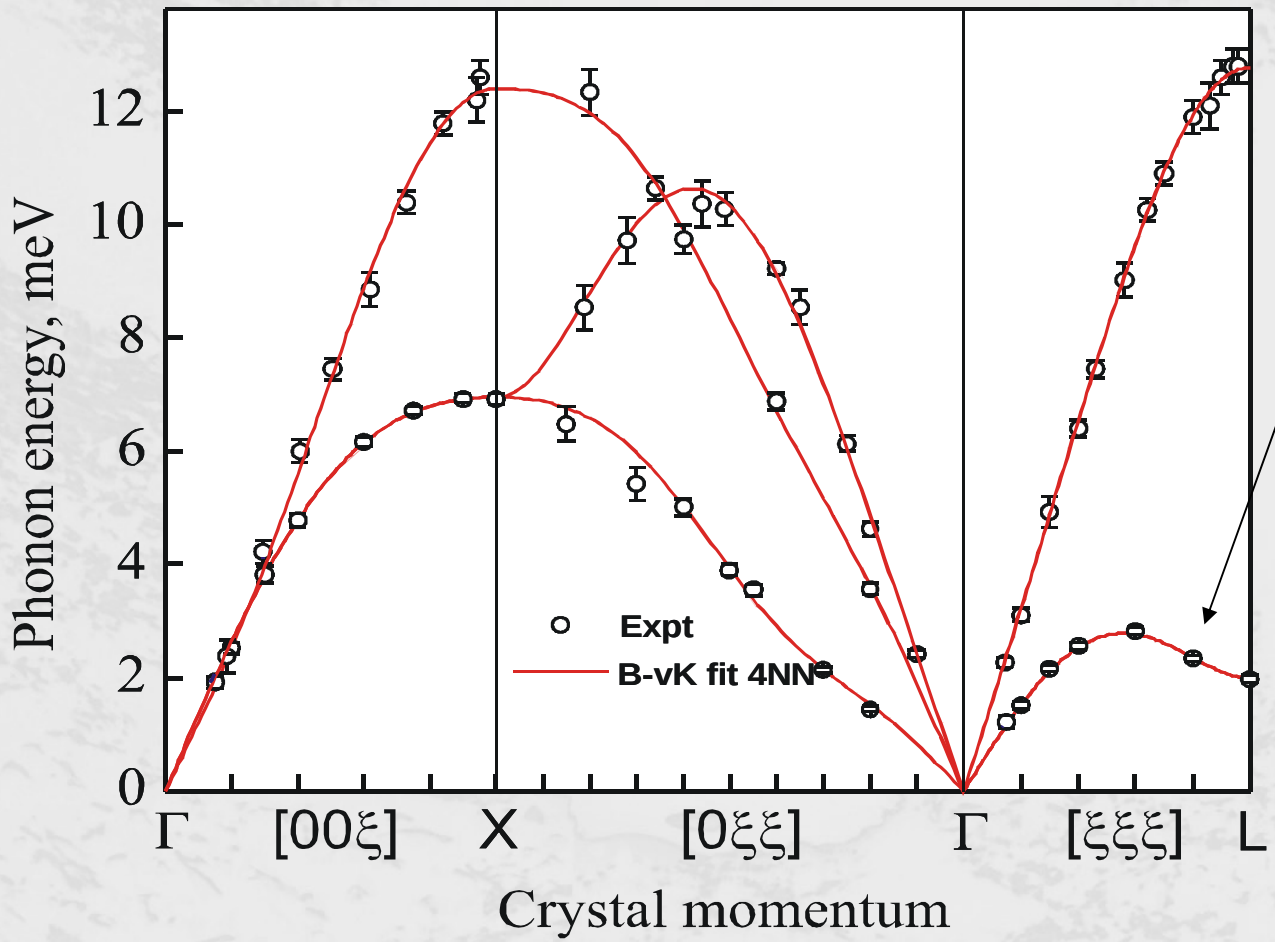
Plutonium: The IXS experiment

ID28 at ESRF
- Energy resolution: 1.8 meV at 21.747 keV
- Beam size: 20 x 60 μm^2 (FWHM)
- On-line diffraction analysis





Plutonium: phonon dispersion



soft-mode behaviour of T[111] branch

proximity of structural phase transition (to monoclinic α' phase at 163 K)

• **Born-von Karman force constant model fit**

- good convergence, if fourth nearest neighbours are included

Plutonium: elasticity

Proximity of Γ-point: $E = Vq$

$V_L[100] = (C_{11}/\rho)^{1/2}$

$V_T[100] = (C_{44}/\rho)^{1/2}$

$V_L[110] = ([C_{11}+C_{12}+2C_{44}]/\rho)^{1/2}$

$V_{T1}[110] = ([C_{11} - C_{12}]/2\rho)^{1/2}$

$V_{T2}[110] = (C_{44}/\rho)^{1/2}$

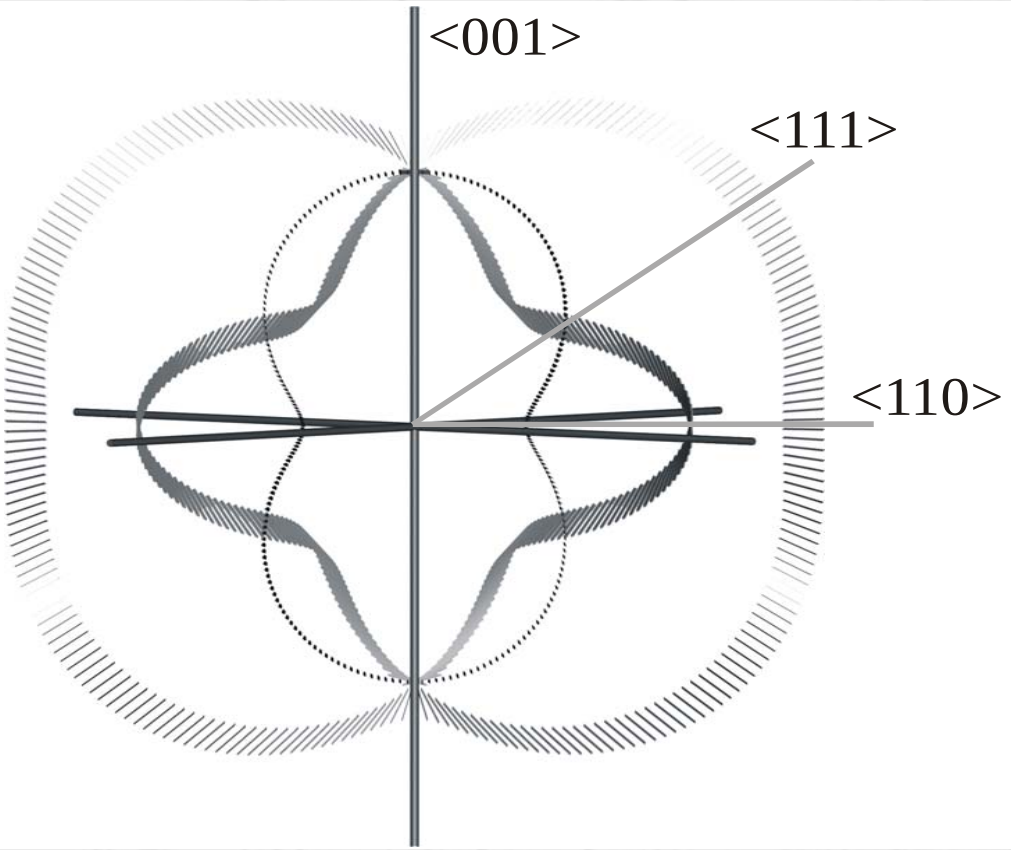
$V_L[111] = [C_{11}+2C_{12}+4C_{44}]/3\rho)^{1/2}$

$V_T[111] = ([C_{11}-C_{12}+C_{44}]/3\rho)^{1/2}$

C_{11} = 35.3±1.4 GPa

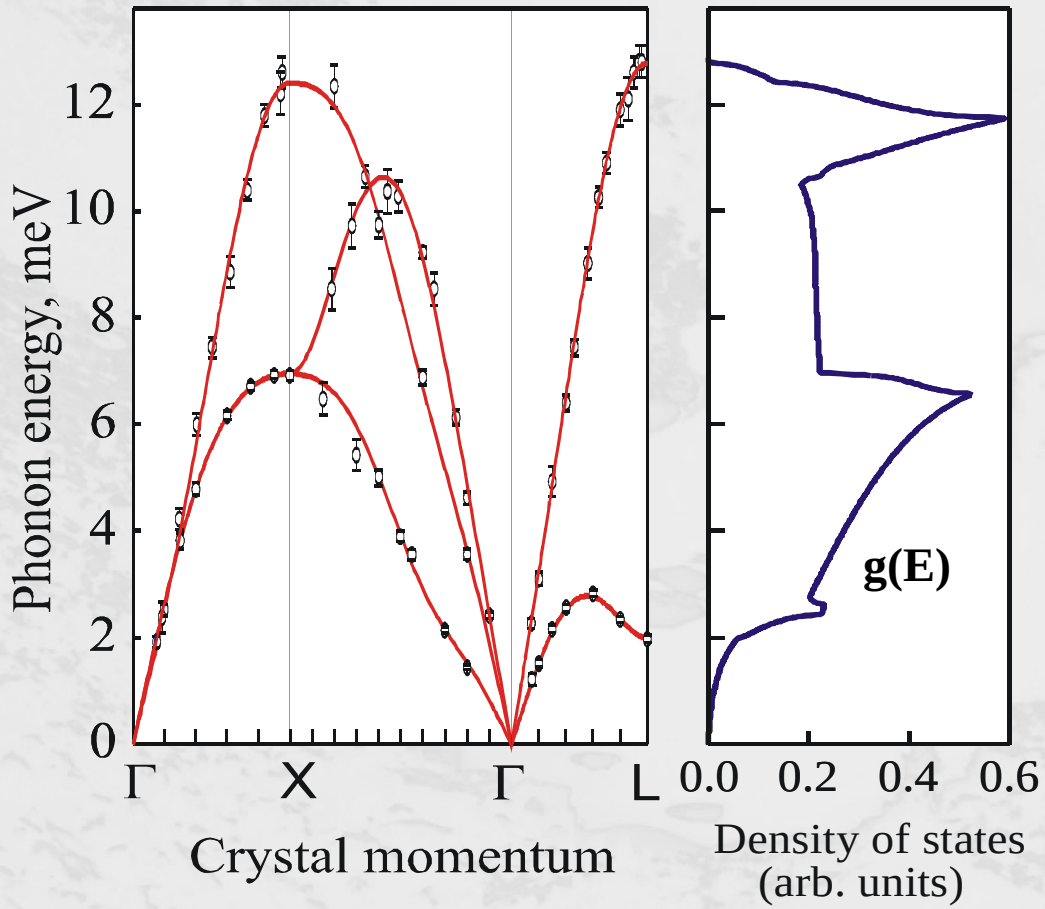
C_{12} = 25.5±1.5 GPa

C_{44} = 30.5±1.1 GPa



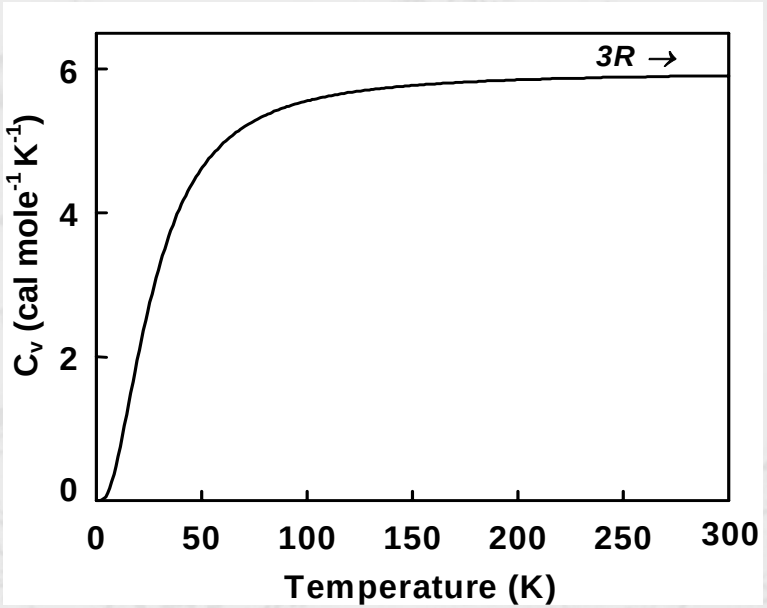
highest elastic anisotropy of all known fcc metals

Plutonium: density of states



Specific heat

$$C_v = 3Nk_B \int_0^{E_{max}} \left(\frac{E}{k_B T}\right)^2 \frac{\exp(E/k_B T)\, g(E)\, dE}{(\exp(E/k_B T)-1)^2}$$



- **Born-von Karman fit**
  - density of states calculated

$\theta_D(T \to 0) = 115K$

$\theta_D(T \to \infty) = 119.2K$