Internal Strain Measurements in Bulk Metallic Glasses (BMG) and BMG Composites using Pair Distribution Function (PDF) Analysis

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TMS

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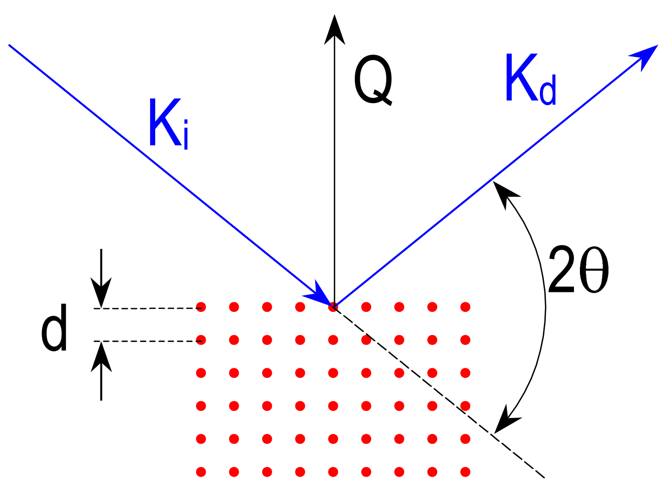
Internal stresses: Why do we care?

- Constitutive performance of structural materials
  - Operating environment and conditions
- Composites
  - Residual stresses in virgin materials
  - Both macro and micro residual/internal stresses
- Bulk Metallic Glass
  - Changes in nearest-neighbor peaks due to applied load

Diffraction

- In-situ measure internal *elastic* strains in bulk material
  - Spatially resolved
  - Changes due to applied “load” (stress, temperature, environment)



$$\lambda = 2d\sin\theta$$

$$\varepsilon^{el}_{hkl} = \frac{d_{hkl} - d^0_{hkl}}{d^0_{hkl}} = \frac{d_{hkl}}{d^0_{hkl}} - 1$$

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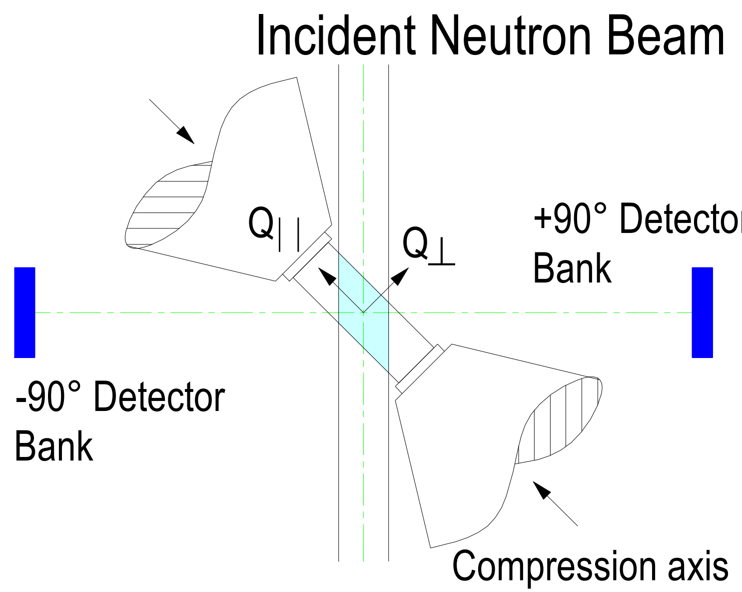
SMARTS

- ±250 kN loading capability
- Measure // and ⊥ strains simultaneously
- 1500 kg translator table
- 1500°C Furnace (1800°C stand-alone)



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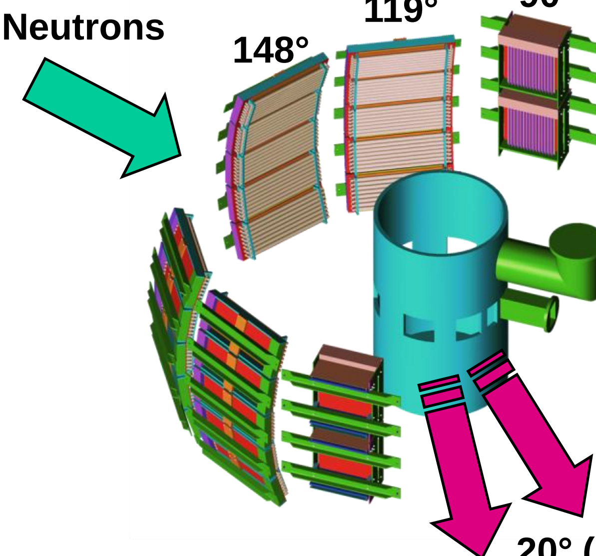
NPDF: Neutron Powder Diffractometer



- High resolution: **Δd/d ~ 0.15%** in backscattering
- Environment: 10-700 K
- Typical data-collection time: 2 hours

- 160 PSDs in backscattering
- 124 SED tubes at 90
- Low-angle detectors in future

Instrument scientist: Thomas Proffen
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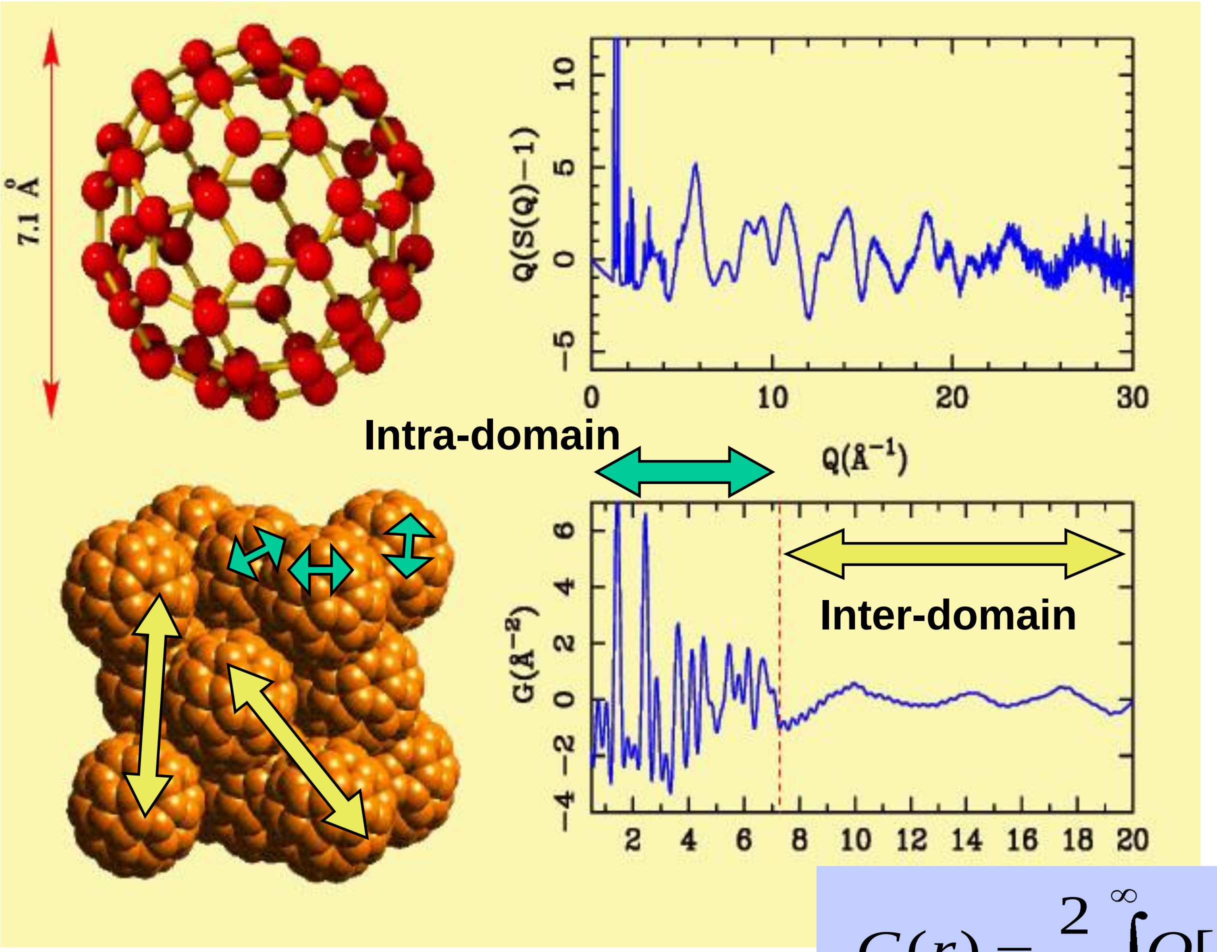
What is a PDF?



Example:
C_{60} - 'Bucky balls'

The PDF is obtained via Fourier transform of the normalized total scattering S(Q):

$$G(r) = \frac{2}{\pi}\int_0^{\infty} Q[S(Q)-1]\sin(Qr)\,dQ$$

$$Q = 4\pi \sin\theta / \lambda$$

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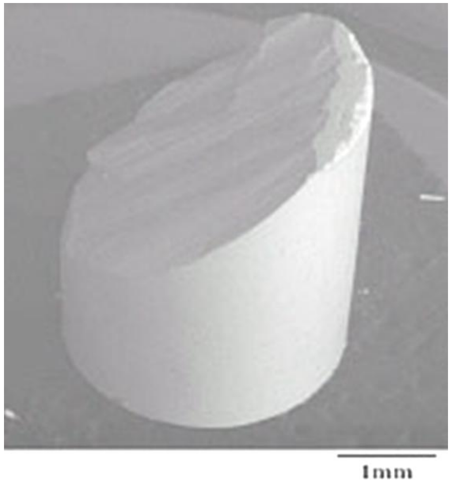
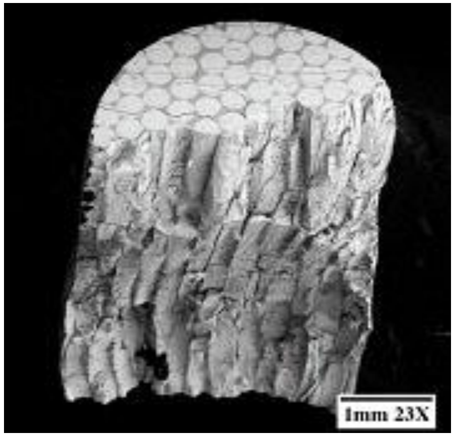
Bulk Metallic Glasses



Brittle fracture of monolithic BMG



Ductile fracture of BMG/W Composite

- Critical cooling rate about 1 degree per second
- High strength (2 GPa), low stiffness (90 GPa), high elastic limit (2%)
- Can be cast into intricate shapes like plastics
- Catastrophic failure due to shear banding

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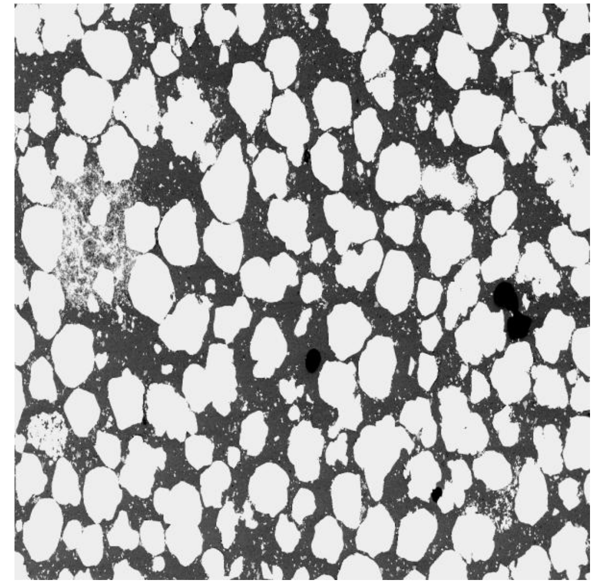
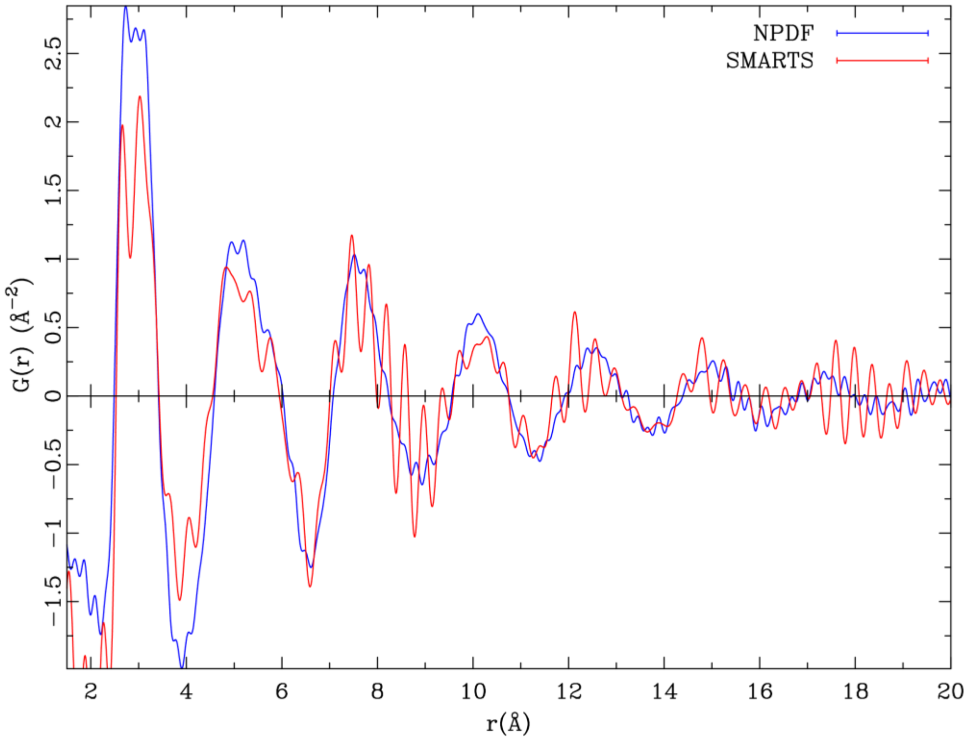
BMG/Tungsten particulate composites

- Vitreloy106
  - $Zr_{57}Nb_5Al_{10}Cu_{15.4}Ni_{12.6}$
  - $E = 85GPa$, $\nu = 0.35$
- Tungsten particles
  - 60 μm size
  - $E = 395GPa$, $\nu = 0.28$



- Volume fraction: 60% Tungsten particles
- Cylindrical samples: Ø6mm by 14.4mm

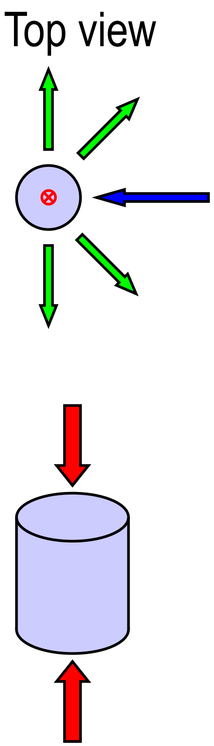
PDF of monolithic Vitreloy106 BMG

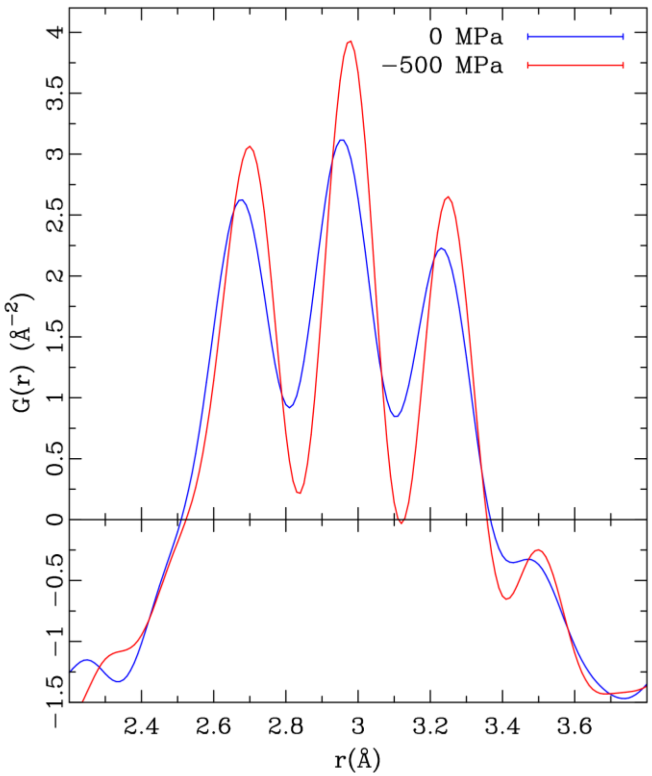


- Three distinct nearest-neighbor peaks
- Structure up to 18 Å $\Rightarrow$ Some medium range order

- Too low Q-range
- Non-trivial geometry

Loading of monolithic Vitreloy106 (NPDF)



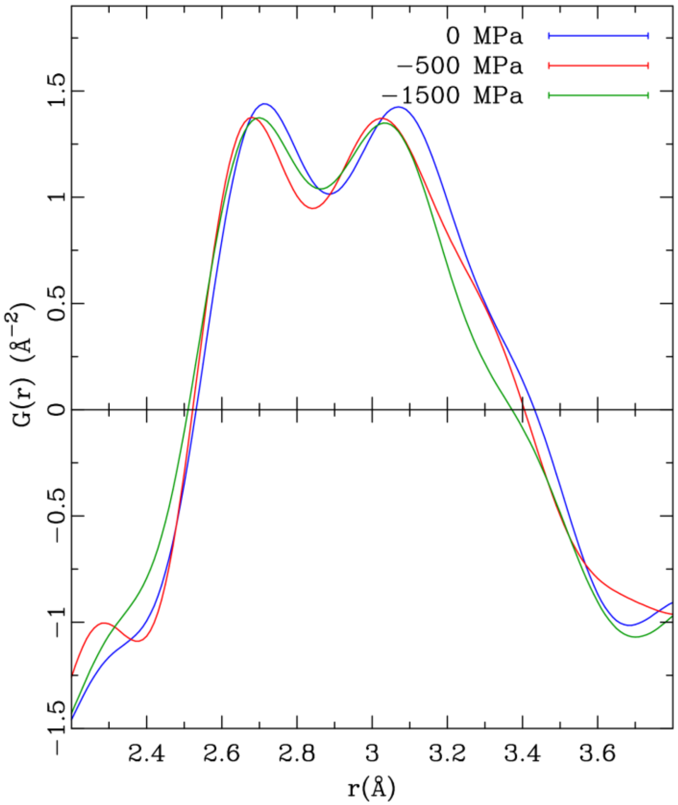


Strain from nearest-neighbor shift in PDF:
Transverse: +0.7%

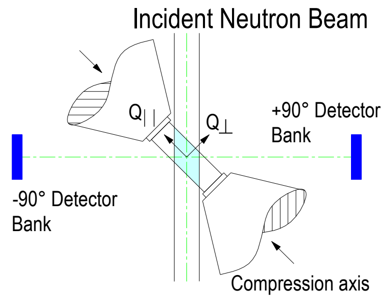
Calculated macroscopic strains:
Longitudinal: -0.5%
Transverse: +0.2%

- Transverse geometry only (standard vertical cylinder)
  - Measuring transverse strains due to Poisson's effect

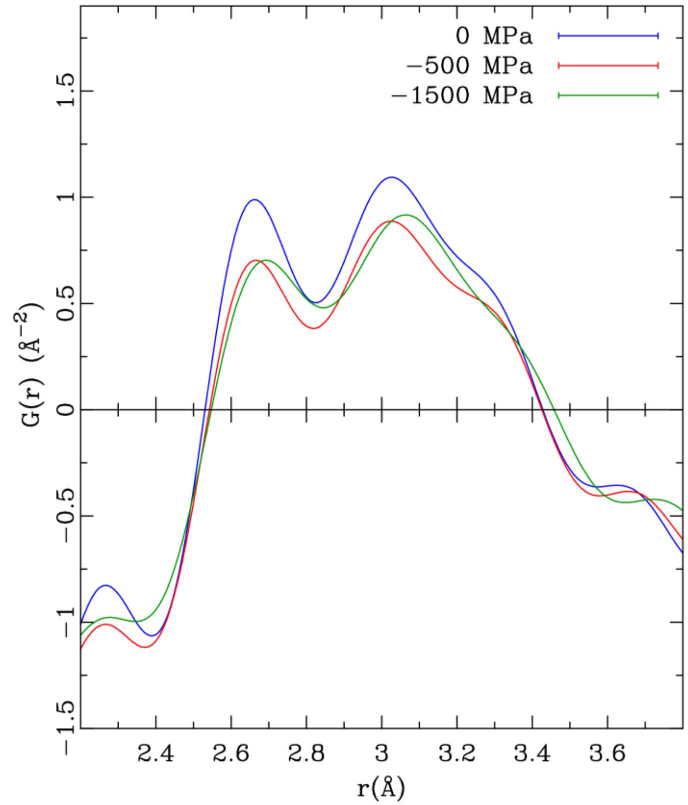
Loading of monolithic Vitreloy106 (SMARTS)



Longitudinal (transmission)



SMARTS geometry



Transverse (reflection)

- Shift in nearest-neighbor peaks are in qualitative agreement with macroscopic strain:

Longitudinal:	-0.8%	[-1.5%]
Transverse:	+0.7%	[+0.6%]

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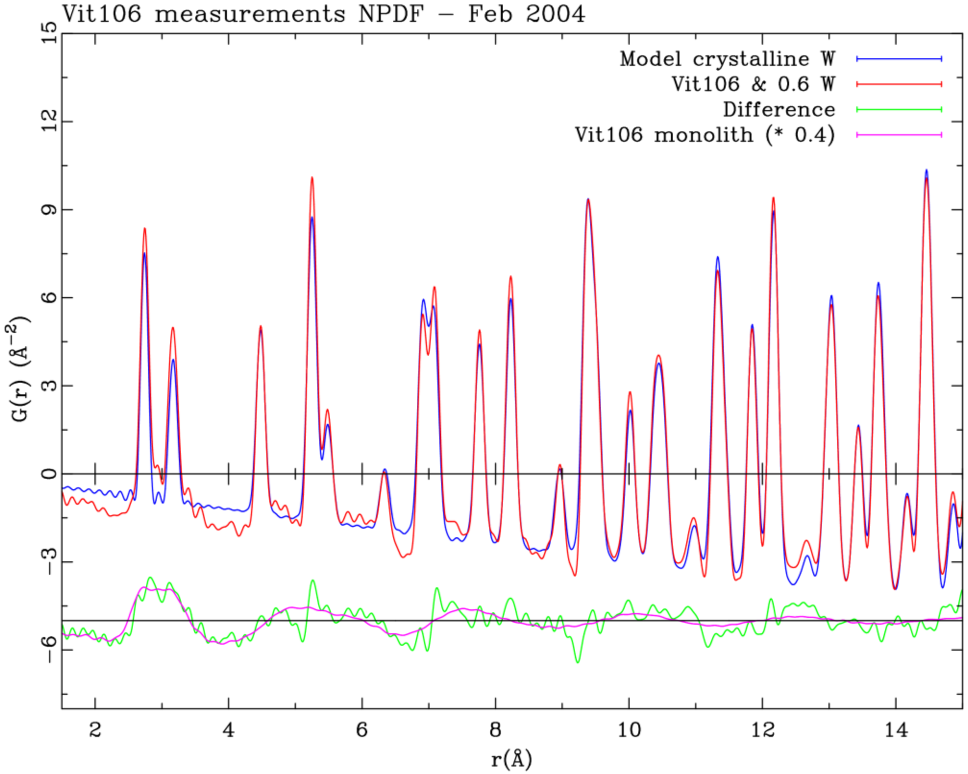
Combined PDF analysis (NPDF)



- Ability to distinguish between phases
  - Difference between measured composite PDF and calculated Tungsten PDF agrees well with measured BMG PDF

Conclusions

- PDF for Vitreloy106
  - Three distinct nearest-neighbor peaks
  - Structure up to 18 Å, indicating medium range order
  - Some sample to sample variation
- Composite
  - Ability to measure both phases simultaneously
- Loading
  - Changes in nearest-neighbor peaks in qualitative agreement with expected elastic strains
  - Not quantitative agreement – yet – work in progress!

Outlook

- Develop a quantitative tool for determining internal strains in amorphous materials
- Expand technique to disordered materials or nano materials
- Improve data analysis software to handle complex sample geometries