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Mechanical properties of muscovite as a function of pressure and temperature

Clay Mineral Society 2011

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National Nuclear Security Administration

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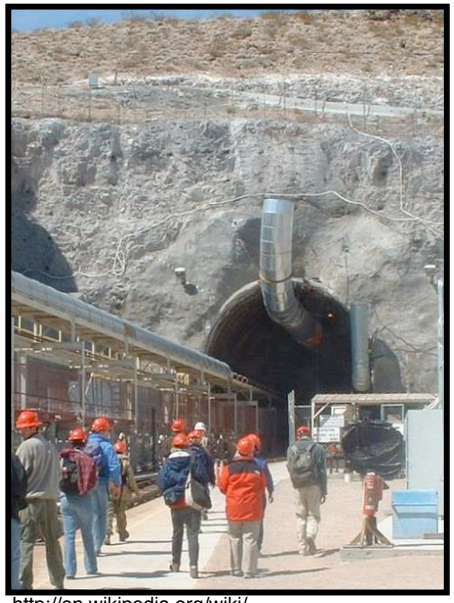
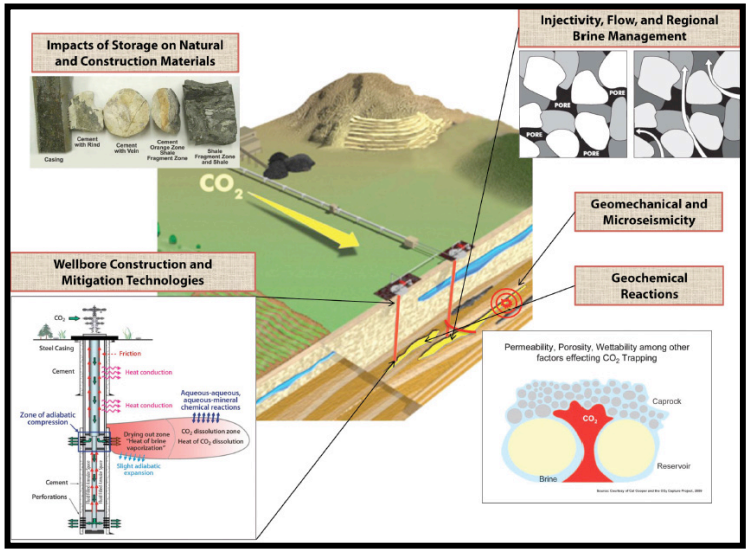
Areas of application of mechanical properties

Waste repositories



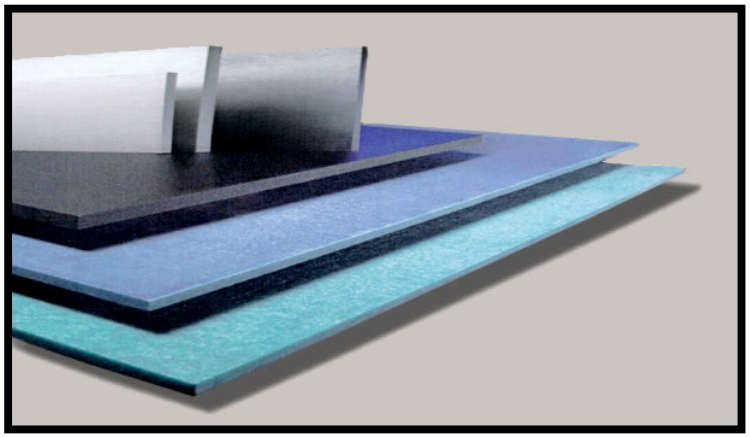
http://en.wikipedia.org/wiki/
Yucca_Mountain_nuclear_waste_repository

Carbon sequestration



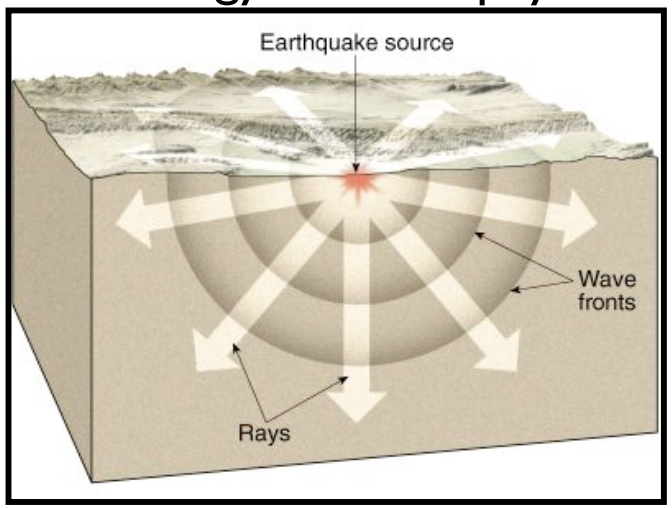
http://www.netl.doe.gov/technologies/carbon_seq/corerd/storage.html#geologic

Composite material properties



http://www.pentagon-ems.com/products/material/esd-composite-material.html

Seismology/ Mineral physics



http://geophysics.ou.edu/solid_earth/notes/seismology/seismo_interior/seismo_interior.html

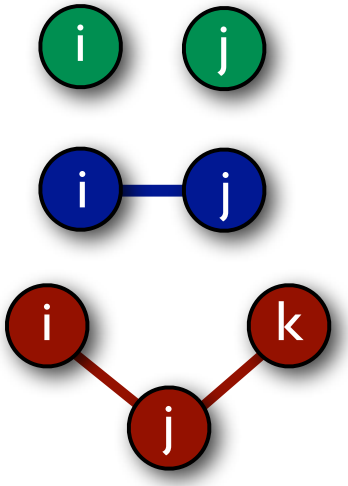
How to model muscovite in a simulation

Accurate description of how atoms interact

Clayff: Flexible model for clays, oxides, aqueous ions, brines

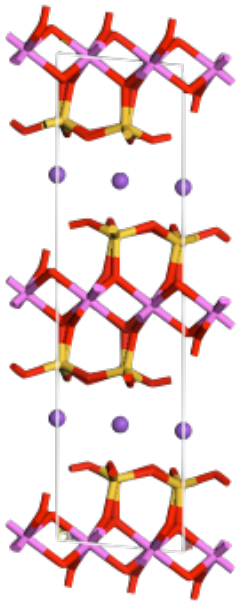
$$U_{ij} = \sum_i \sum_j \left(\frac{A_{ij}}{r_{ij}^{12}} + \frac{B_{ij}}{r_{ij}^{6}} + \frac{q_i q_j}{\varepsilon r_{ij}} \right) + \sum_{ij} \frac{1}{2} k_b (r_{ij} - r_o)^2 + \sum_{ijk} \frac{1}{2} k_\theta \left(\theta_{ijk} - \theta_o \right)^2$$

Short-range terms | Electrostatic terms | Bonded terms | Angle terms



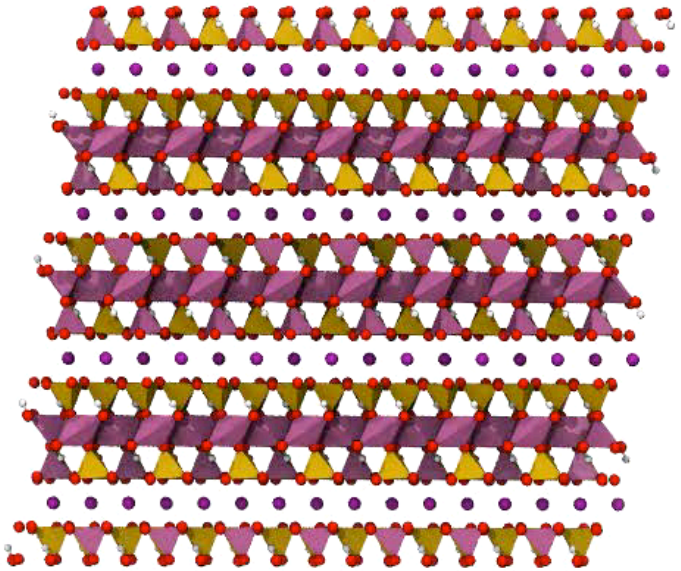
Cygan, Liang, and Kalinichev (2004) *Journal of Physical Chemistry B*

Accurate chemical and structural description



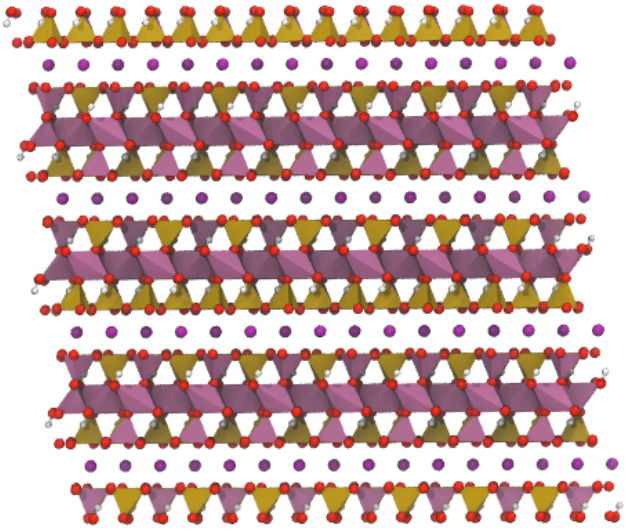
Muscovite unit cell
$KAl_2(Si_3Al)O_{10}(OH)_2$

Monoclinic C2/c 2M1 unit cell
Supercell 8 x 4 x 2 (5376 atoms)
4.1 nm x 3.6 nm x 4.0 nm



Simulation methods to determine mechanical properties

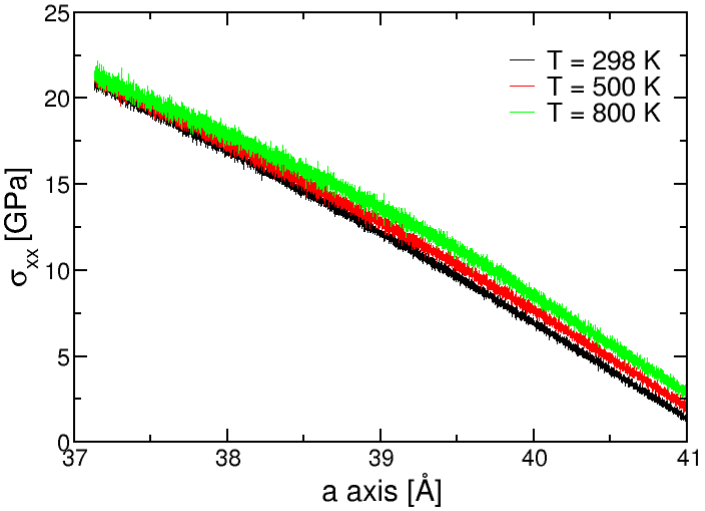
Molecular dynamics
Sandia's LAMMPS code



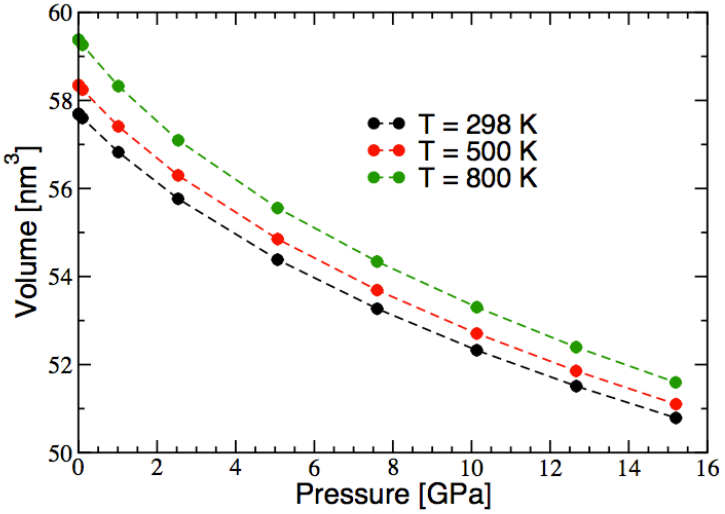
Simulation evolves

T = 298, 500, 800 K

Non-equilibrium NPT: ε = -10 to 10%



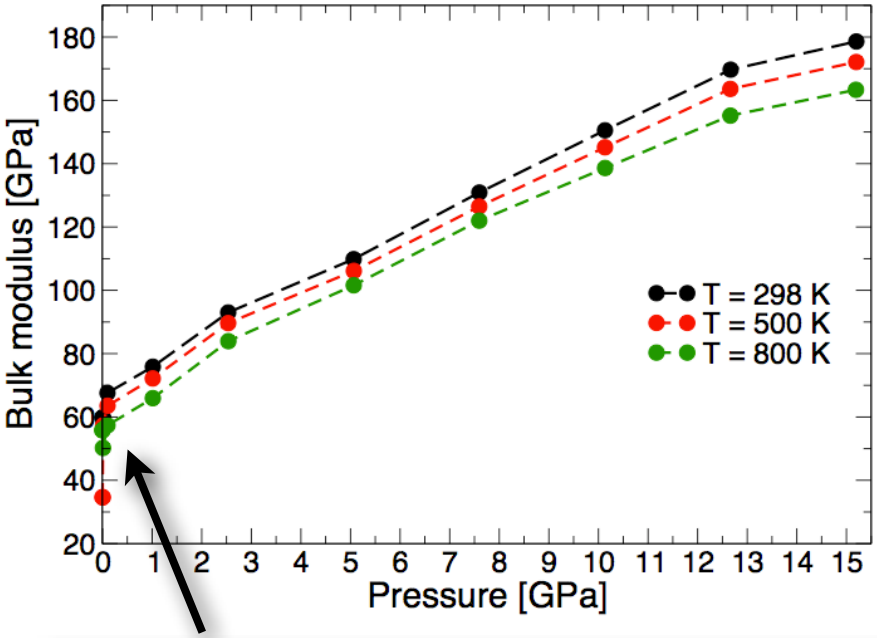
Equilibrium NPT: P = 1E-3 to 15 GPa

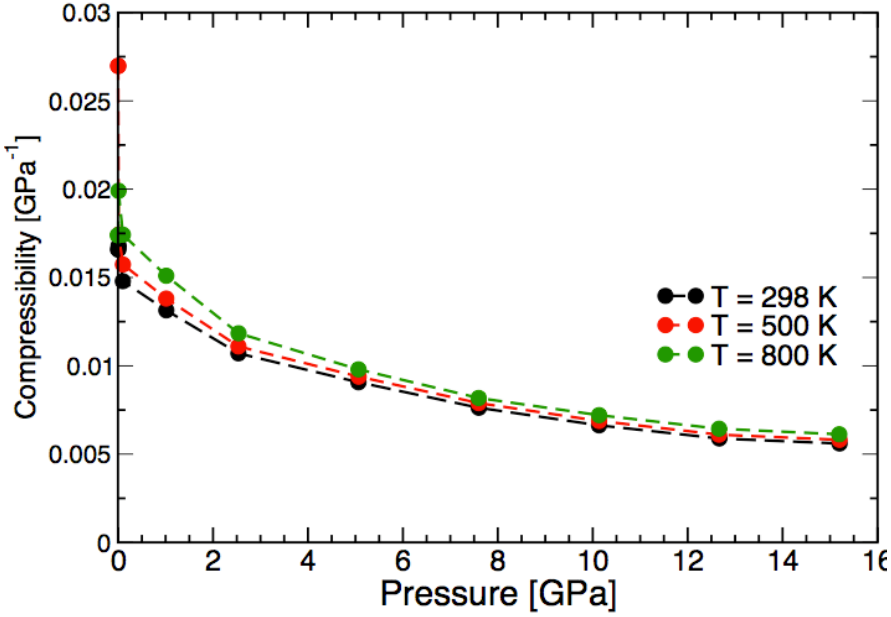


Bulk Modulus and Compressibility

Bulk modulus = $-V(\partial P/\partial V)_T$

Compressibility = $-1/V\,(\partial V/\partial P)_T$



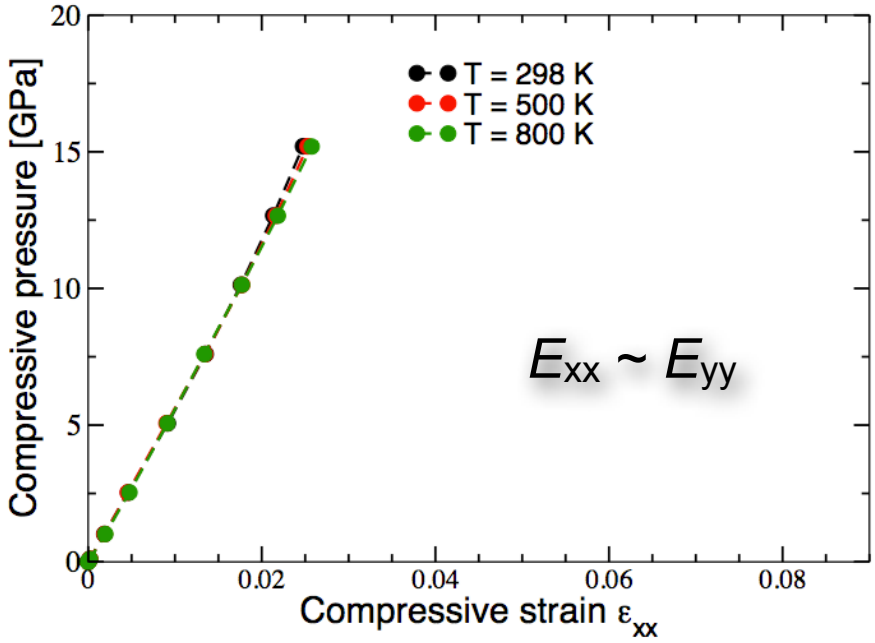


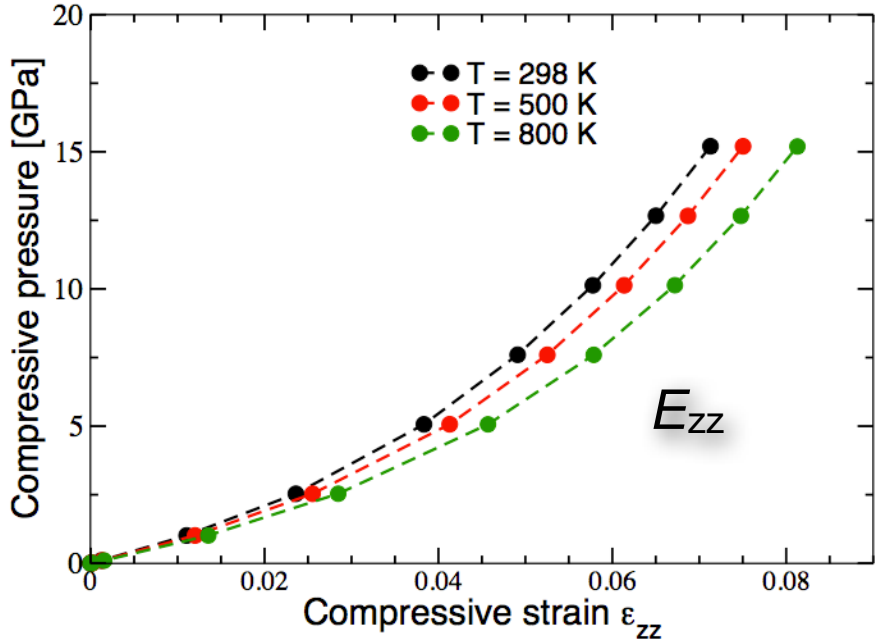
[a]Experimental value (T = 300 K) ~ 61.0

Temperature effects are small over pressure ranges studied

[a]Faust *et al.,* Journal Geophysical Research, 1994

Equilibrium stress-strain curves

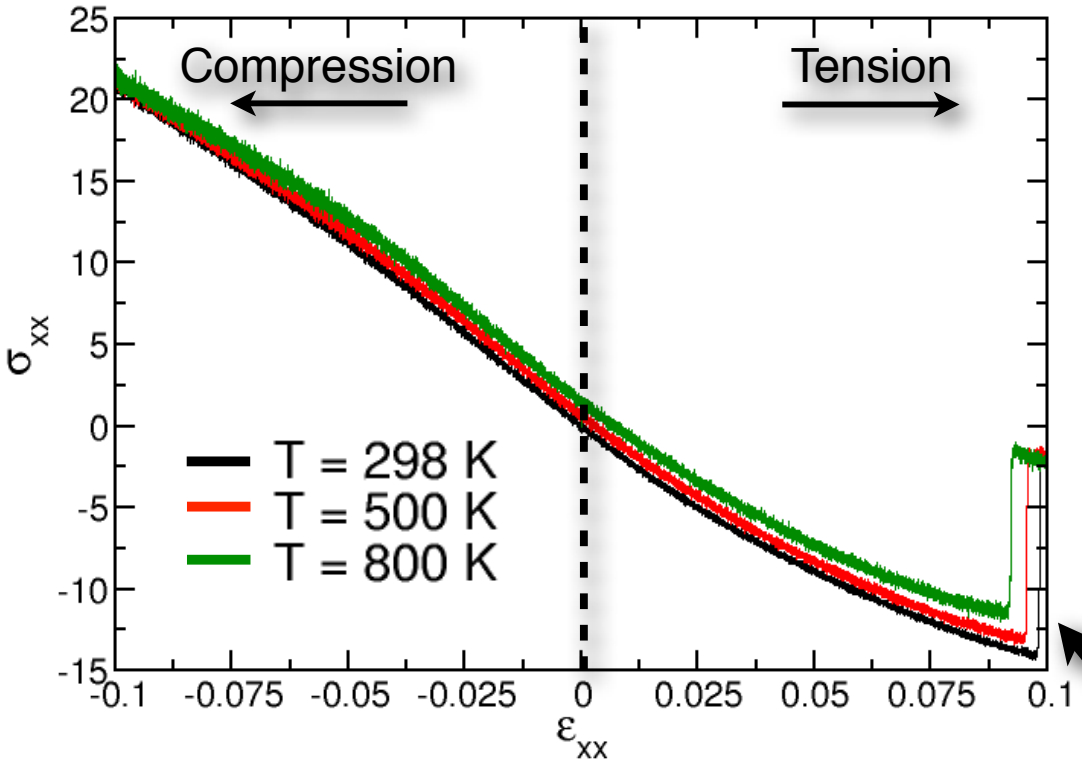




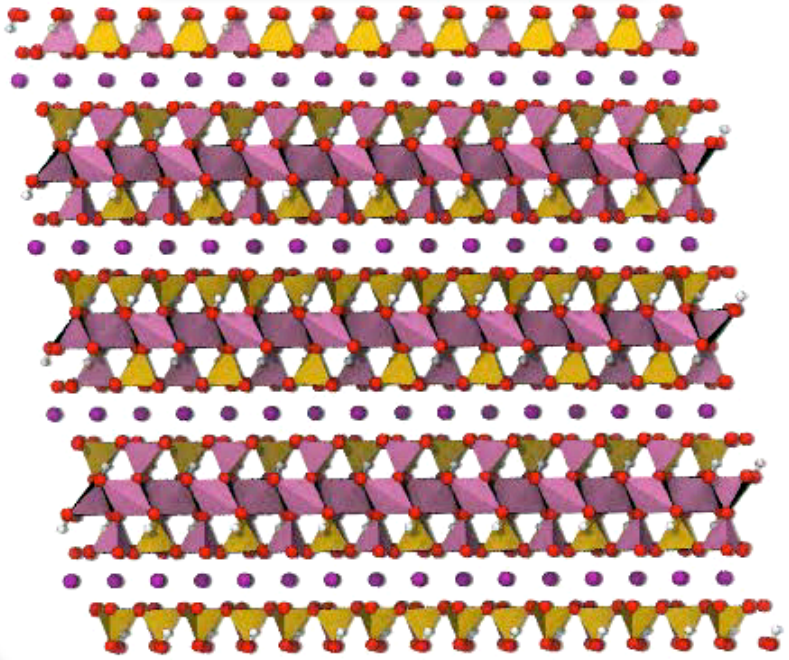
Temperature effects are greater in the z direction perpendicular to the cation interlayer

Uniaxial stress strain curves

Compression and tension simulations are conducted at constant strain rate



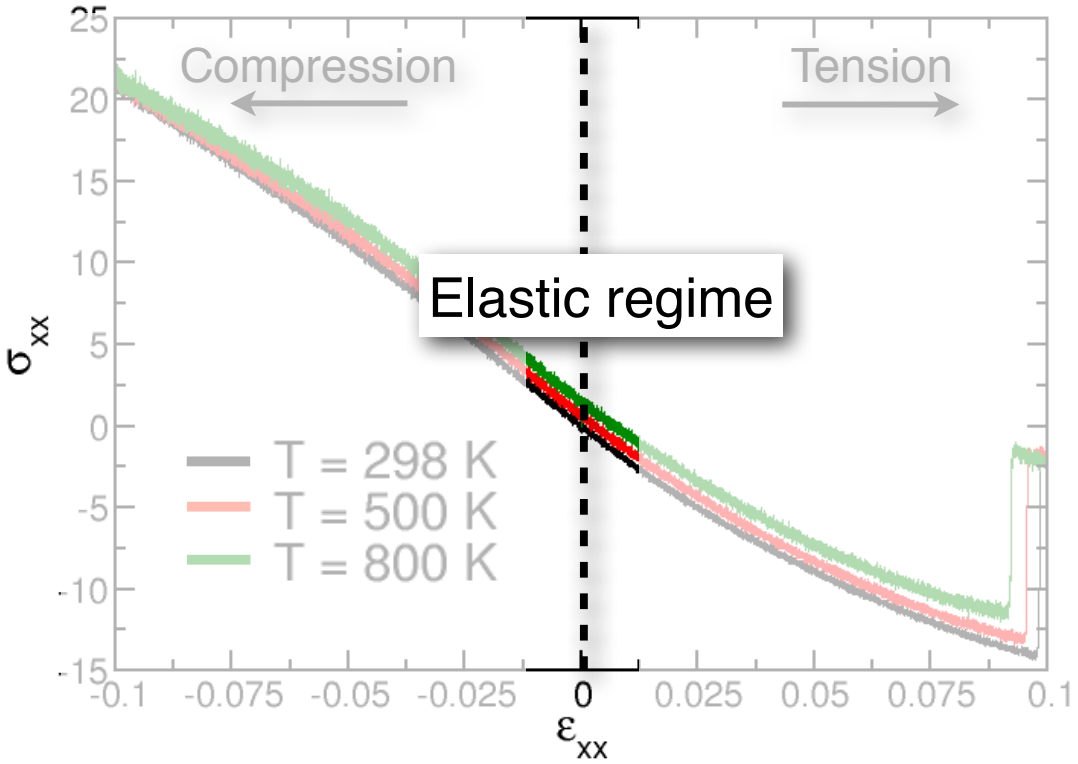
T = 298 K, tension

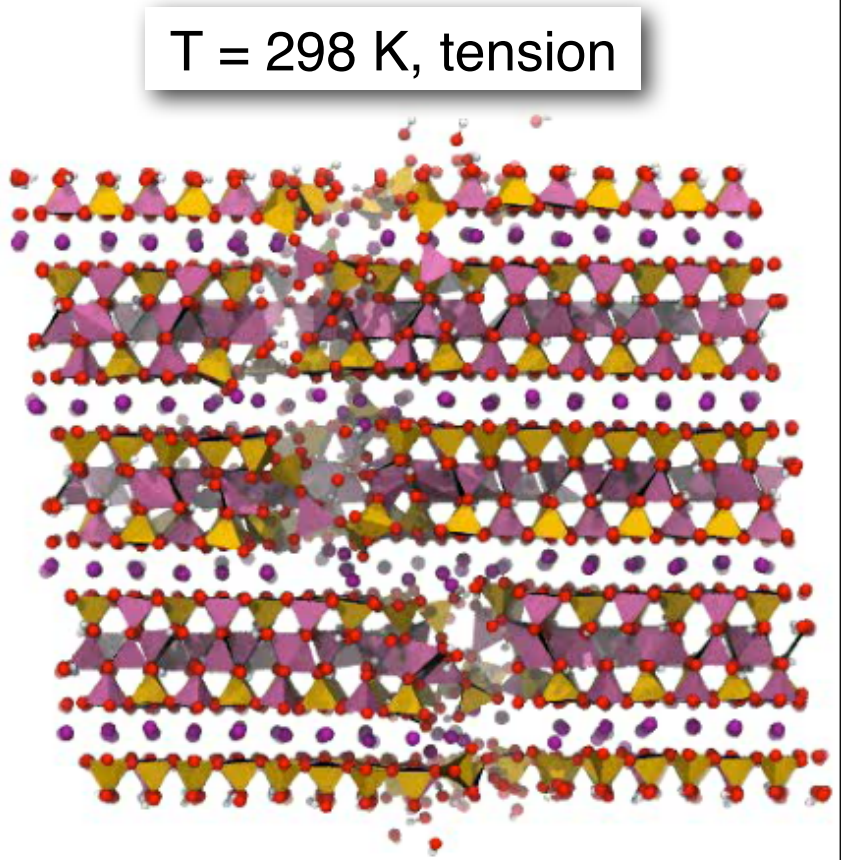


Model breaks apart at high strain

Uniaxial stress strain curves

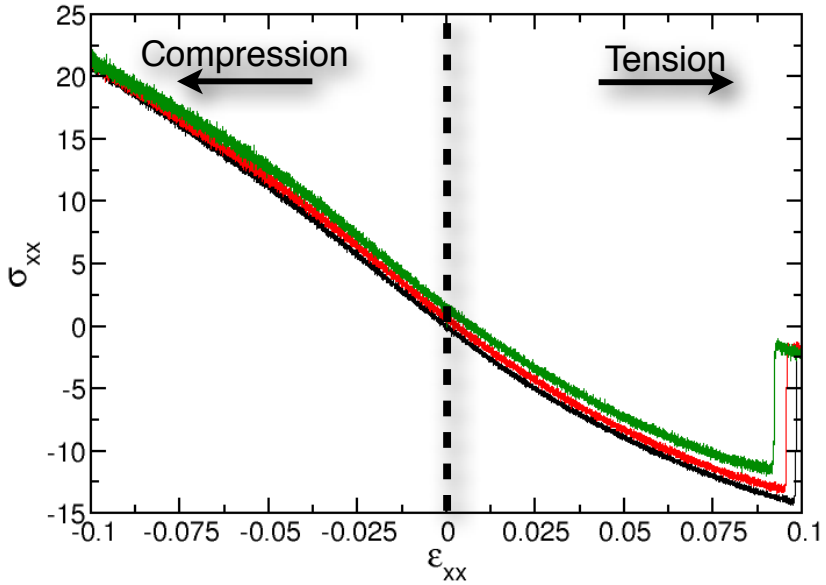
Compression and tension simulations are conducted at constant strain rate





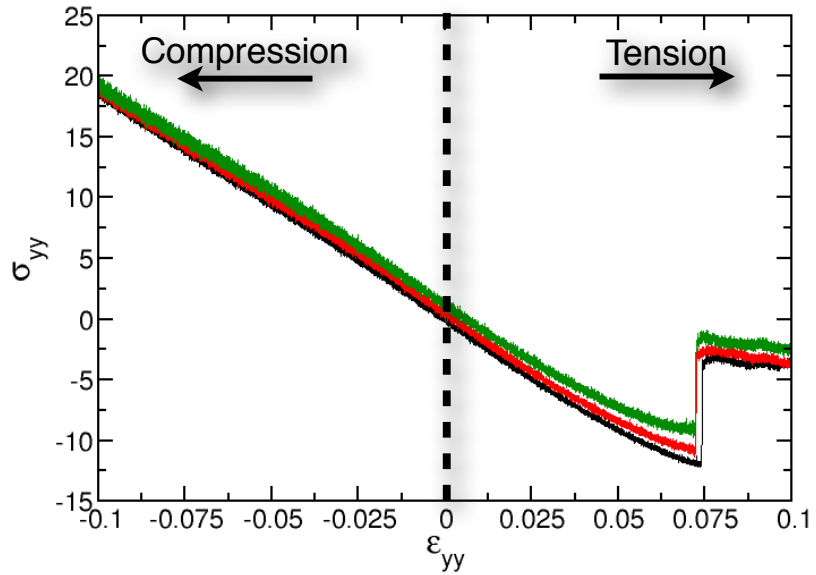
Calculate Young's moduli and shear moduli from data within the elastic regime

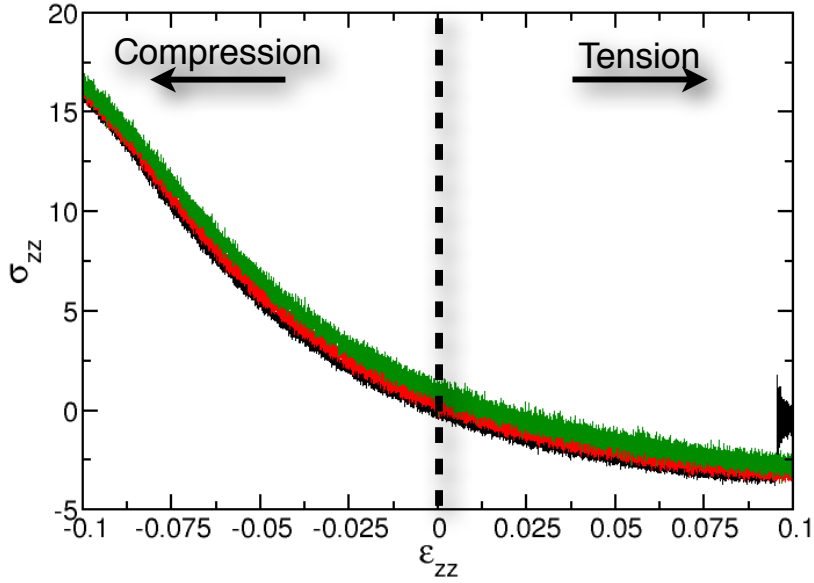
Young's modulus



T = 298 K
T = 500 K
T = 800 K

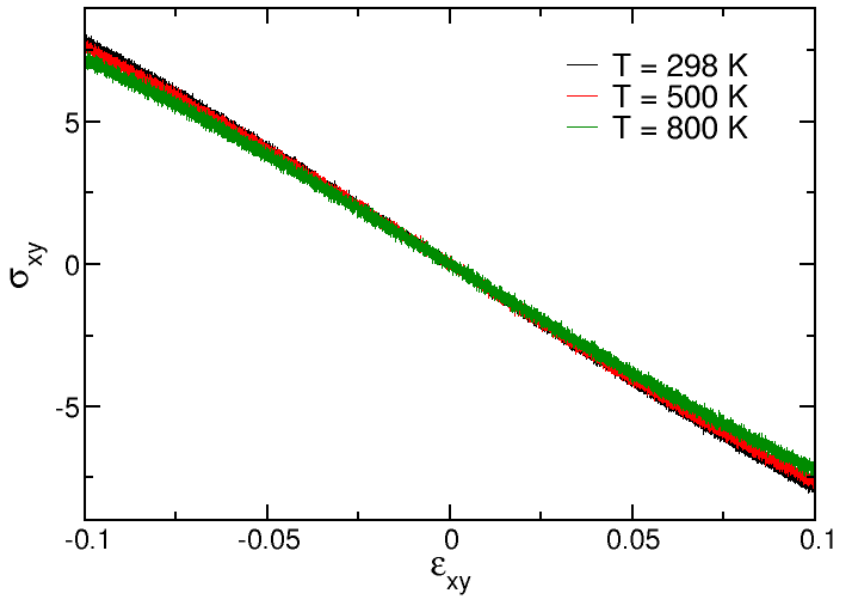
E [GPa] / T [K]	Exp	298	500	800
xx	160.9[a]	220.7	219.9	215.4
yy	161.3[a]	199.6	198.2	192.6
zz	77.4[b]	69.4	69.7	74.3



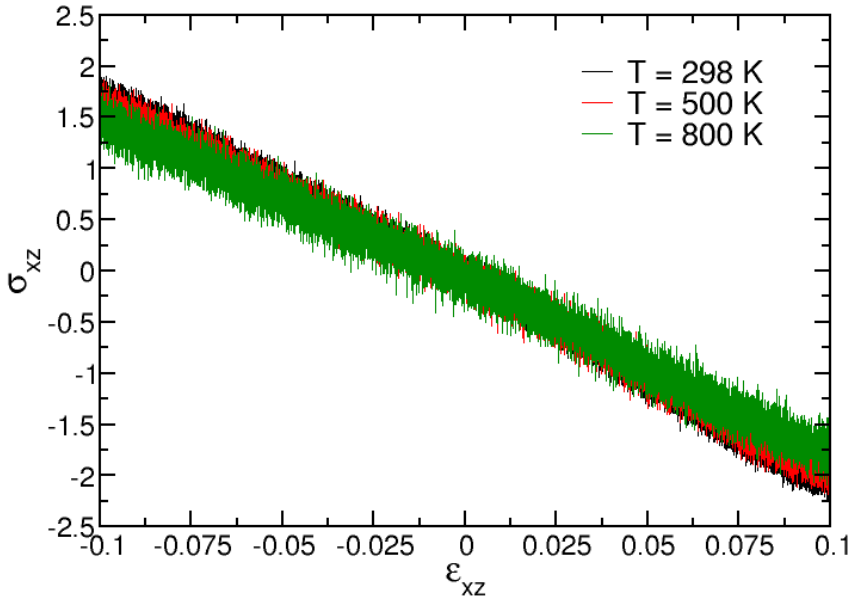


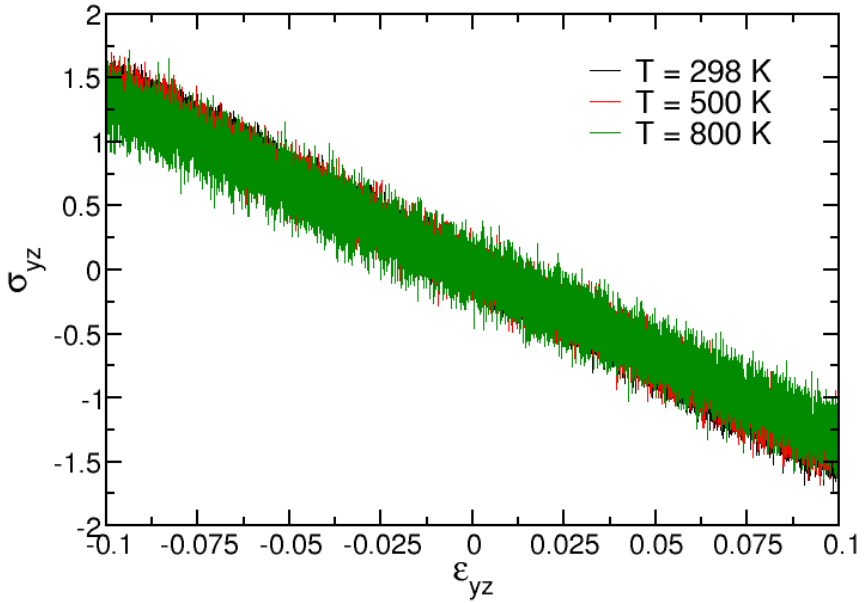
[a]Vaughan *et al.*, Journal Geophysical Research, 1986; [b]Zhang *et al.,* American Mineralogist, 2010

Shear modulus



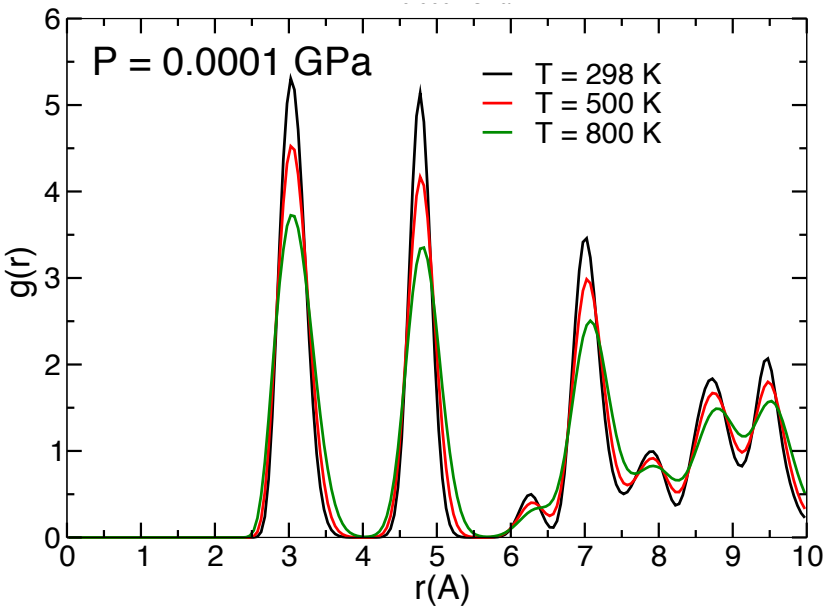
E [GPa] / T [K]	Exp	298	500	800
xy	71	83.9	81.7	78.7
xz	17	18.8	17.7	16.4
yz	15	15.1	13.6	12.7

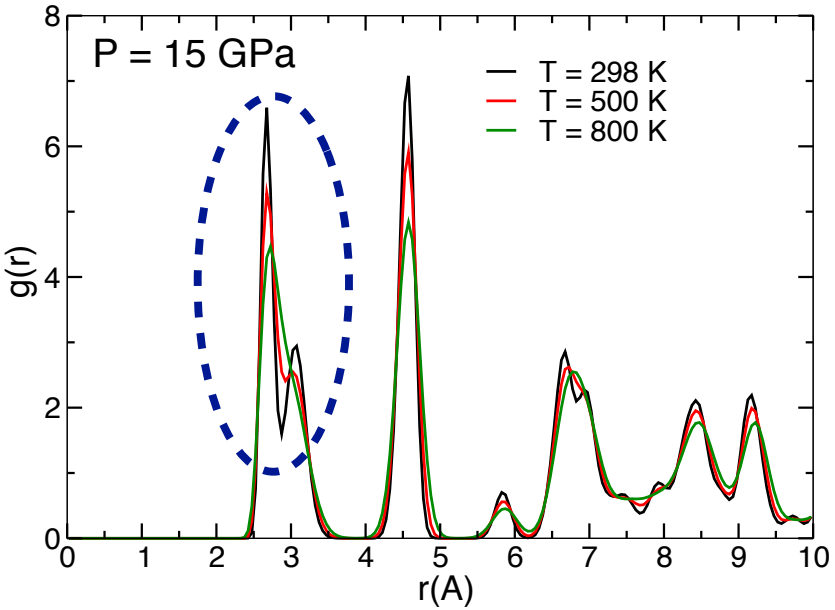




[a]Vaughan *et al.*, Journal Geophysical Research, 1986

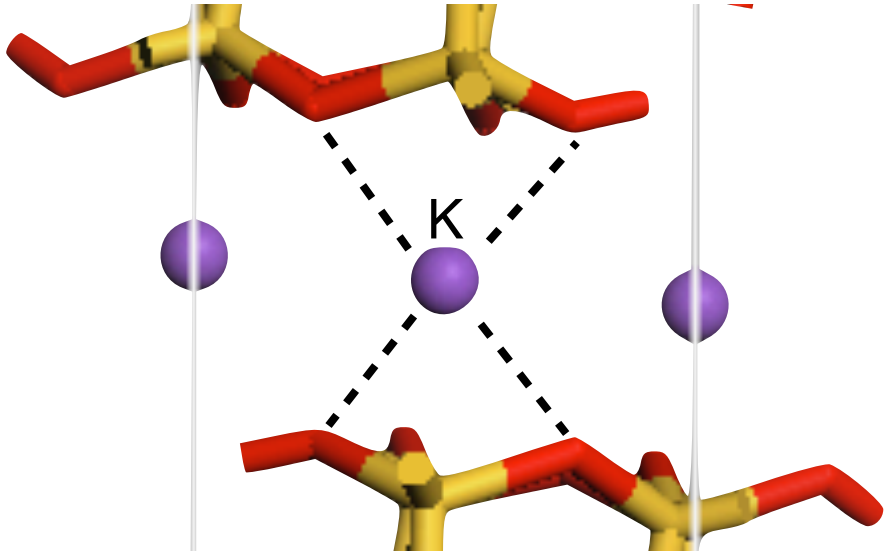
Structural changes with deformation





K-O radial distribution function

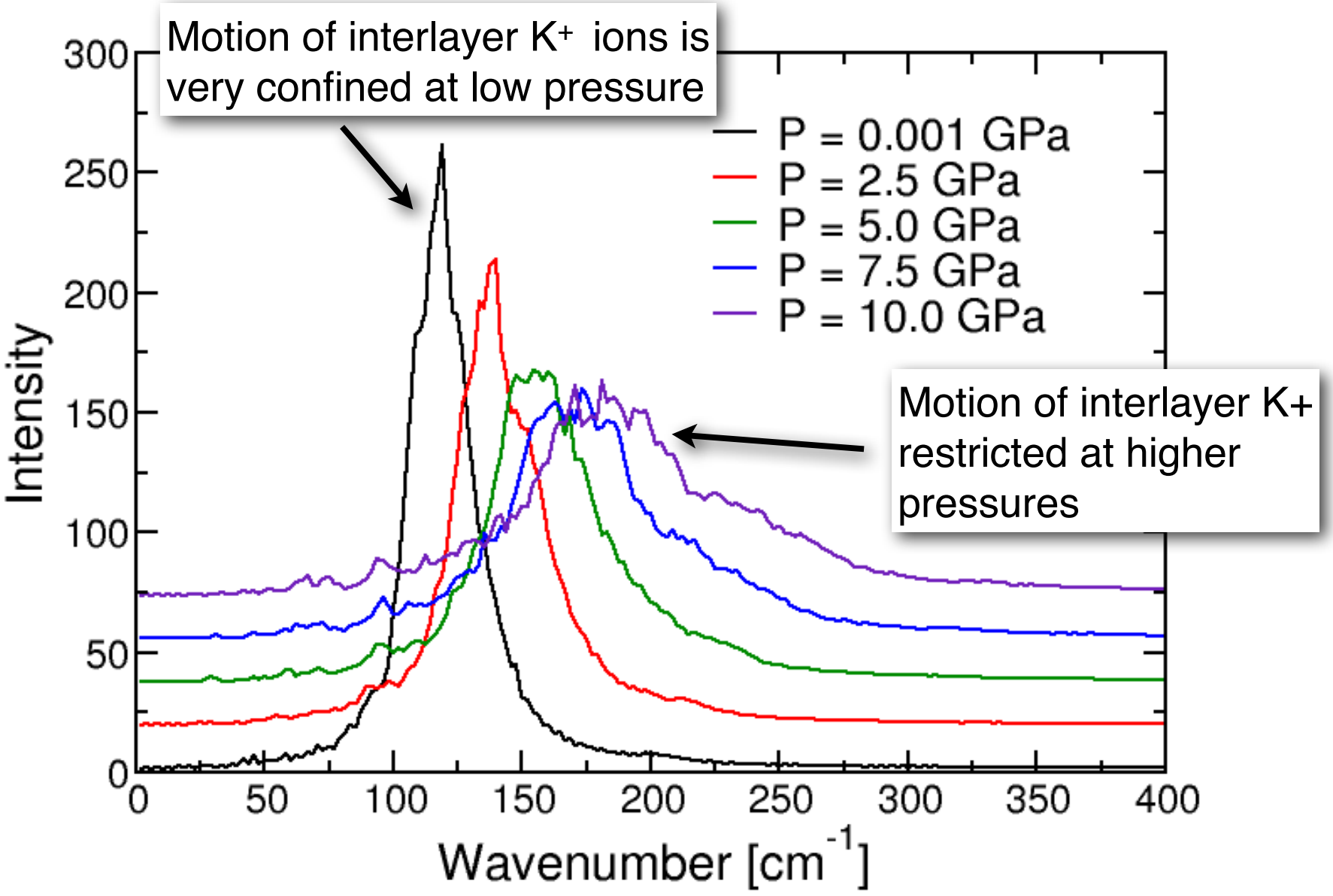
$$g(r) = \int 4\pi r^2 \rho dr$$



At high pressure see change in first neighbor peak

This change is reduced at higher temperatures

Power spectra - interlayer K^+



Conclusions

- Our simulation results matches well with experiment
- The clayff force field does a good job at capturing the mechanical properties of muscovite in the elastic regime
- Temperature does not greatly impact the mechanical properties of muscovite in the elastic regime
- Pressure has a greater effect on the mechanical properties of muscovite than does temperature