Relaxation phenomena in bulk metallic glasses: from beta relaxations to nano shear bands

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I.Physik. Institut, Univ. Göttingen

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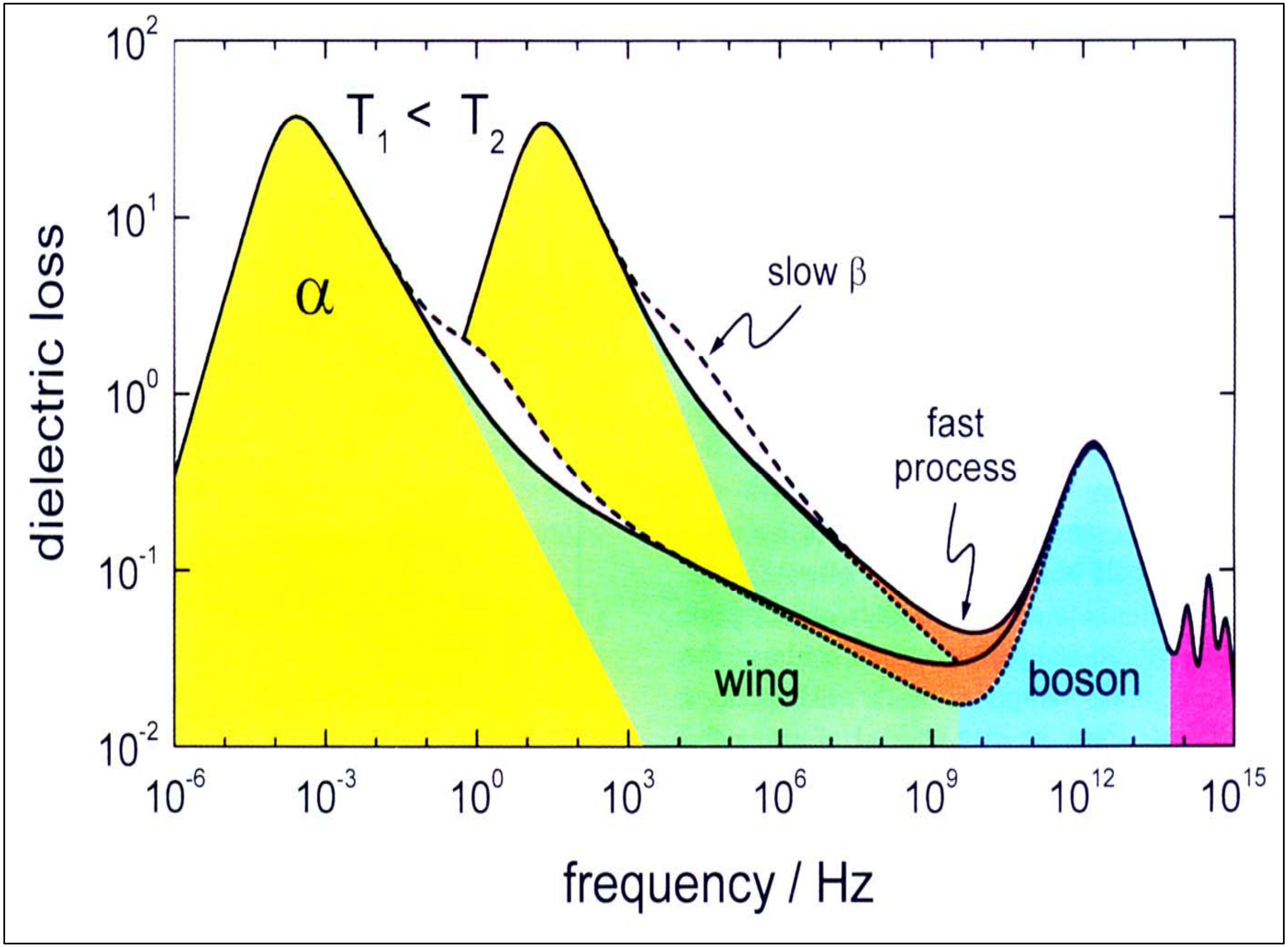
**** Weizmann Inst., Rehovot**

Financial support by GIF, DFG- FOR 1394 ,EU-ITN VitriMet Tech

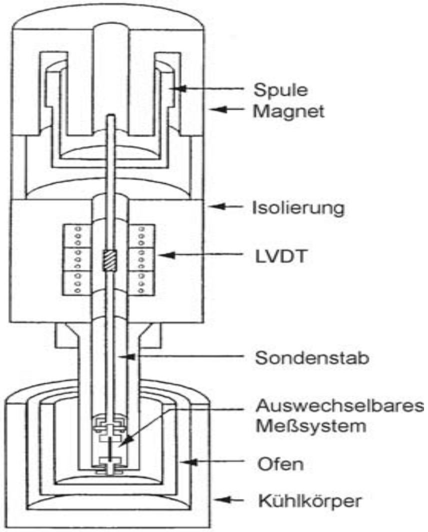
Frequency dependence of dielectric loss



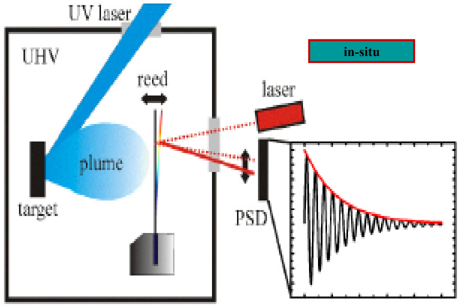
P. Lunkenheimer et al., Contemp. Phys.(2000)

Mechanical Spectroscopy in Göttingen

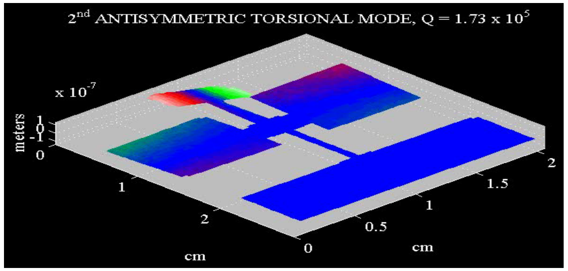
DMA 7: 0.01-50 Hz
DMA 8000 : 300Hz

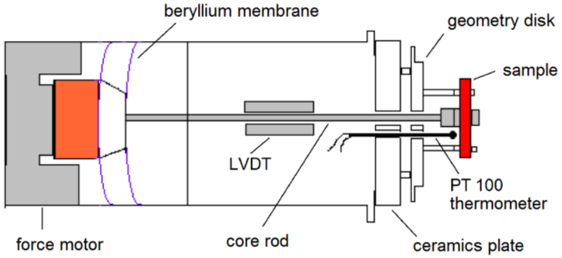


Vib. Reed : 200- 500 Hz (H.U Krebs)

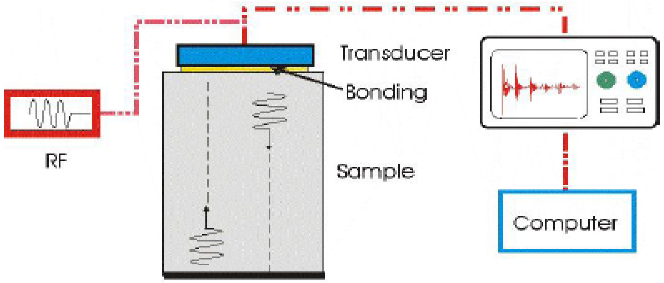


DPO: 0.4- 5 kHz

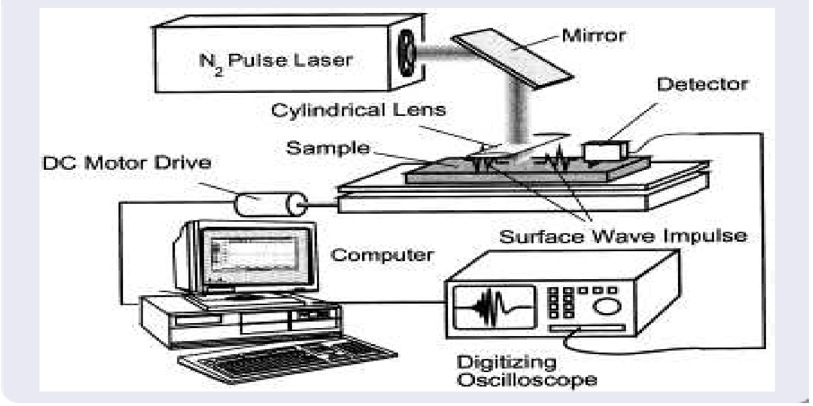




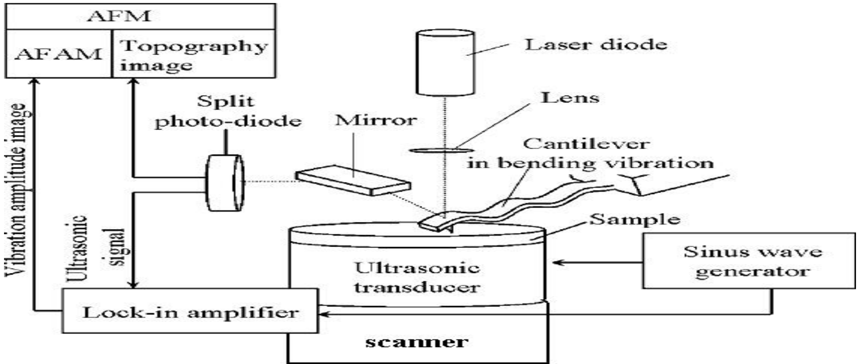
Ultra sound : 5- 20 MHz



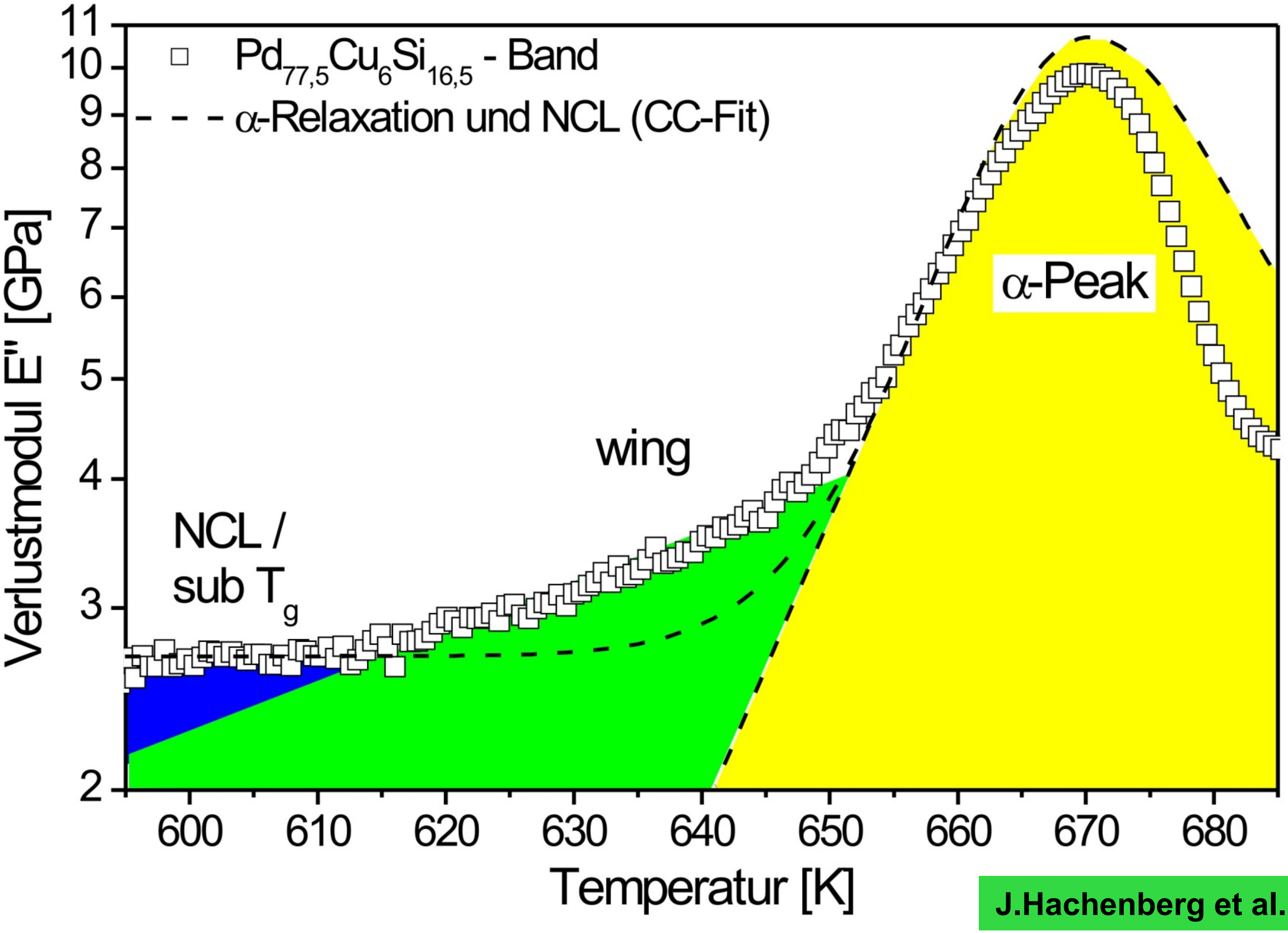
LASW : 5 - 300 MHz



AFAM: 1 - 2 MHz/ 3 GHz



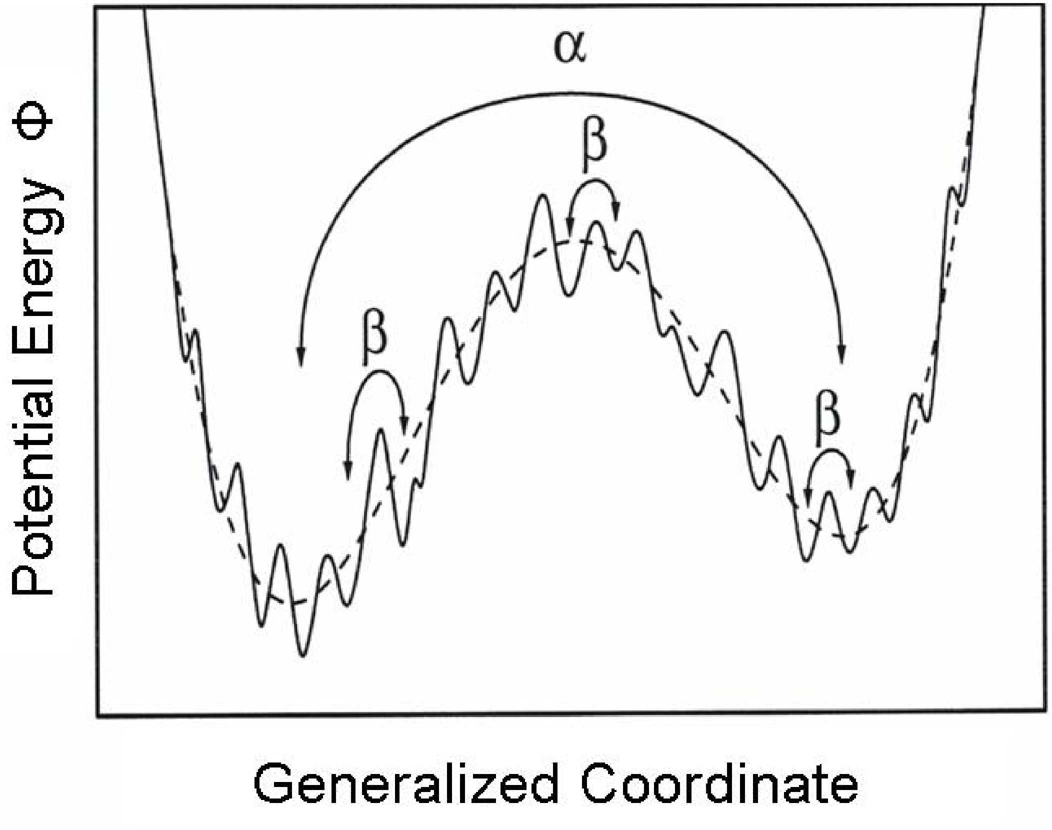
Slow beta-relaxation in metallic systems



J.Hachenberg et al. JNCS 2006

Potential Energy Landscape

- **„unhappy atoms“-T.Egami**
- **TL –systems – R. Pohl**
- **Vibrations – H. Schober**
- **Jumps**
- **Strings (β - relaxation)**
- **Plastic events (STZ)
(α - relaxation)- A. Argon**



Stillinger,Weber

Dynamical crossover in colloidal systems

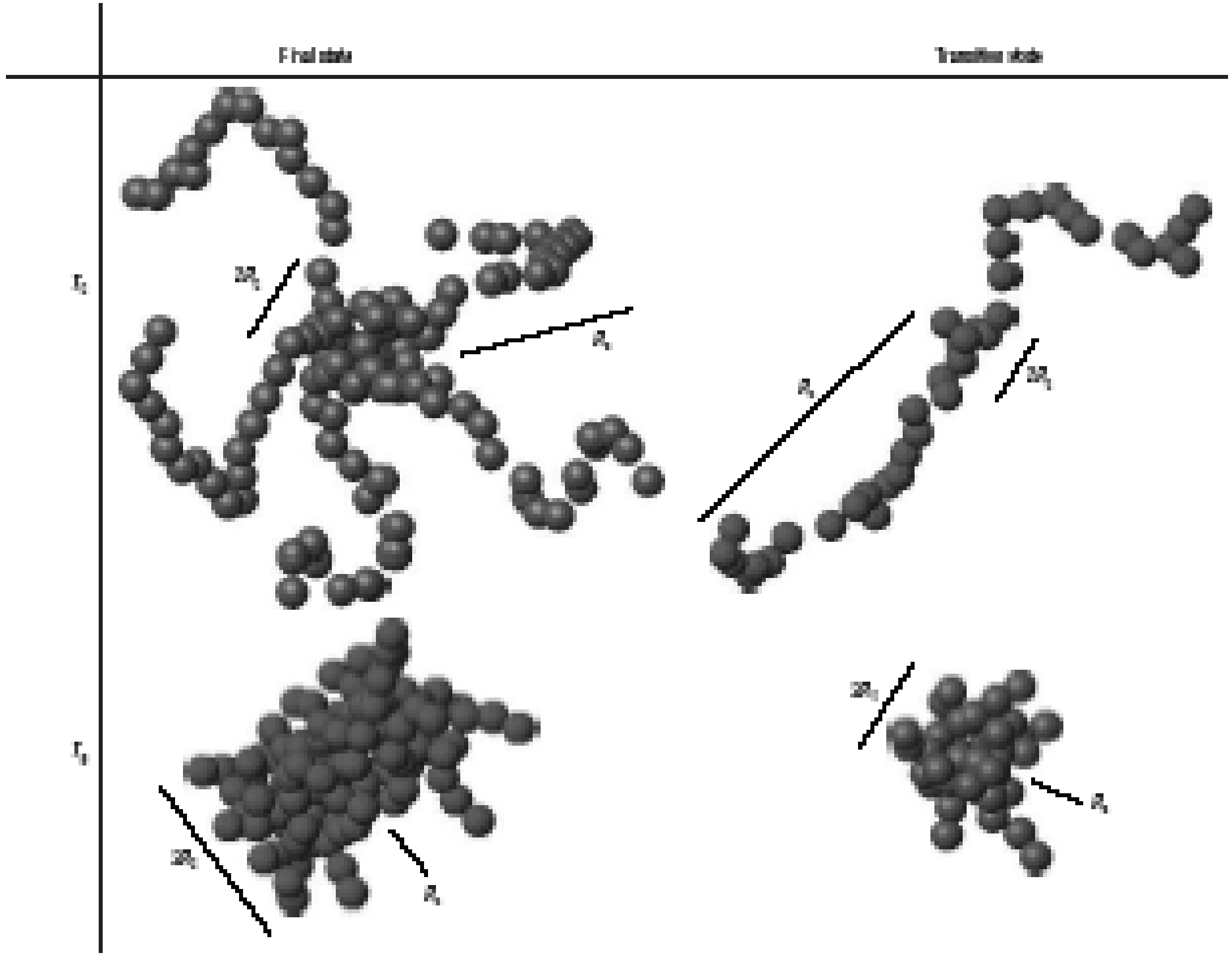


Figure 1 The shape of CRRs at T_c and T_g. The schematic appearance of the reconfiguring regions predicted by RFOT theory according to the free-energy profiles of the fuzzy-sphere model (see text) at T_g and the crossover transition temperature $T_c^{(1)}$. The shapes are shown for both the rearranged CRR (the final state) and the partially rearranged transition state. The radius of the core, R_0, and the radius of the stringy halo, R_s, are shown in the figure.

JACOB D. STEVENSON[1]*, JÖRG SCHMALIAN[2] AND PETER G. WOLYNES[1]*

Nature Physics,2006

STZ‘s and network forming in colloidal systems – P.Schall, D.Weitz and F.Spaepen

Science 2007

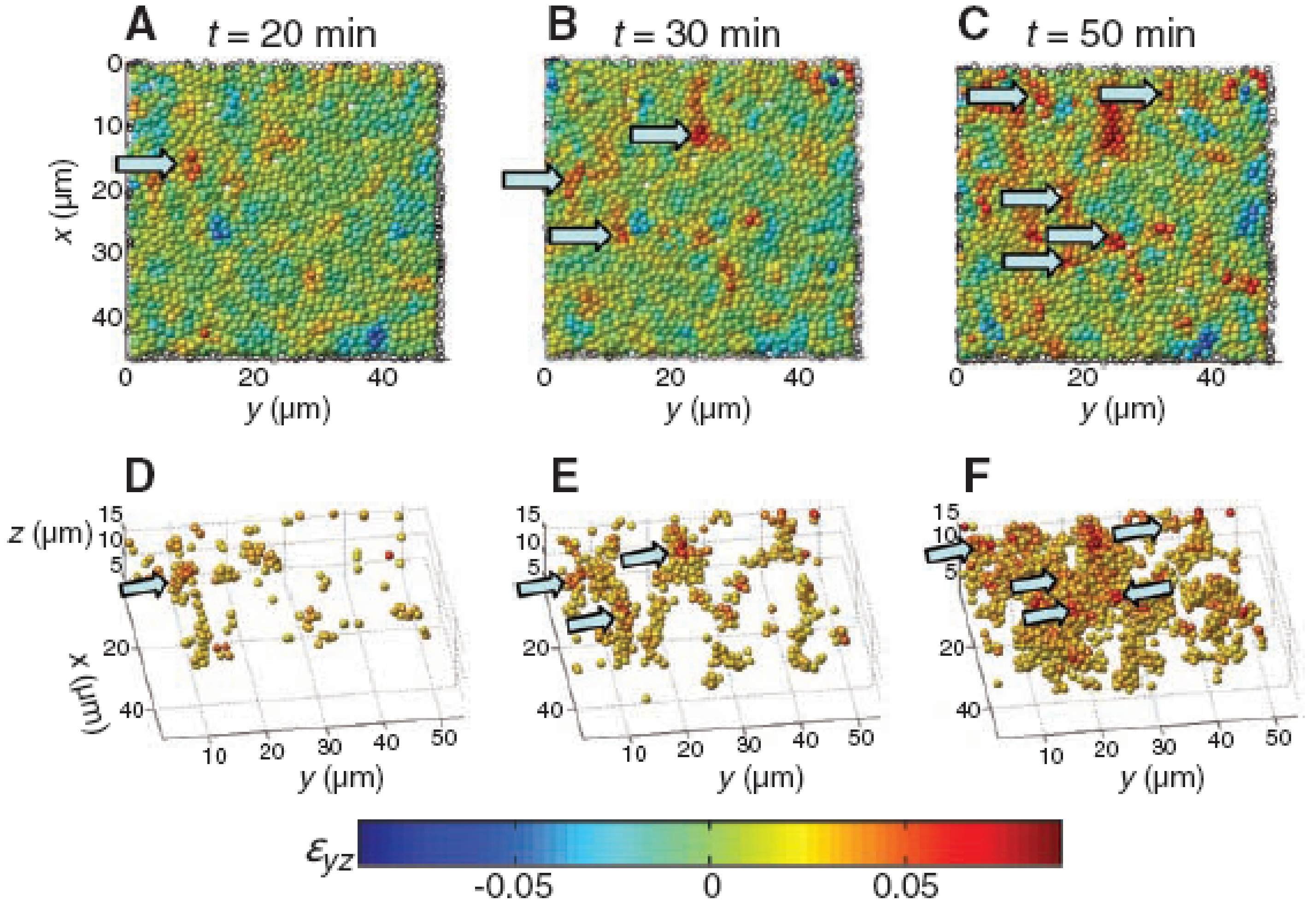


Fig. 4. Strain evolution during shear. Distribution of the cumulative shear strain after 20, 30, and 50 min of shear. For each frame, arrows indicate shear transformation zones that have been formed in the time interval before the frame shown. Shear transformation zones appear to form a connected network at $t = 50$ min. (**A** to **C**) *x*-*y* sections (5 μm thick) centered at $z = 13.5$ μm. (**D** to **F**) Perspective view of 16-μm-thick sections showing particles with shear strain values larger than 0.025 only.

Local shear transformations in deformed and quiescent hard-sphere colloidal glasses

K.Jensen,D.Weitz, F Spaepen Phys.Rev E 90 (2014)

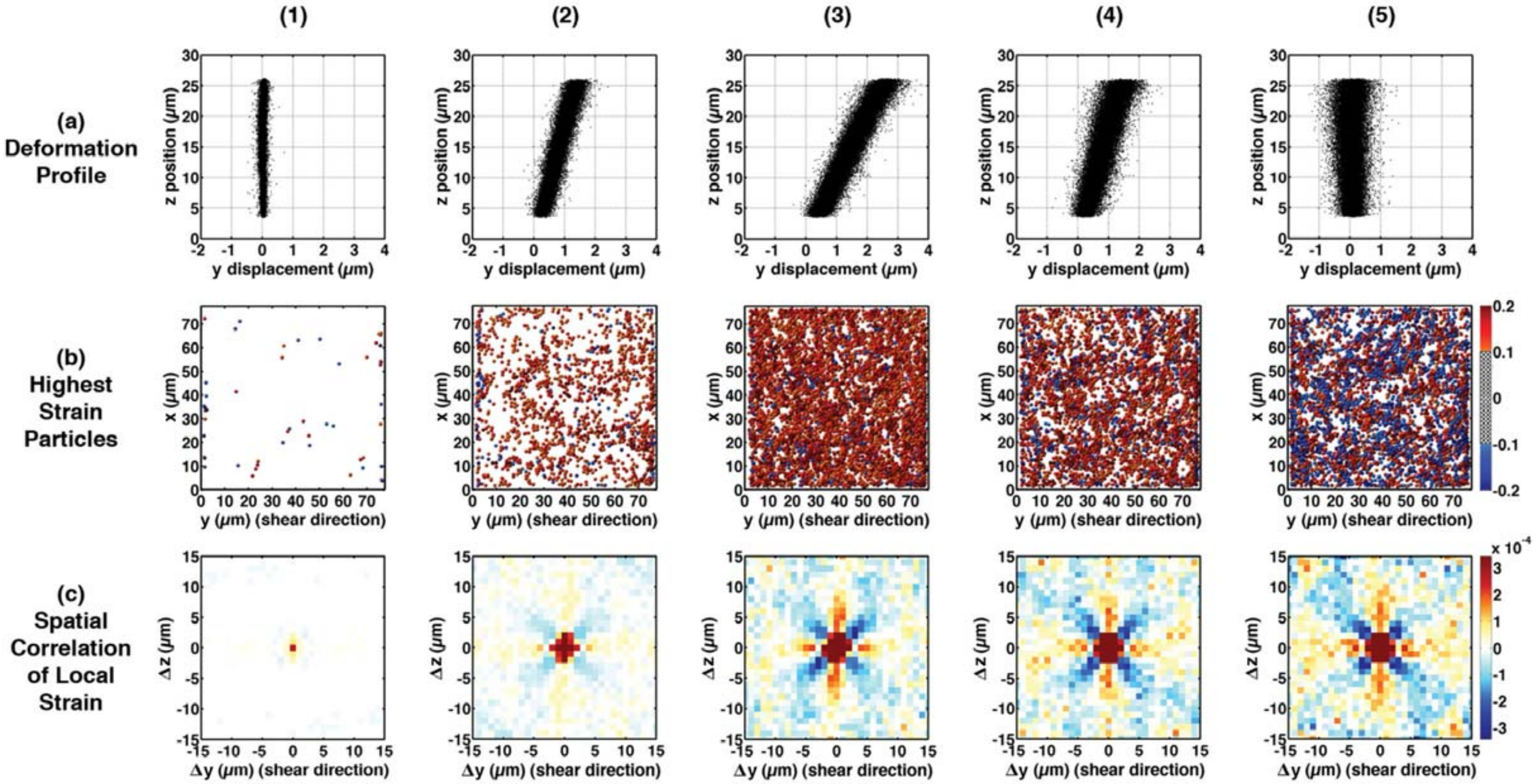
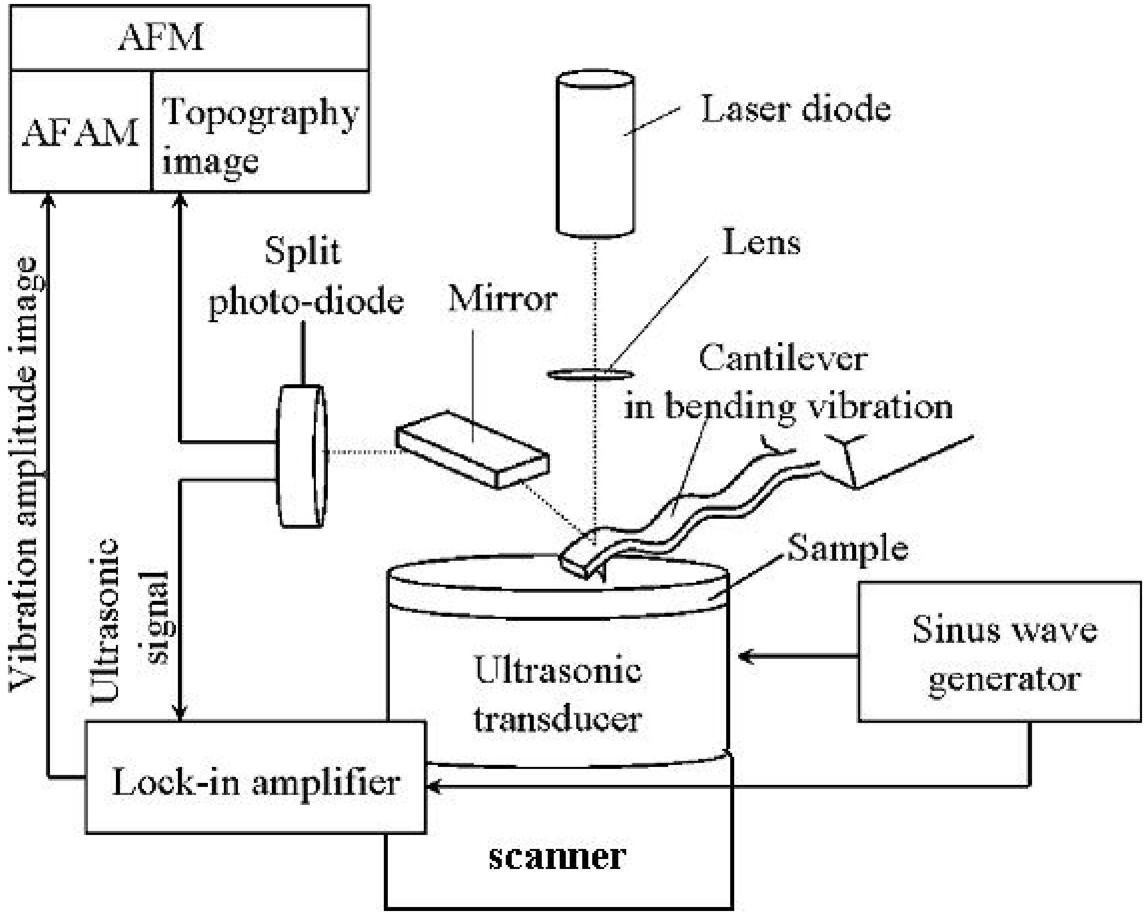


FIG. 6. (Color online) Evolution of strain and strain correlations in the colloidal glass during a shear experiment. The time and macroscopic strain corresponding to columns (1)–(5) are indicated in Fig. 5(c). Row (a) shows the deformation profiles. Row (b) shows the top-view reconstructions showing only those particles with individual strain $|\epsilon_{yz}| > 0.1$, colored according to their strain. On strain reversal, some of the regions of particles that acquire a high positive strain (red) return to a low-strain configuration and disappear from the reconstruction; others experience an irreversible local deformation and remain in a high-strain state at the end of the experiment. These are compensated for by other regions that deform in the opposite direction (blue) so that at the end the average strain is zero at time (5). Row (c) shows the y-z plane cross sections of ϵ_{yz} spatial autocorrelations, showing the evolution of the fourfold pattern that is the signature of Eshelby inclusions active in the material.

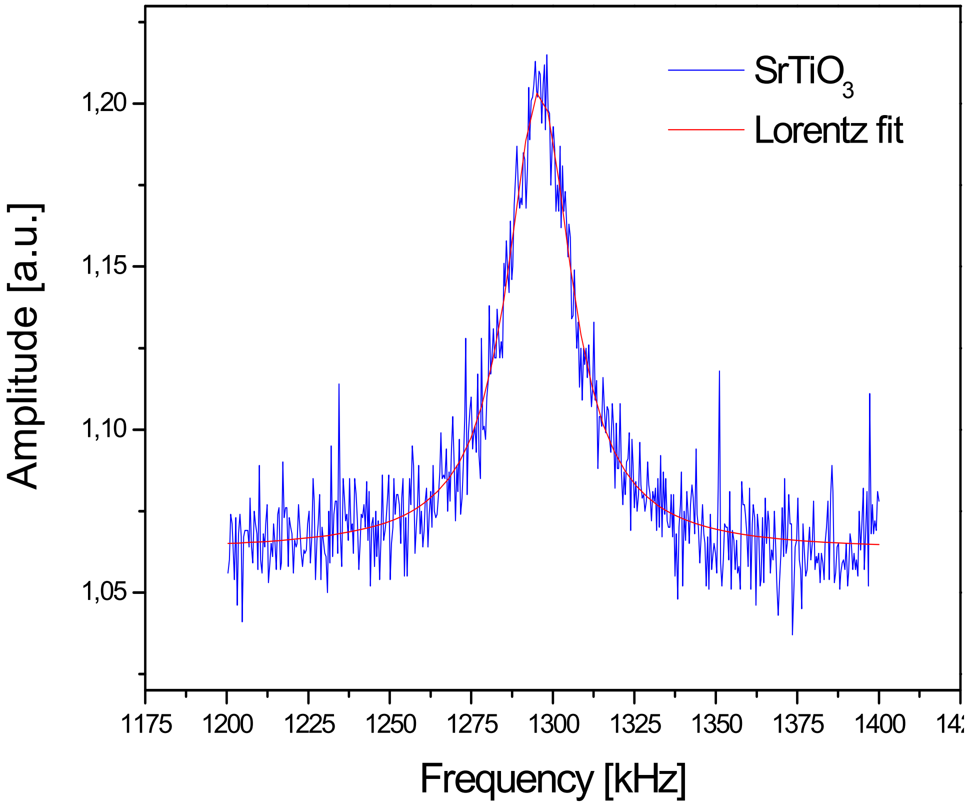
AFAM: setup used by the Arnold group (IZFP Saarbrücken)



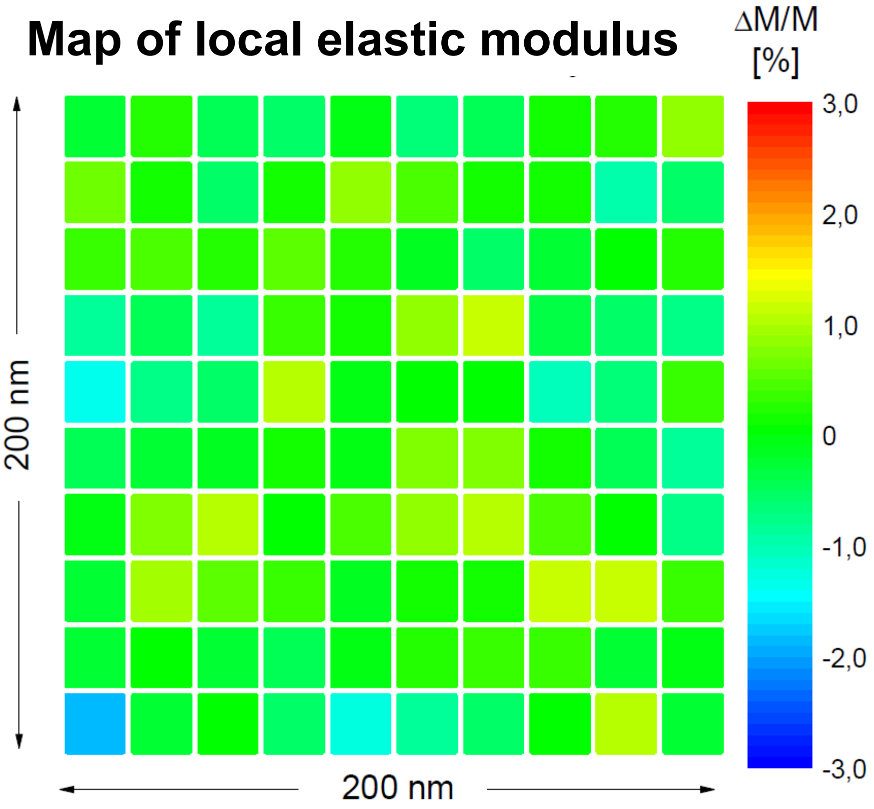
M. Kopycinska-Müller, A. Caron, S. Hirsekorn, U. Rabe, H. Natter, R. Hempelmann, R. Birringer and W. Arnold
Z. Phys. Chem. **222** (2008) 471–498

AFAM spectroscopy

Contact-resonance spectra of a $SrTiO_3$ sample and map of local elastic modulus



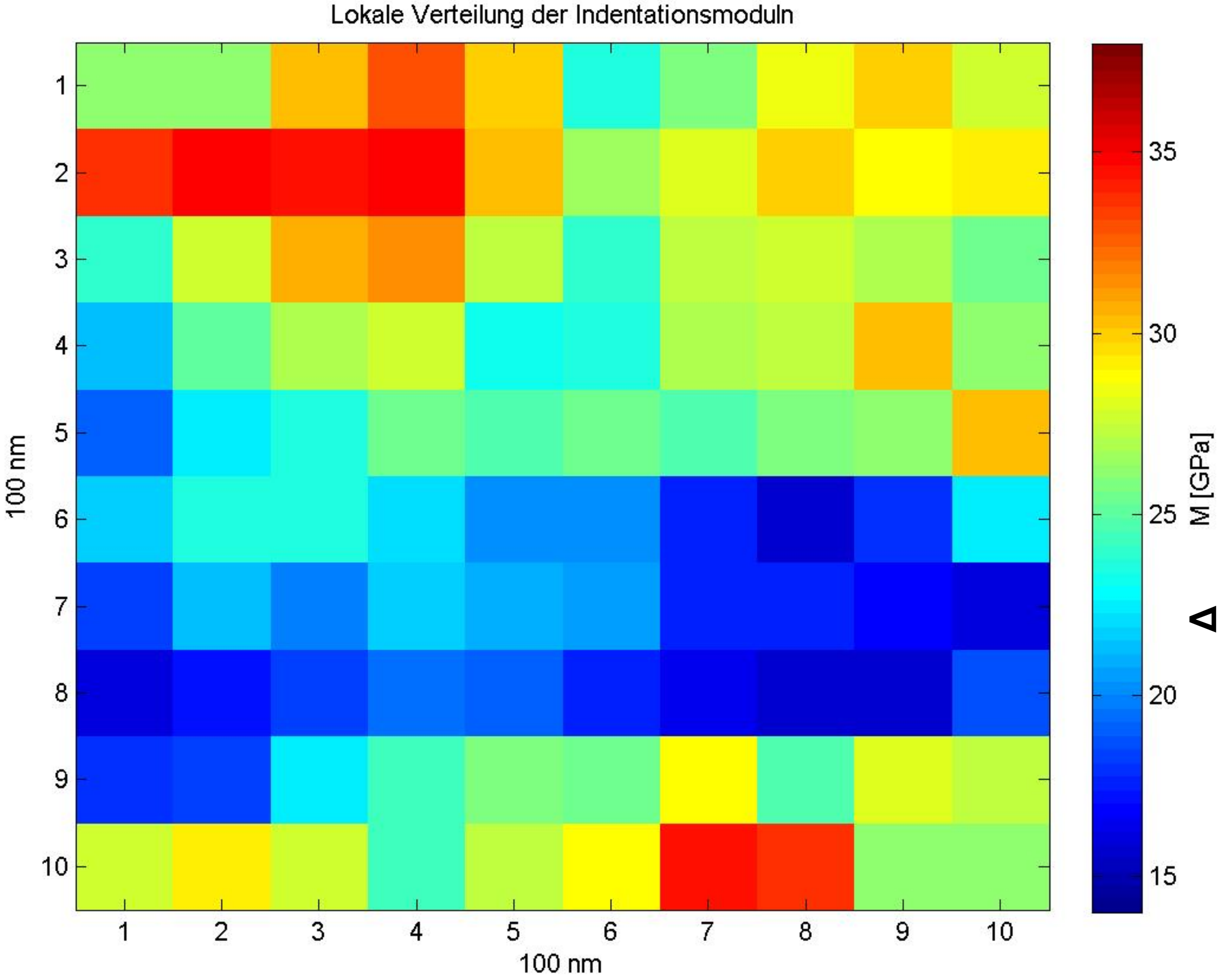
Map of local elastic modulus



Bulk metallic glasses

Sample: PdCuSi, Reference samples: STO, SiO2

Map of local elastic modulus

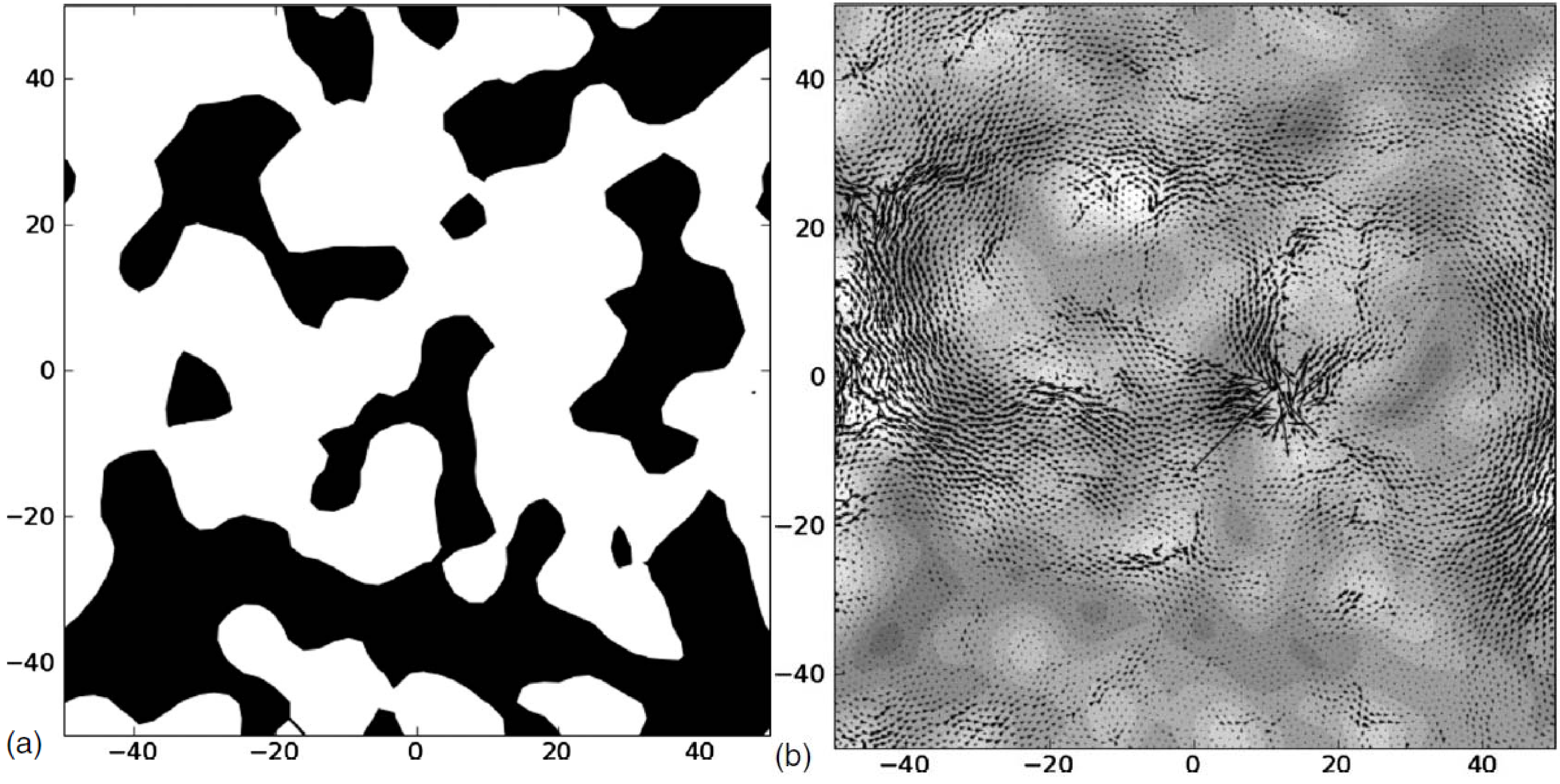


Lokale Verteilung der Indentationsmoduln

H.Wagner et al. Nature Mat. 2011

Local elastic map & plasticity (2-D-LJ system)

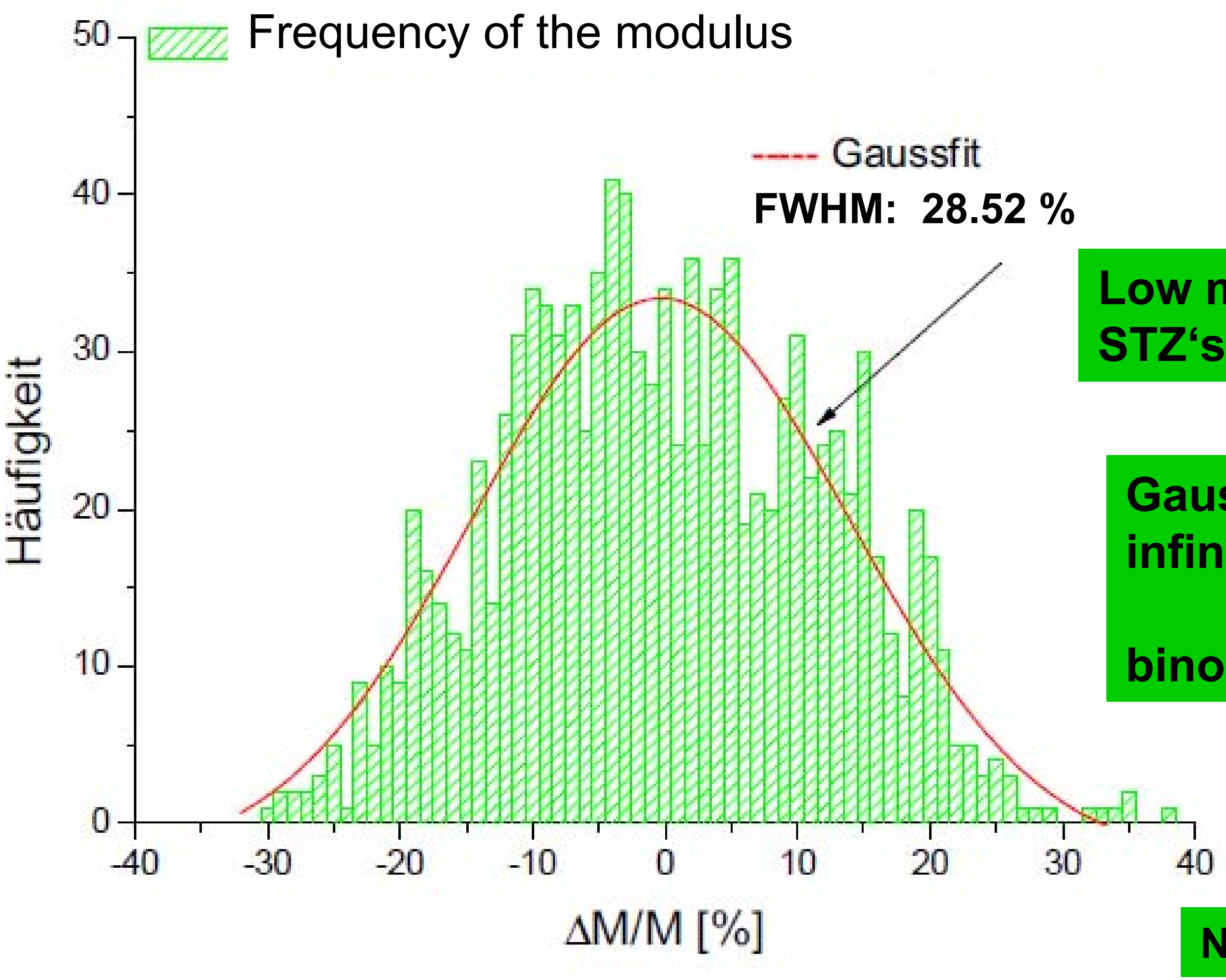
M.Tsamados, J-L Barrat et al. PRE 80 (2009)



G in rigid (black) and soft (white) zones
2.5% strain (100x100 atoms)

Overlap of nonaffine displacement field
(x 300) with elastic map for 2.55% strain

Frequency distribution of local modulus with M= 105 GPa – amorphous PdCuSi (H. Wagner)



FWHM: 28.52 %

Low modulus „soft spots“: STZ‘s in the „elastic„regime

Gaussian not good due to infinite tails –

binomial or Hughes distr.

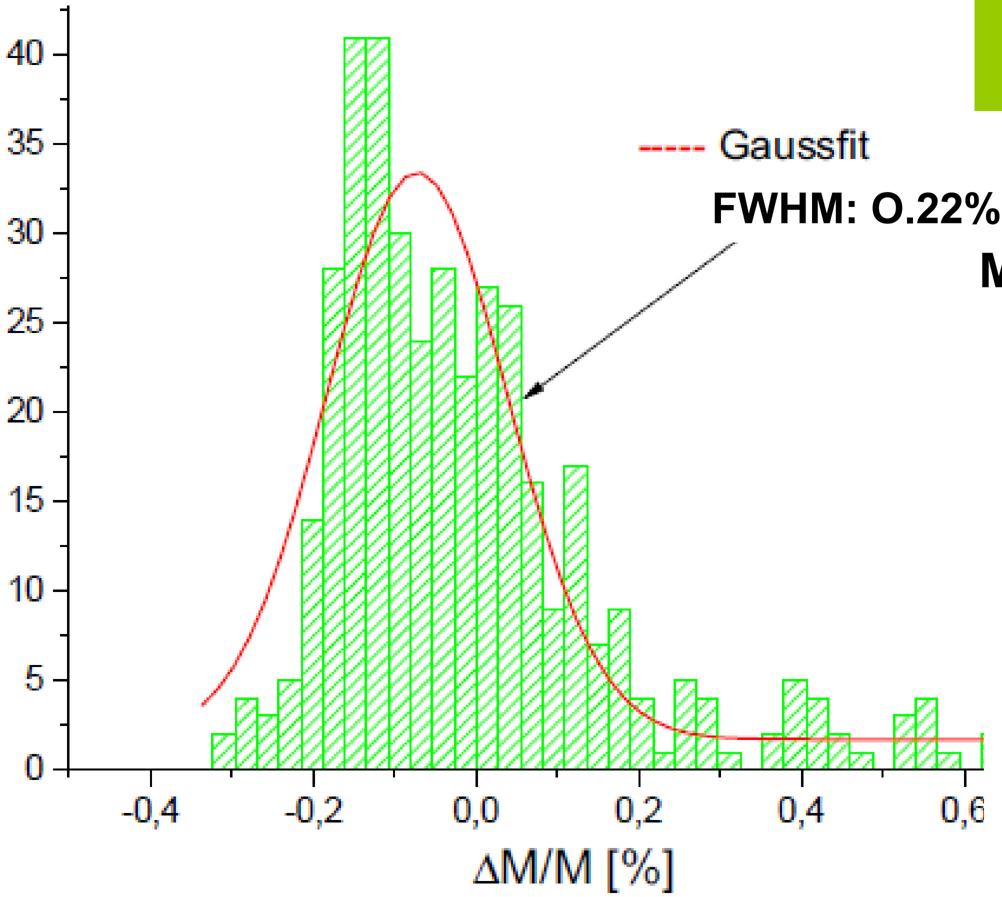
Nature Mat.,10 (2011) 439

Probability distribution of local modulus with M= 174.5 GPa – at least partly crystalline PdCuSi (H. Wagner)

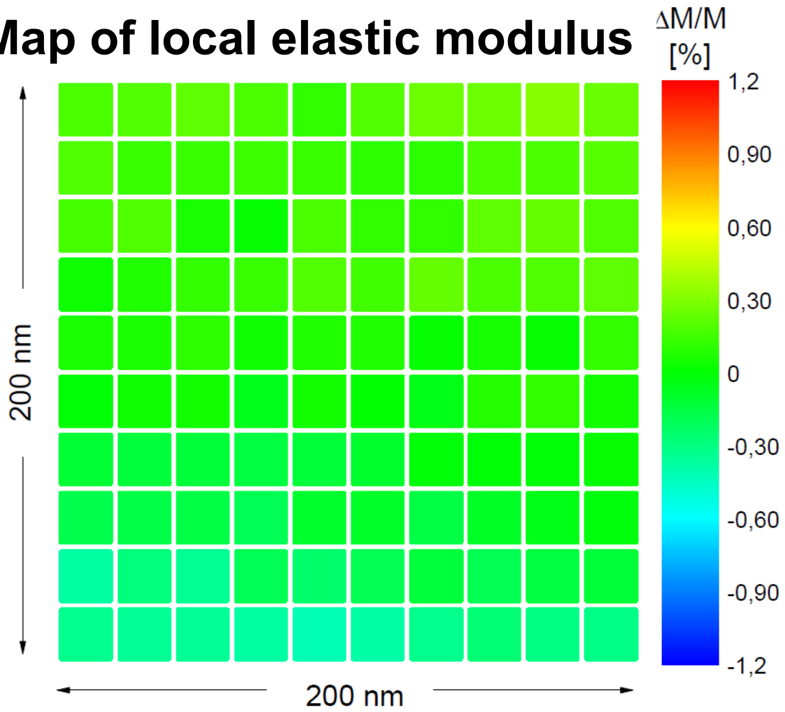
Polycrystalline material with grain size
orientation distribution
= Modulus distribution

Note: HWHH a **factor 100** smaller
compared to glass
and
soft parts are missing in
Gauss distribution
(first to crystallize)

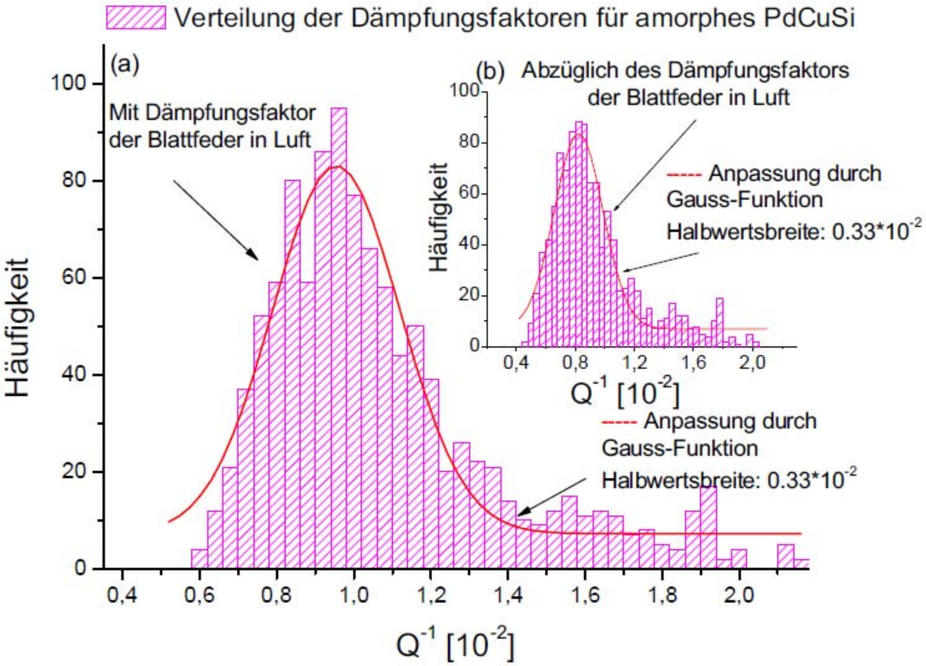
Frequency of the modulus

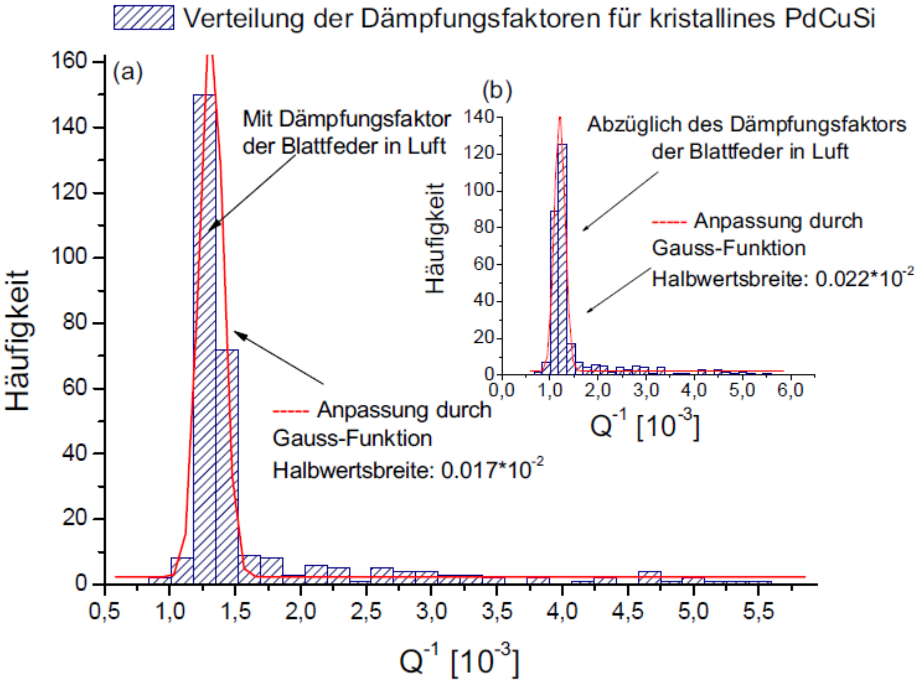


Map of local elastic modulus



Loss distribution of amorphous and x-talline PdCuSi

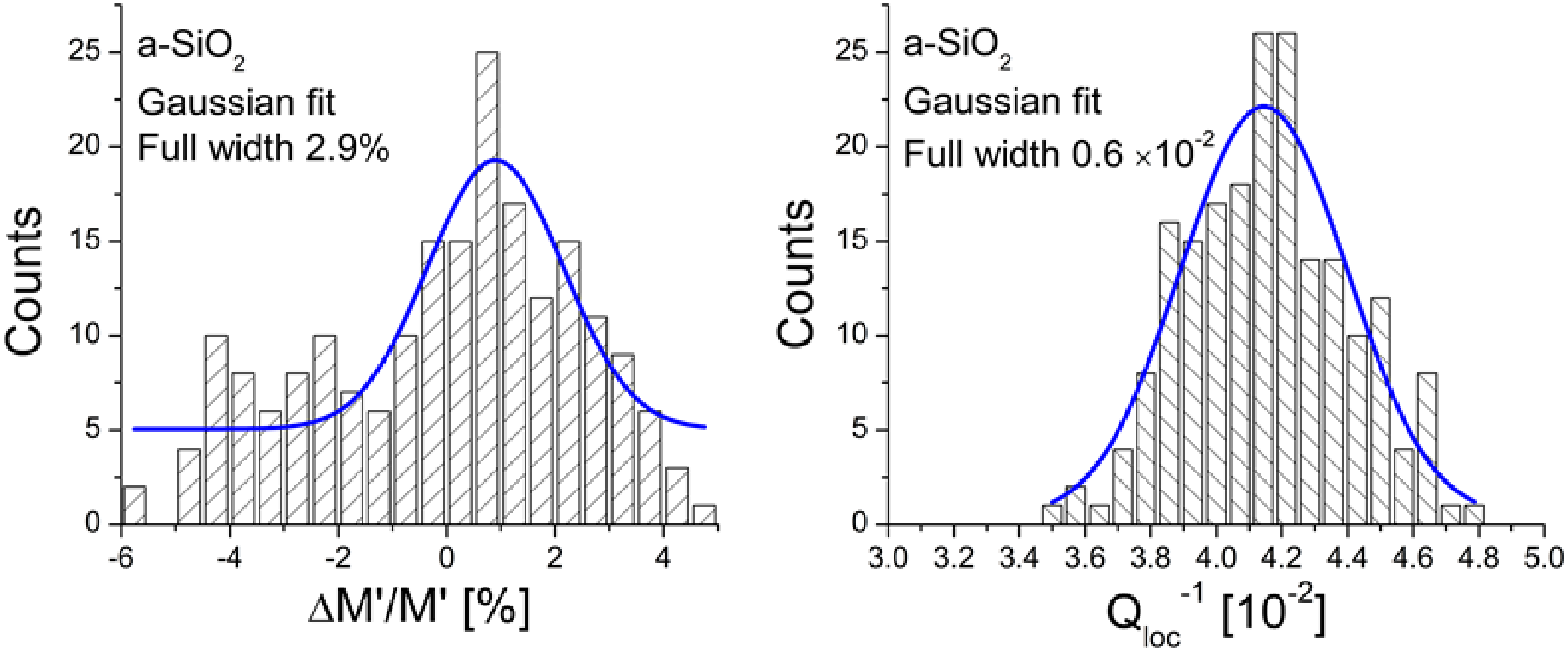




FWHM (a-PdCuSi) ~ 0.33 x10^{-2}

FWHM (x-tal PdCuSi)~ 0.017 x 10^{-2}

Frequency distribution of local modulus and loss– amorphous SiO_2 -a strong glass forming system



H.Wagner et al. accepted by JAP 2014

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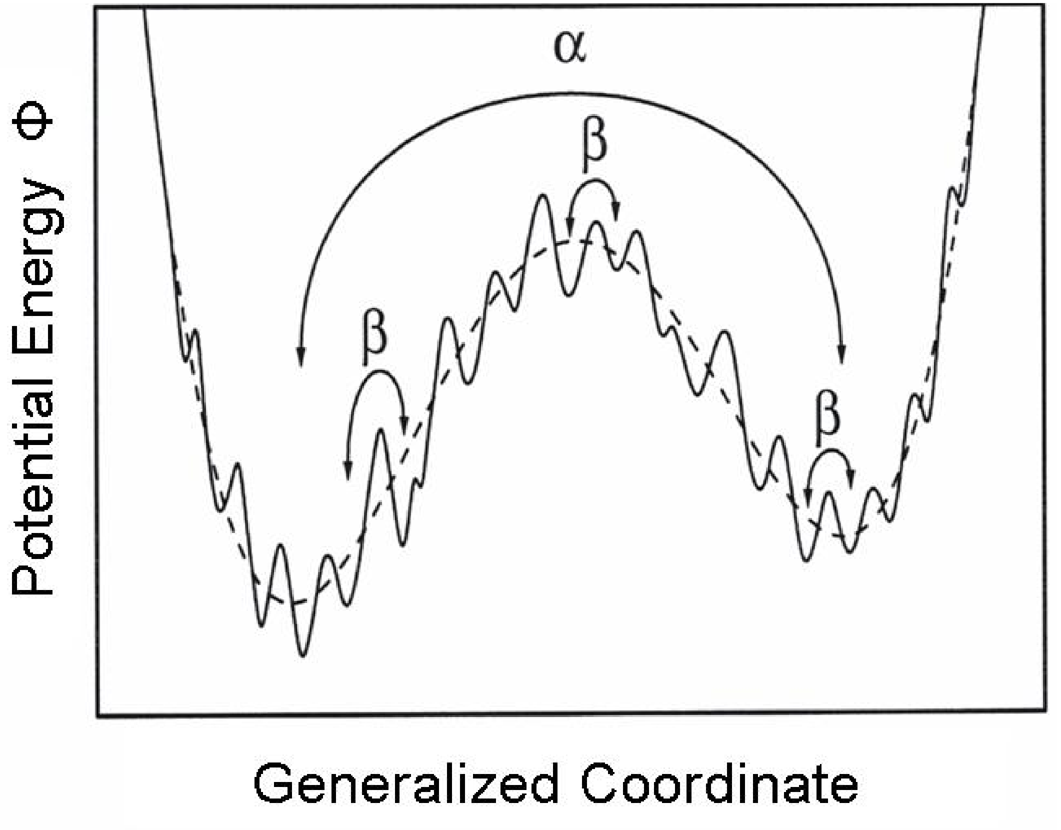
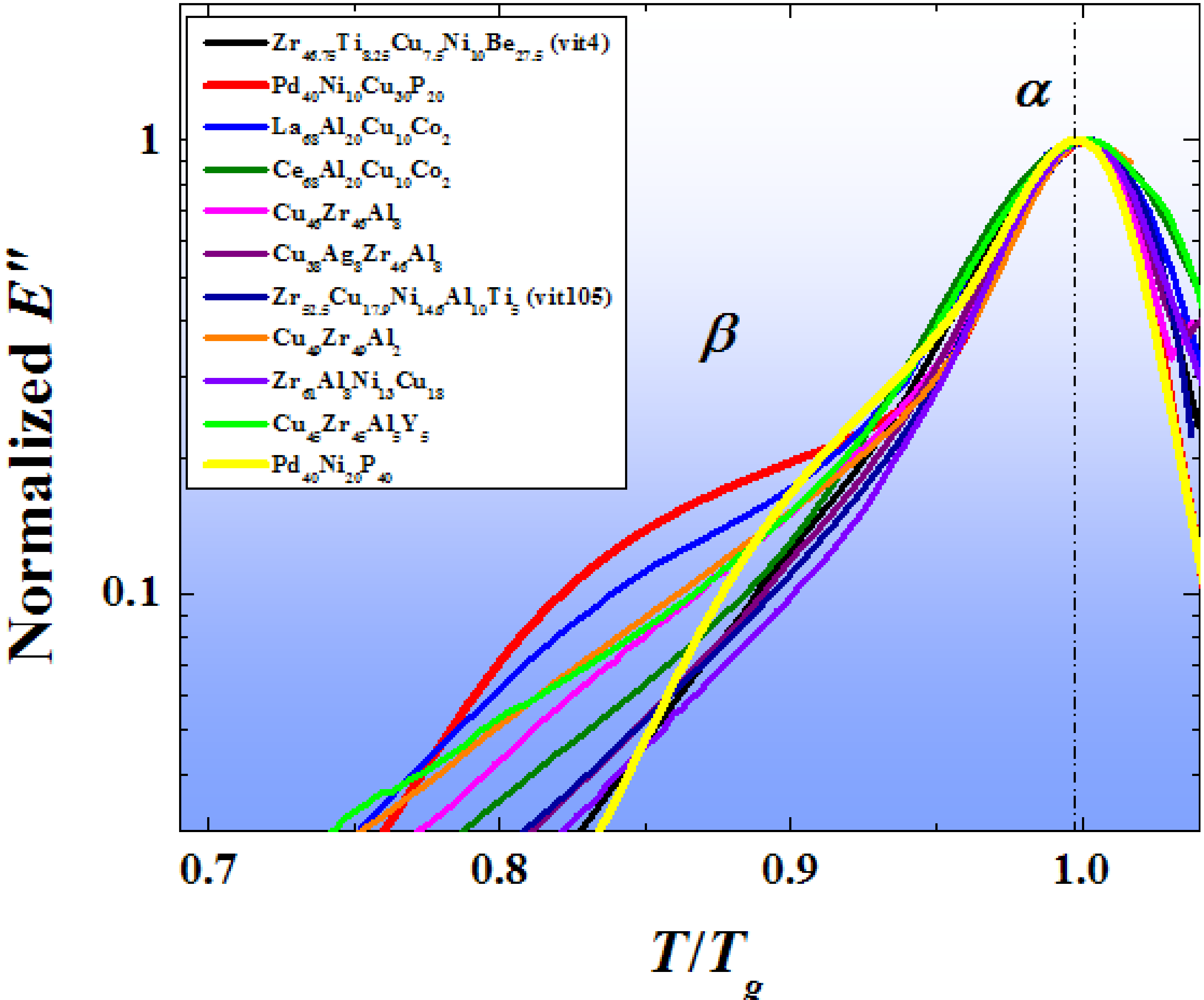


Stillinger,Weber

Universal character of the slow beta-relaxation in metallic systems

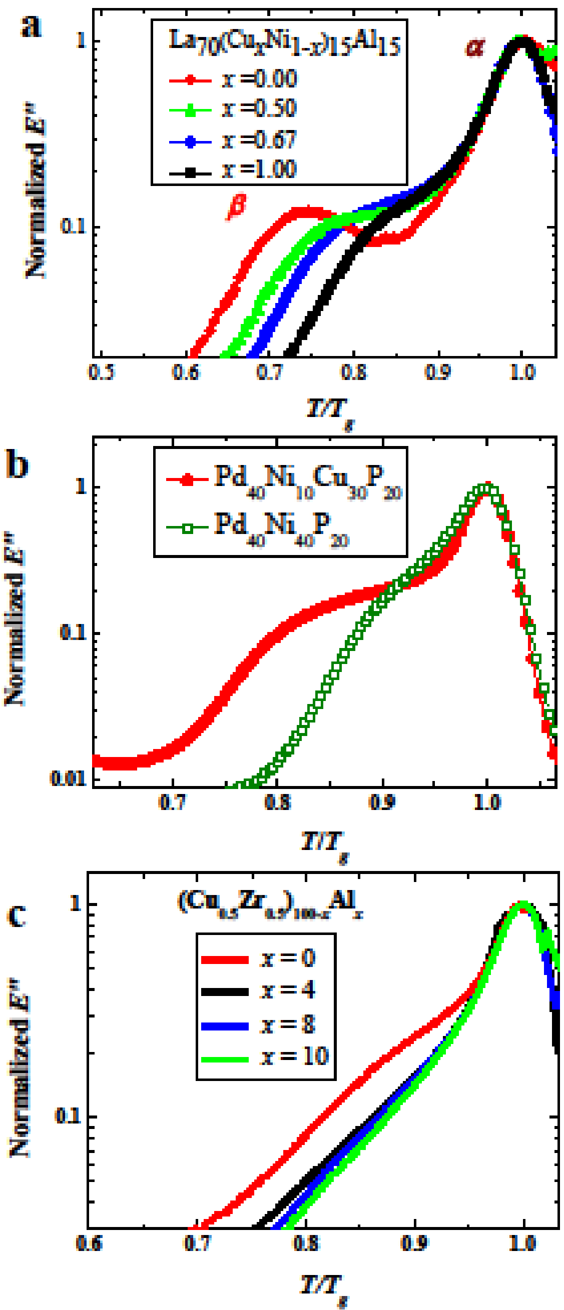


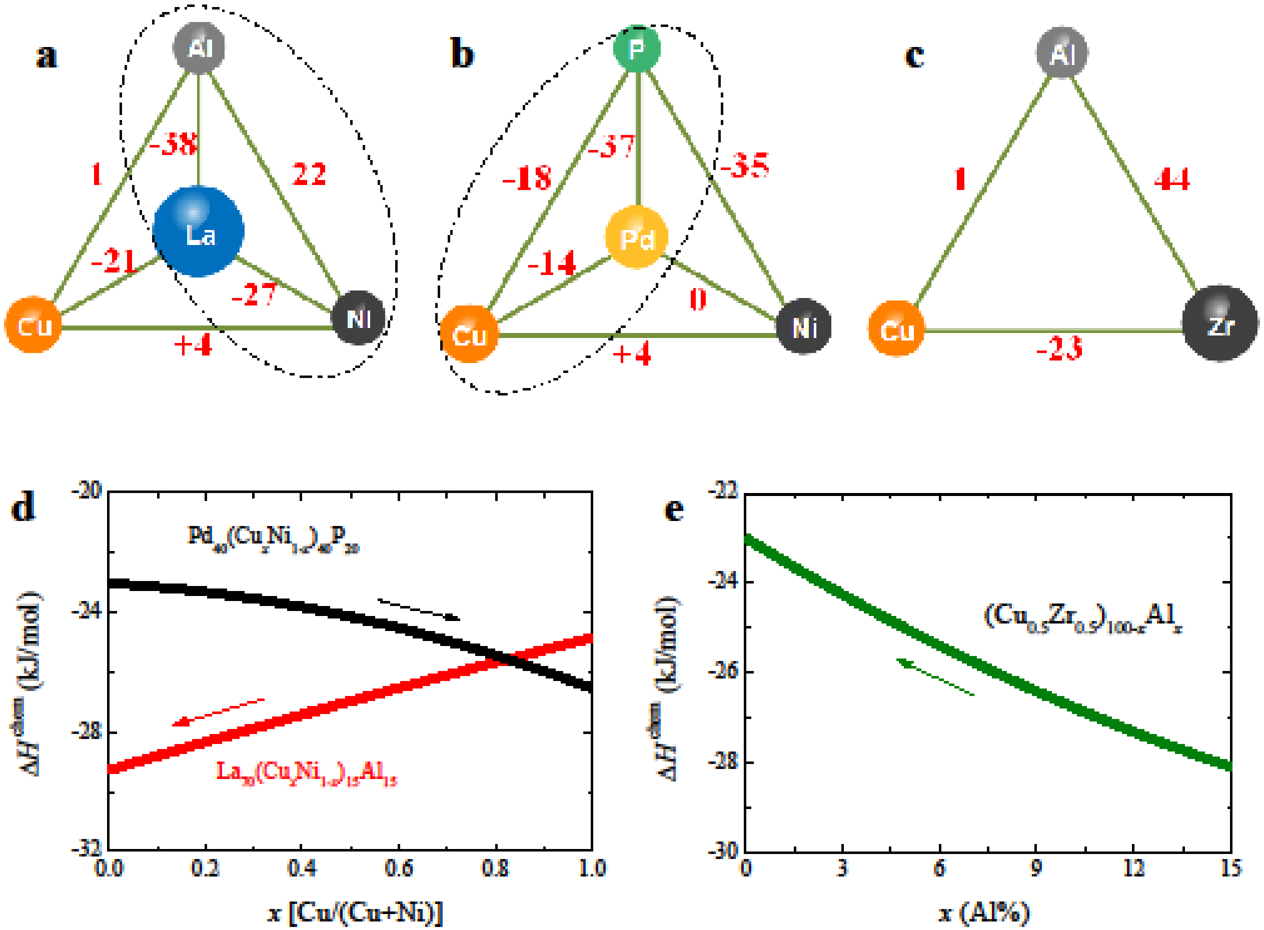
Prof Wei Hua Wang Group,Beijing,China

Type **A** and type **B**-Glasses (Roessler): for metallic systems depending on **„molecule-like“** metallic glass types.

Nature Comm.(2013)

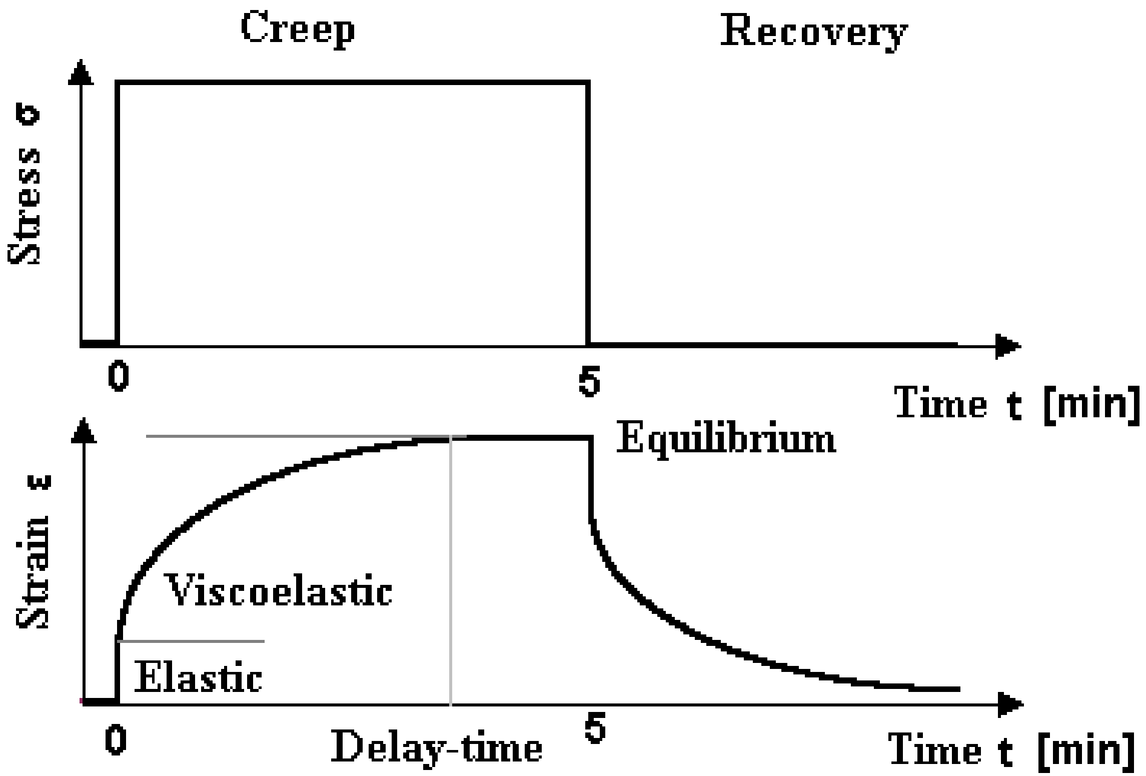
„Molecule –like“ metallic glasses: Chemical influence on β relaxations

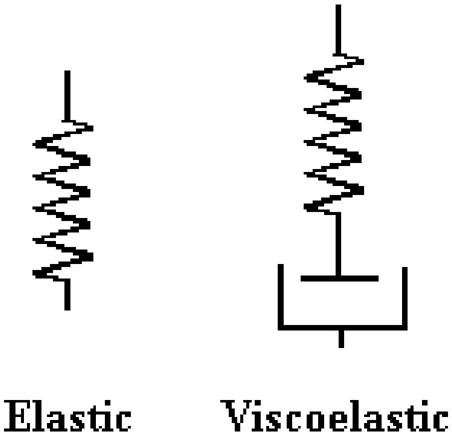




H.B.Yu, K.S., W.H.Wang and H.Y.Bai: Nature Comm. 2013

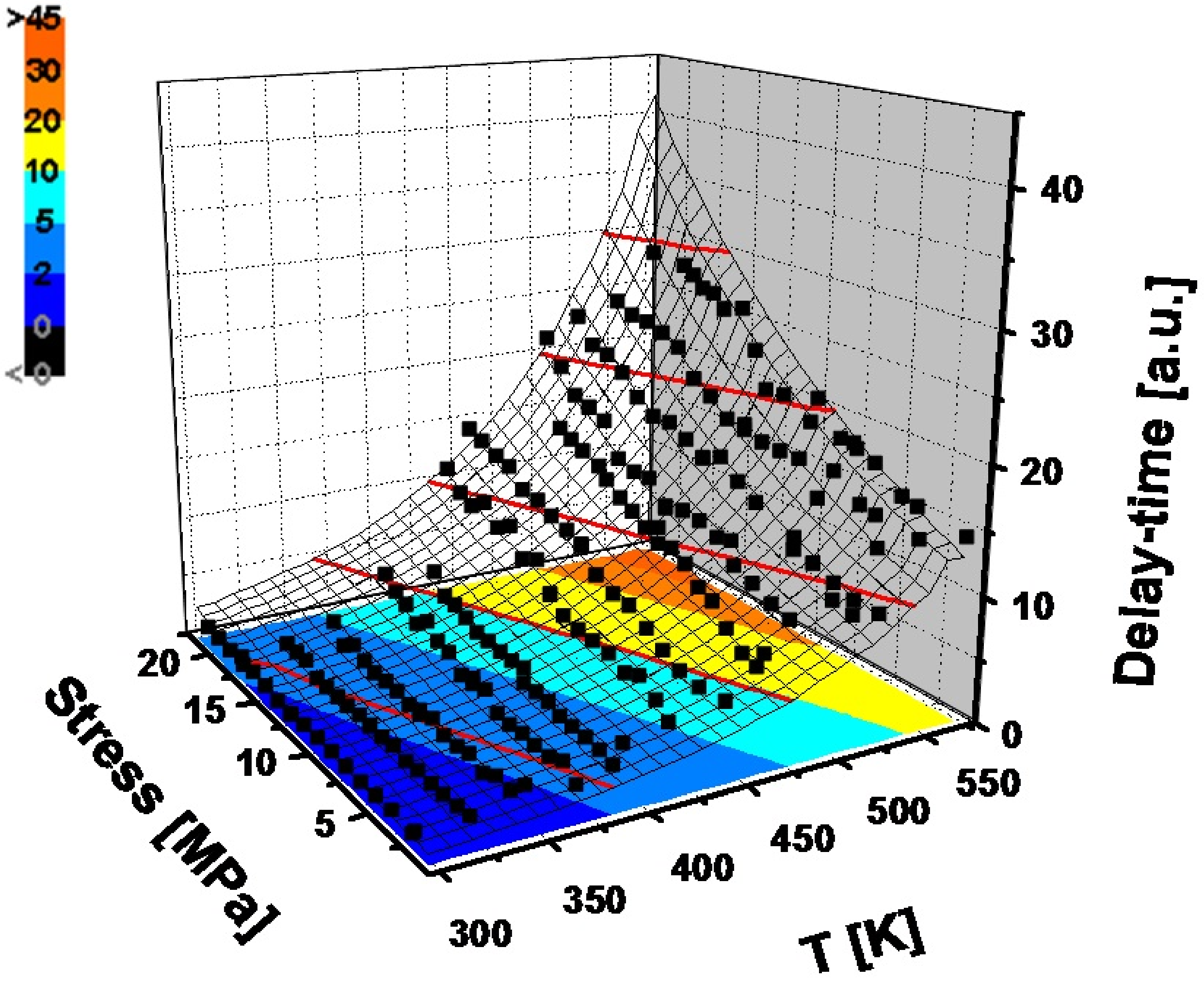
Creep- recovery experiment for glassy PdCuSi below Tg to test the β - relaxation





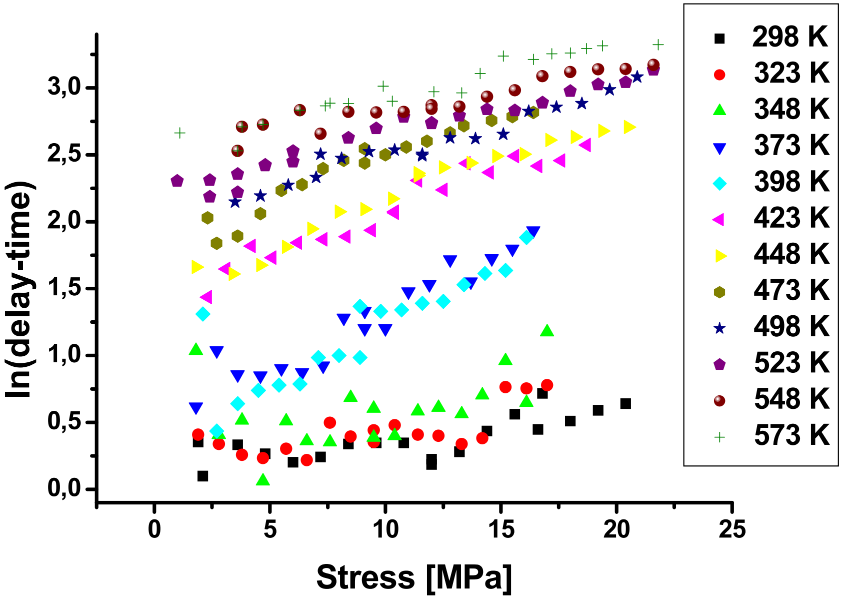
M.Schwabe et al., EJPE,2011

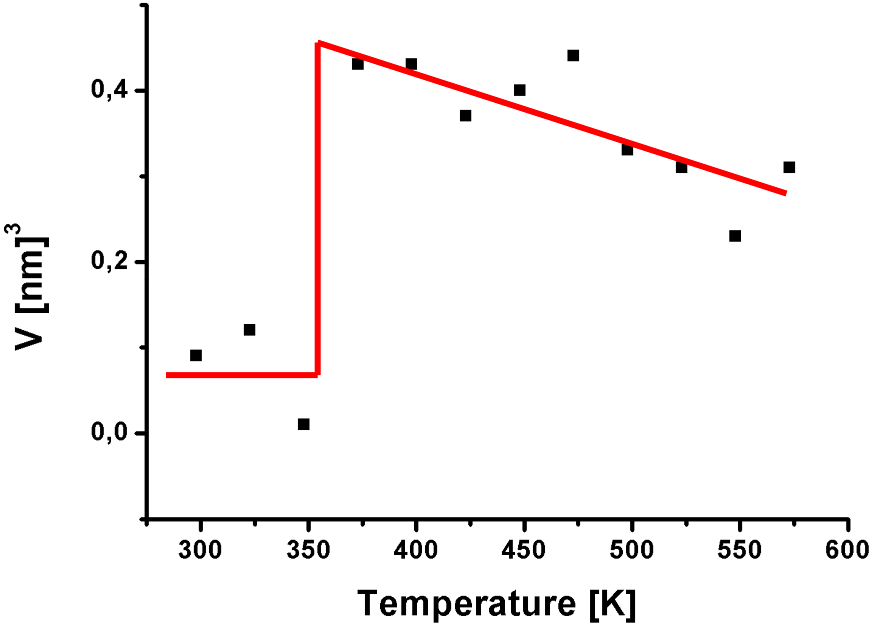
Loss landscape for the secondary - JG- β - relaxation versus temperature and stress



Activation volume for the secondary- JG- β relaxation for glassy PdCuSi

$$V = k_B T \left(\frac{\partial \ln \text{delay} - \text{time}}{\partial \sigma} \right)$$



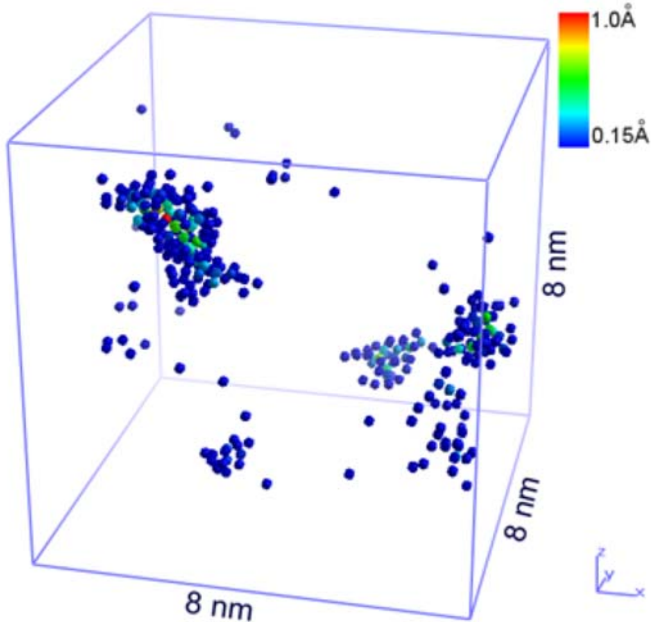


String volume only 0.4 nm^3 ~ 20-30 atoms– factor 20 less than STZ size and <u>decreasing length scale</u> with increasing temperature

see also MW Chen, H.Schober, F. Faupel et al.

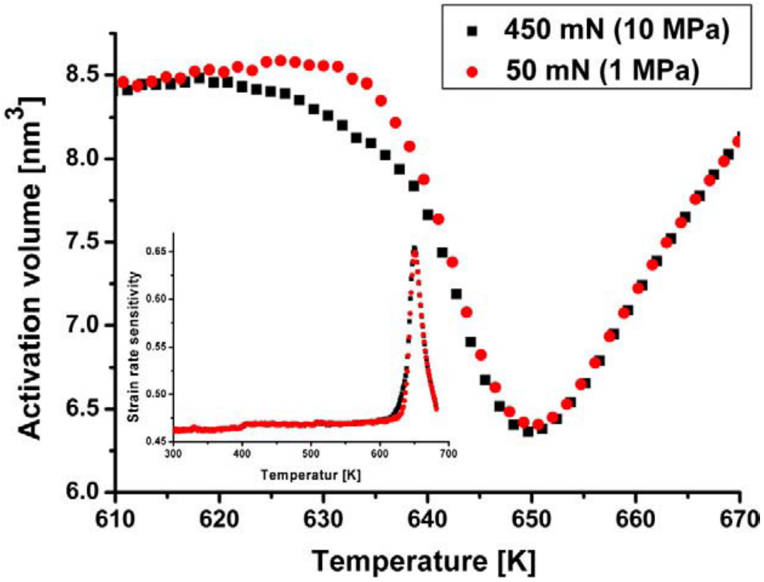
Size of plastic events (STZ) – α - relaxation

Computer simulations:



[M. Neudecker, S. G. Mayr, Acta Mater. 57, 1437 (2009)]

Experiments on bulk samples:
(strain rate sensitivity)



[M. Schwabe et al, J. Non-Cryst. Solids 357, 490 (2011)]

STZ – size ~ 120 Atoms

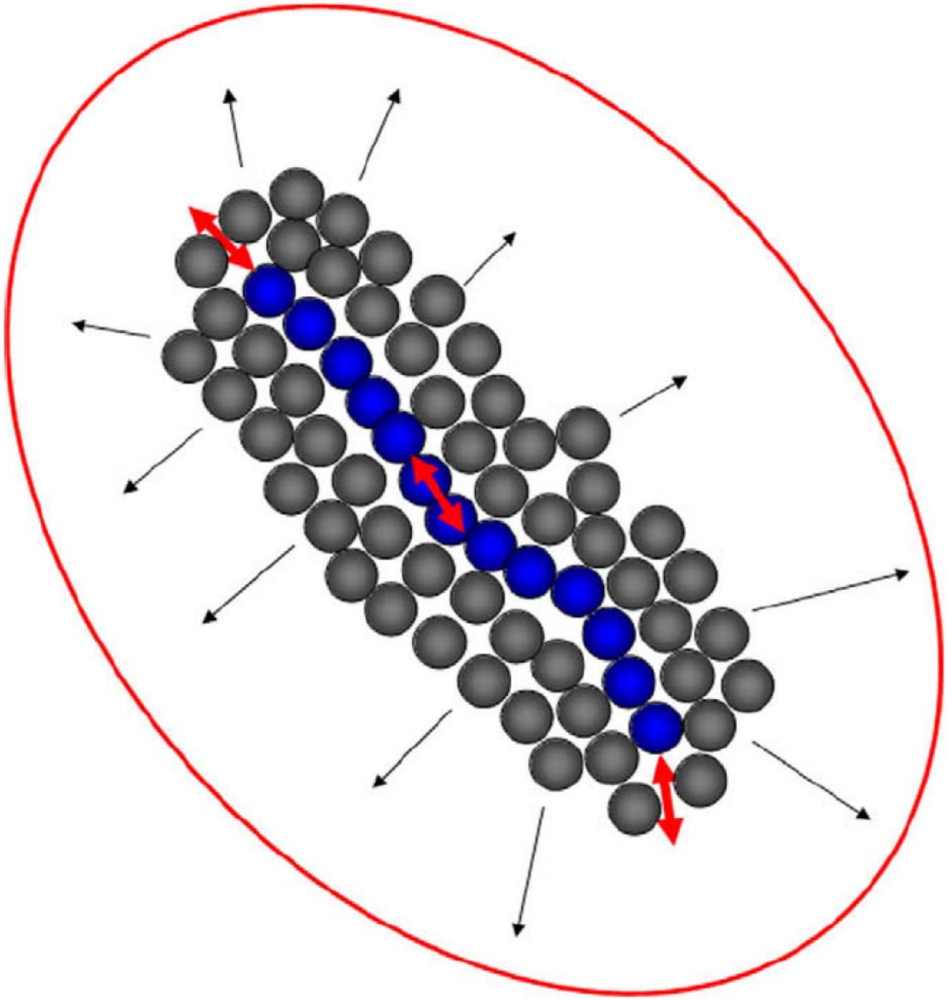
STZ size ~ 560 Atoms

See experimental results from D. Pan, MW Chen et al. PNAS 2008 and Y.H.Liu et al. PRL(2011) : Correlation length ~ 2.5nm (Phase)

β-excitation or string acts as an elastic quadrupol !!

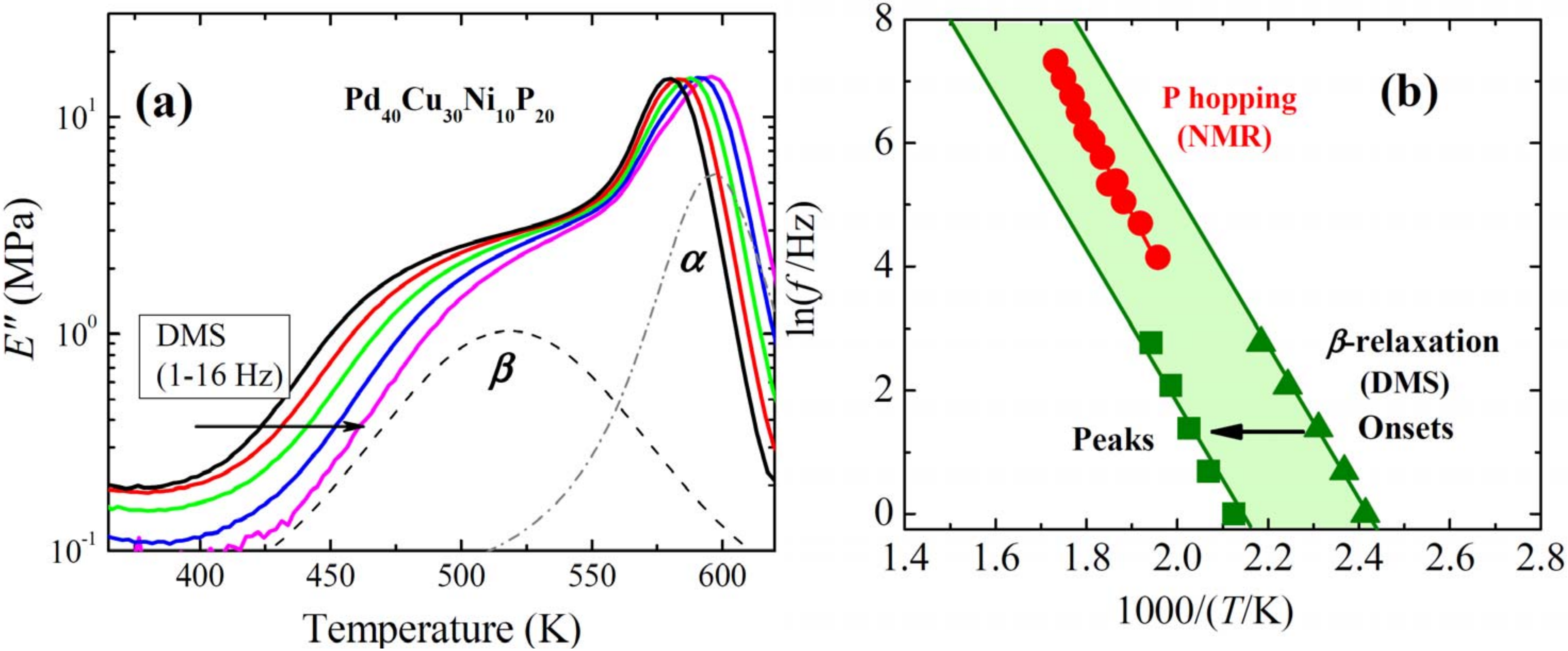
H. Schober1993 (from Miracle MRS Bull. 2007

String with Eshelby stress field (not correct scale)



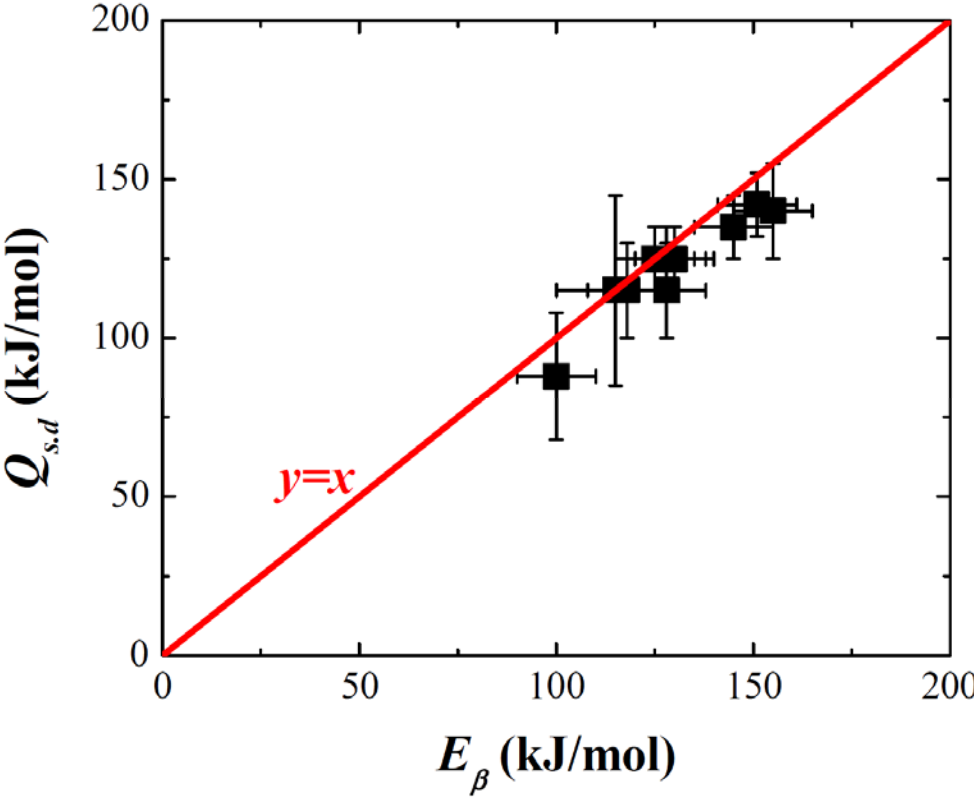
D.Bedorf, K.S. JNCS, 2010

Activation energy for beta relaxation and small atom diffusion

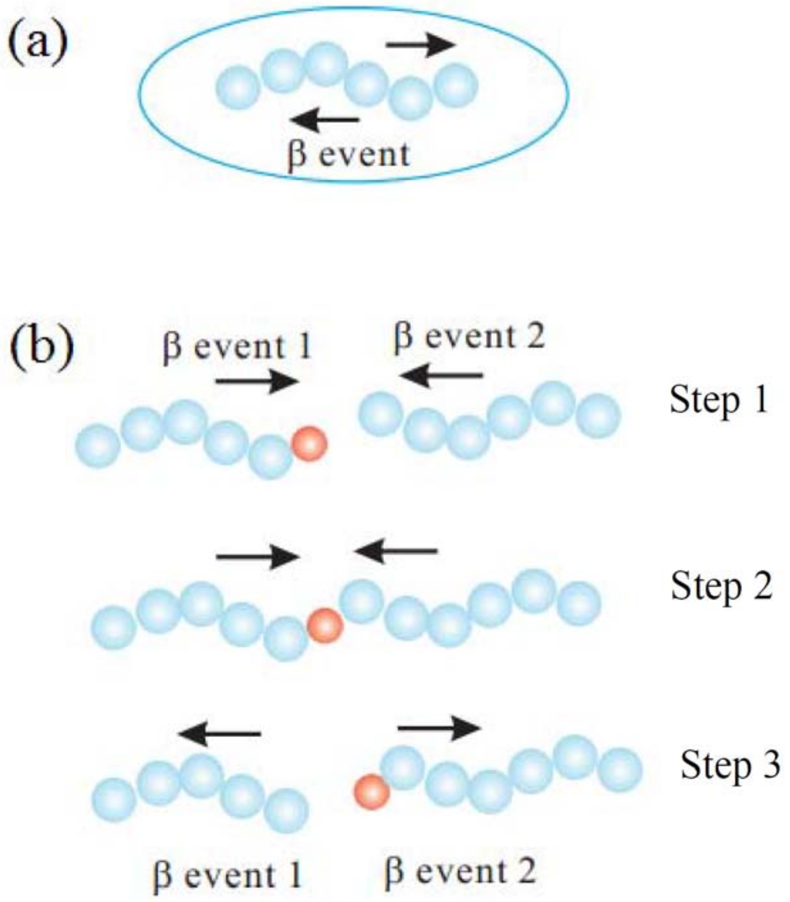


Hai Bin Yu et al. PRL 2012

Activation energy for beta relaxation and small atom diffusion



Sliding event for diffusion (here shown only in 1D)



H. B. Yu et al. PRL 2012

MD simulation(2-D) for beta relaxation without and with pinning centers

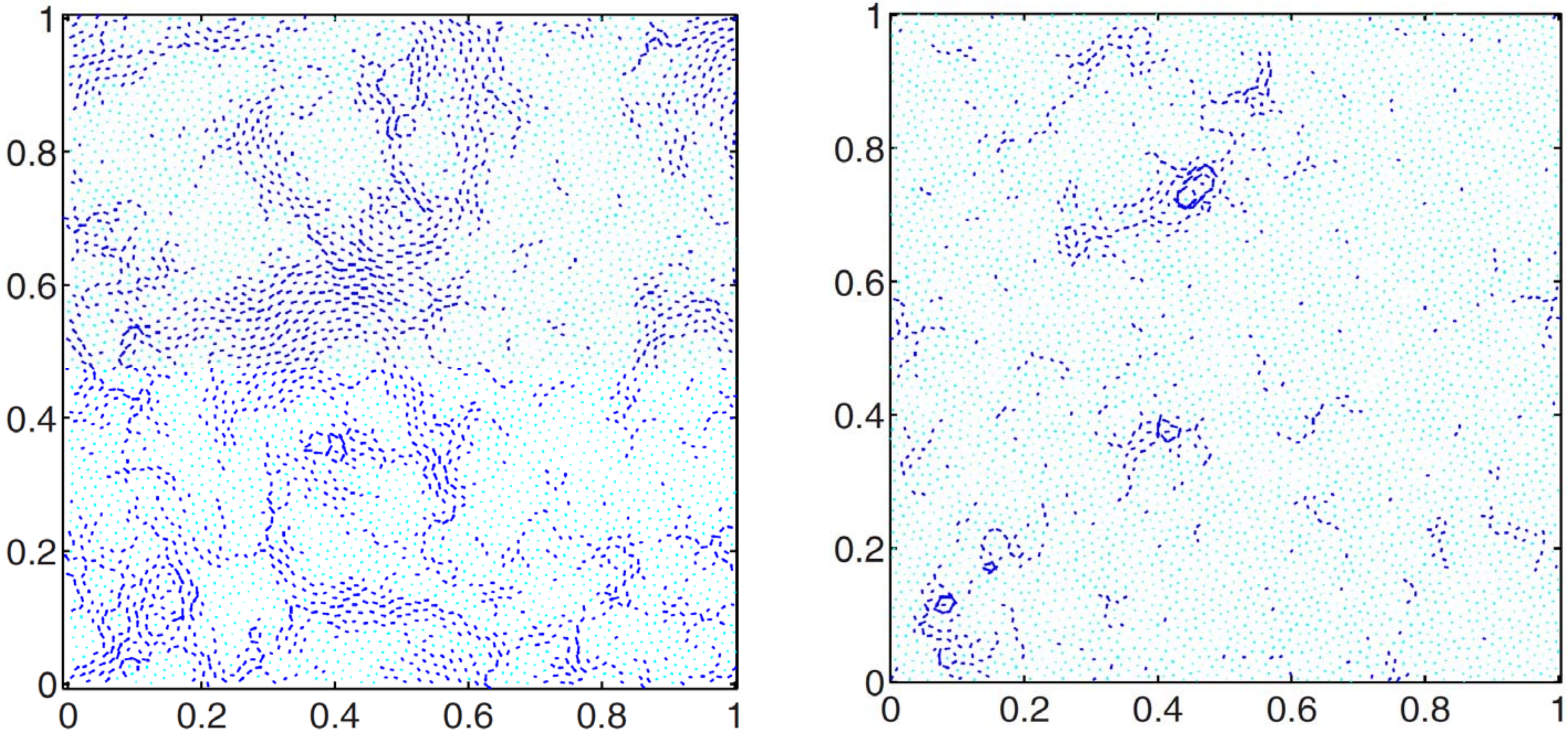
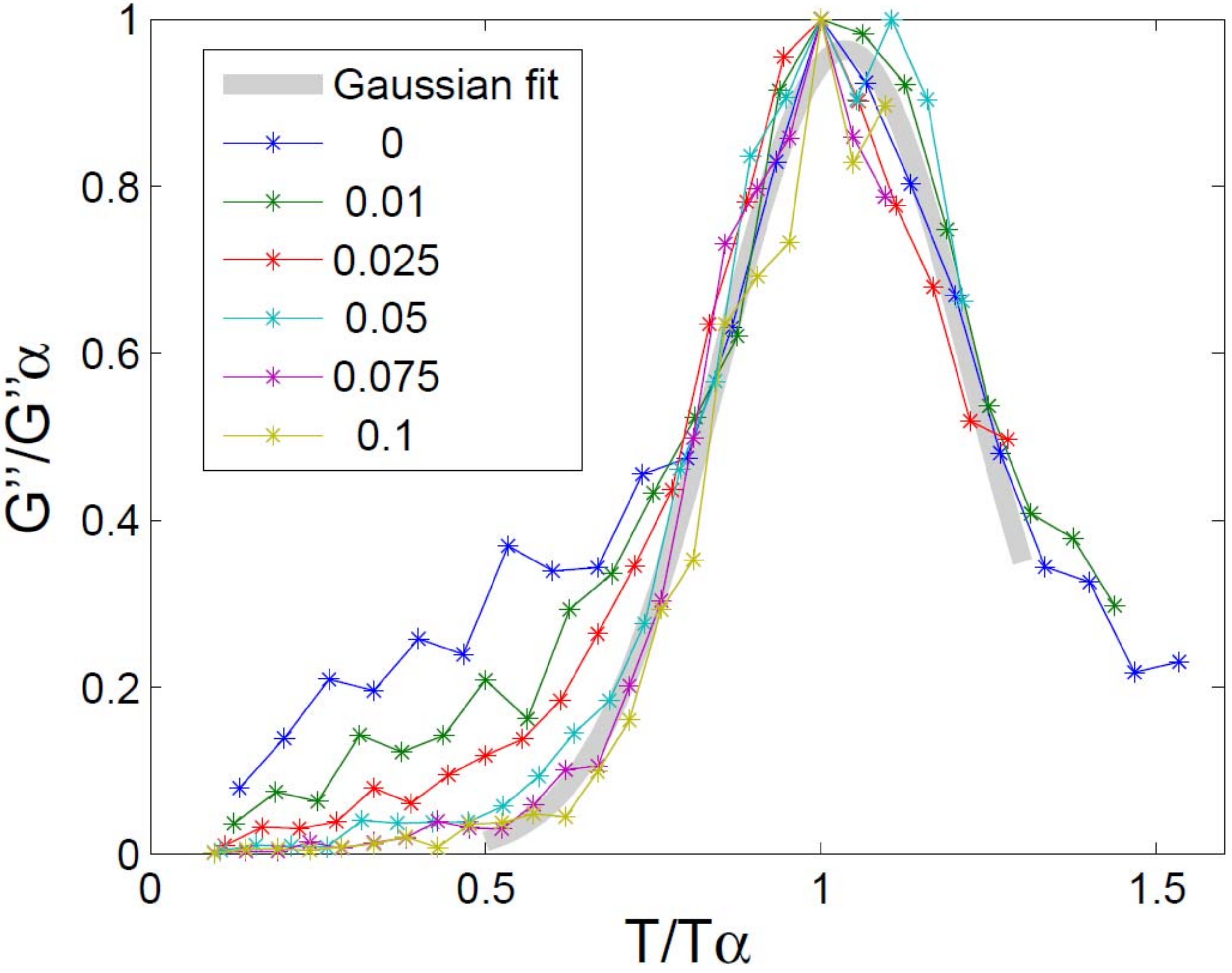


Fig. 5: (Color online) Left panel: a graphic representation of the cooperative motion that is associated with the β-wing. Note the chains of particles that have moved coherently during a time span of four time units. The particles that move more than 40% of the typical inter-particle distance are marked in dark blue. Right panel: similar graphic representation of the suppression of the majority of the cooperative motion that is responsible for the β-wing by the addition of 2.5% pinned particles. In contrast to the previous figure, here one needs to look at cumulated motions for 15 time units to see the remnant correlated motion.

Y.Cohen, I.Procaccia, K.S. et al. EPL 100 (2012) 36003

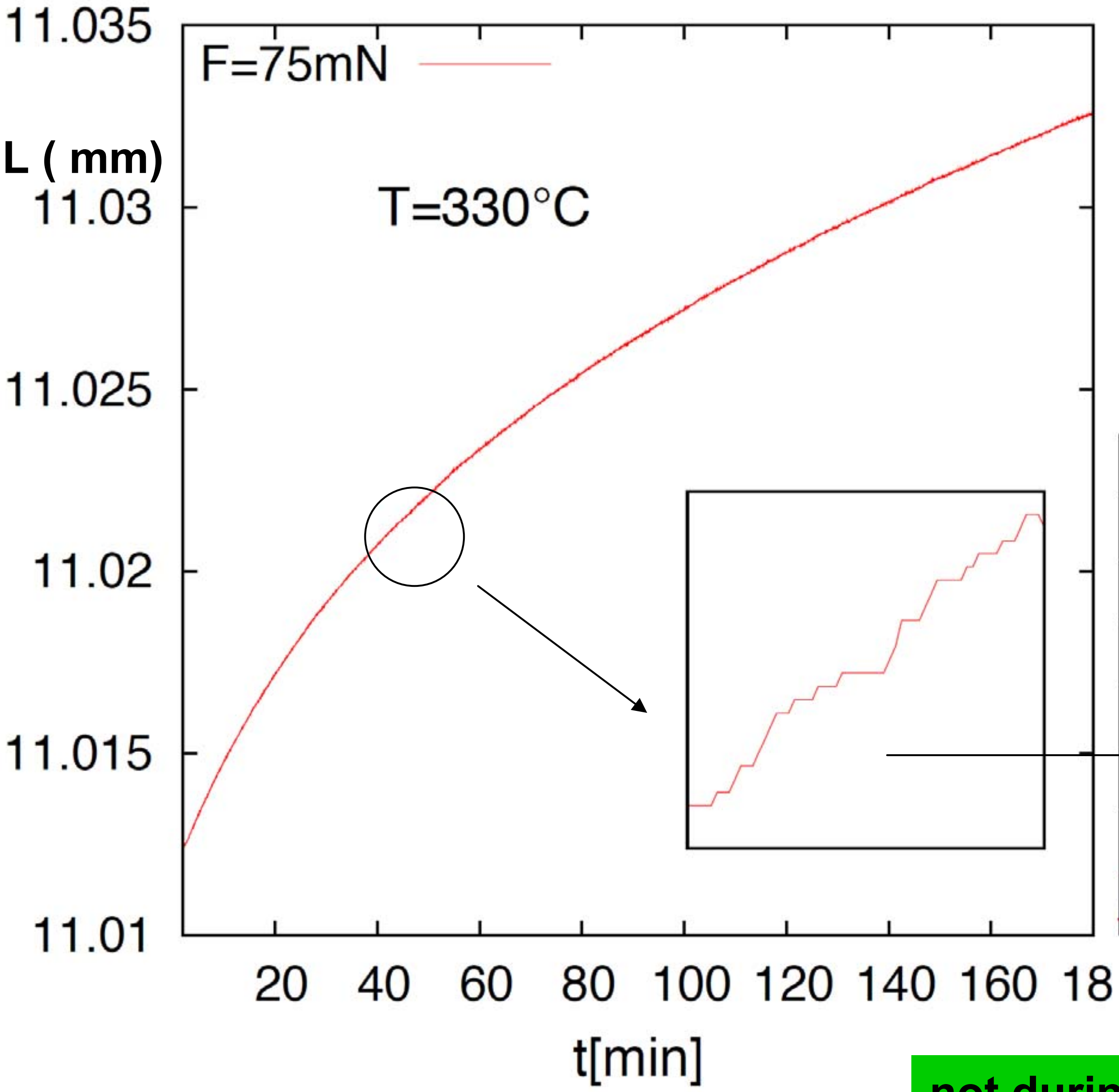
Suppression of beta relaxation (wing) due to pinning centers (5%)

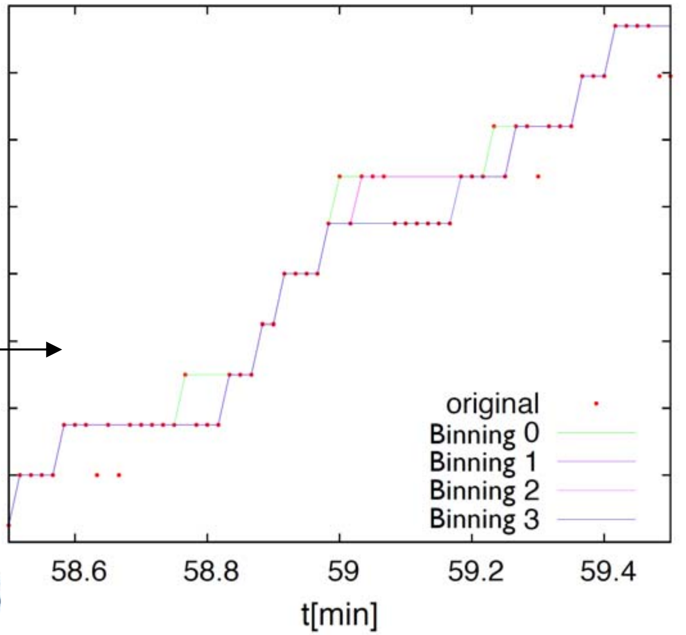


Y.Cohen, I.Procaccia, K.S. et al., EPL 100 (2012) 36003

Crackling or Barkhausen noise (minimal resolution 15 nm)

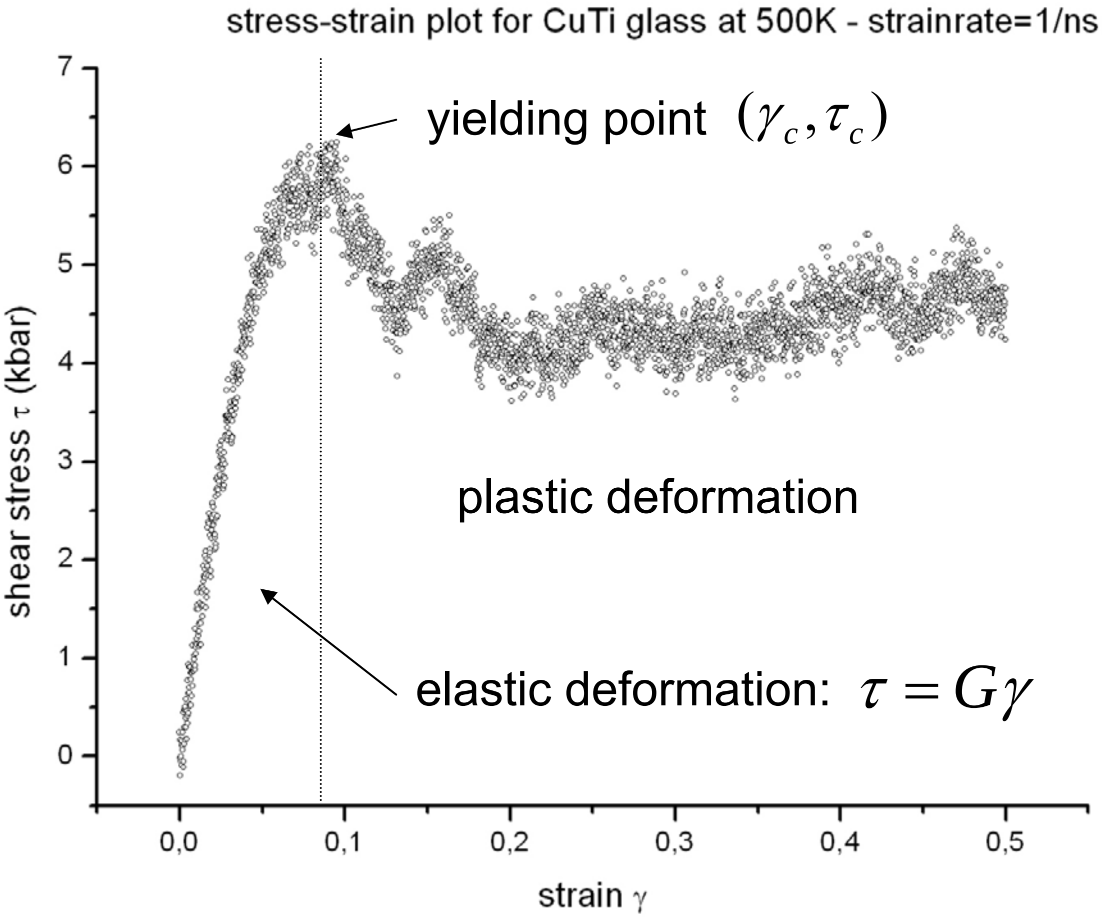
PdCuSi





not during recovery (like pop in‘s)

MD-simulation: Stress-strain behavior



yielding point (γ_c, τ_c)

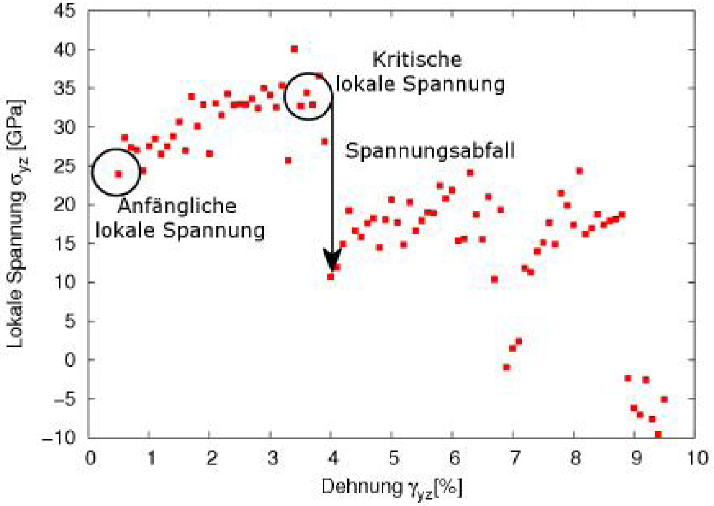
plastic deformation

elastic deformation: $\tau = G\gamma$

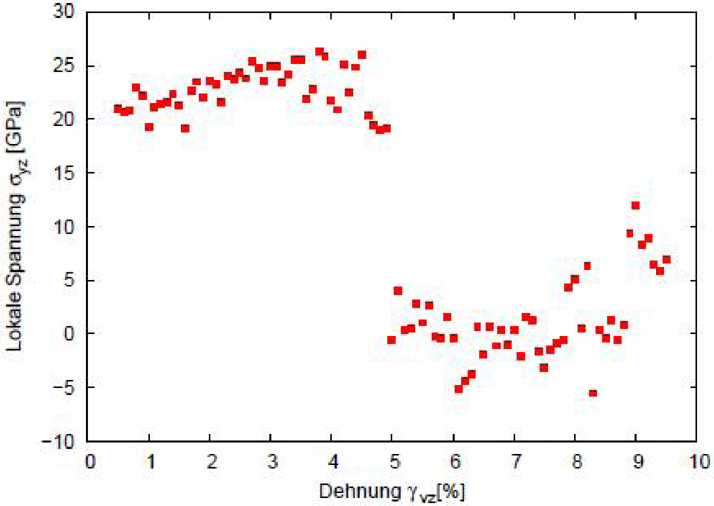
M. Zink, K. Samwer, W. L. Johnson, S. G. Mayr , Phys. Rev. B 74 (2006) 012201

MD-Simulation below critical yield strain- local STZ

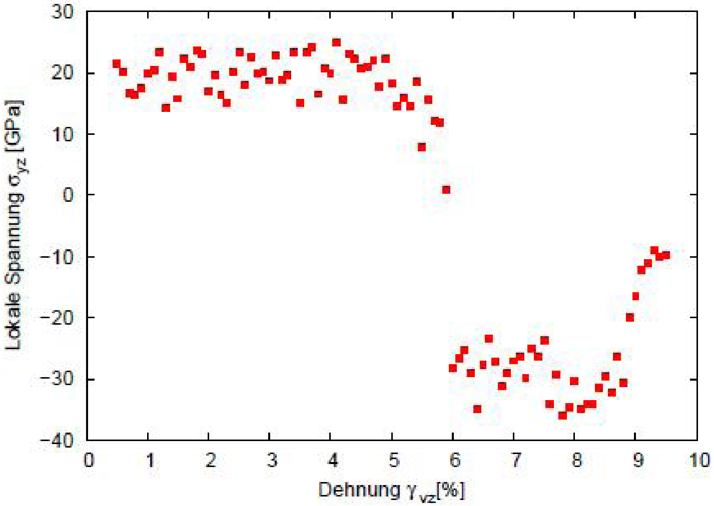
(M.Neudecker,S.G. Mayr, (Acta Mat. (2009))



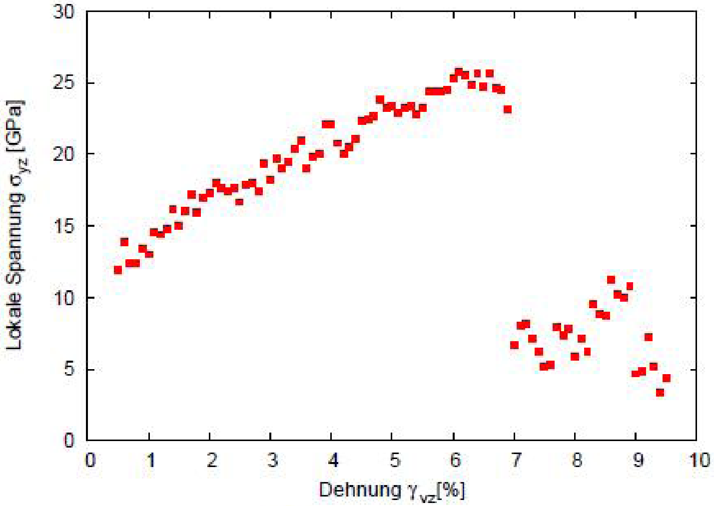
(a) $\gamma_i = 3.9\,\%$



(b) $\gamma_i = 4.9\,\%$



(c) $\gamma_i = 5.9\,\%$

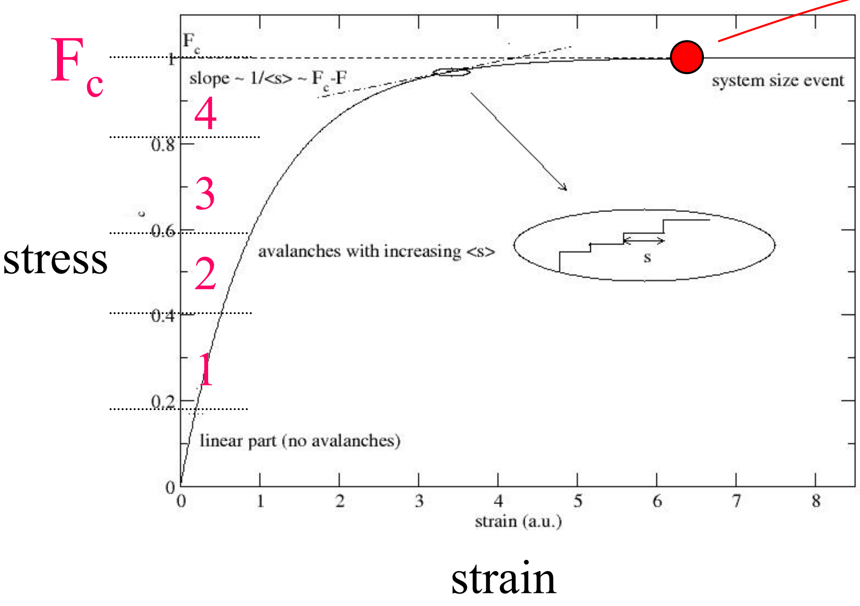


(d) $\gamma_i = 6.9\,\%$

Fixed stress boundary condition: Results for $\varepsilon=0$:

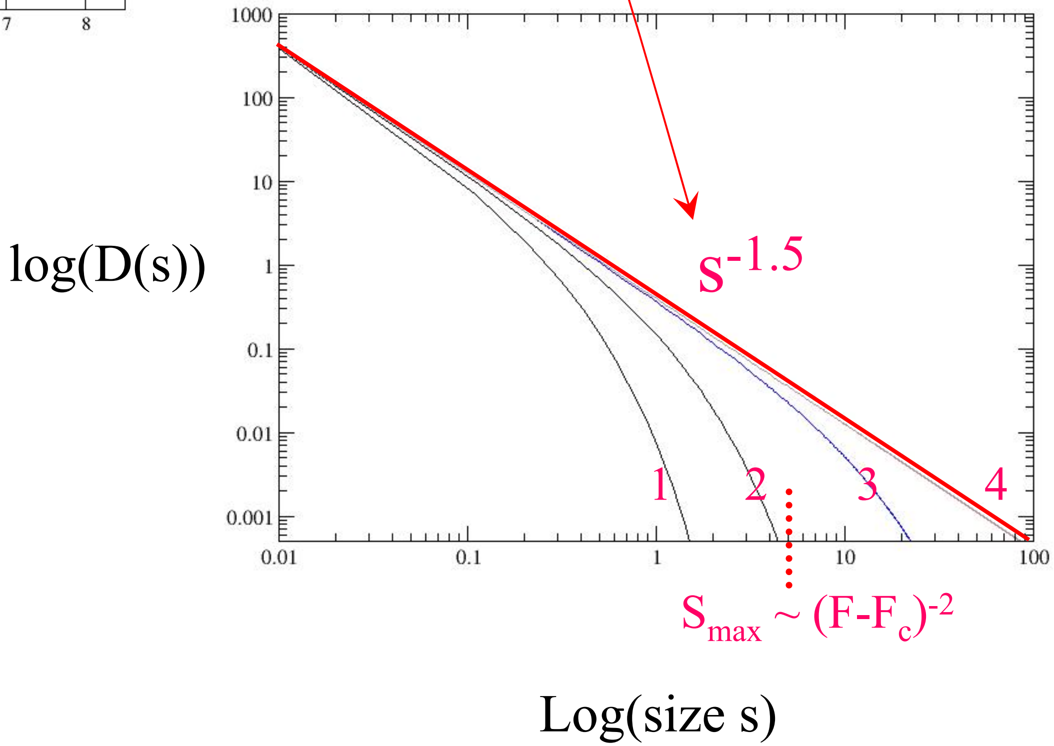
K.Dahmen,Nature 2010

Stress strain curve (ductile)

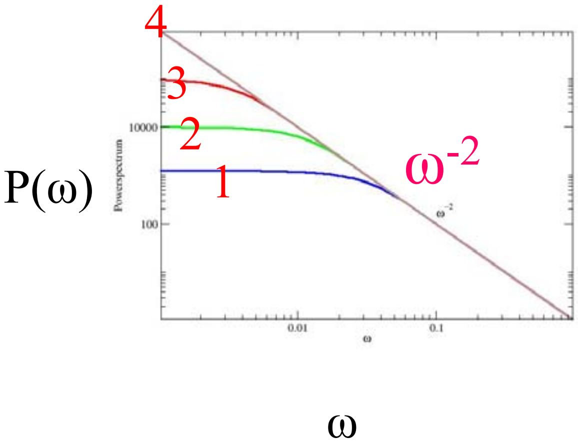


critical point

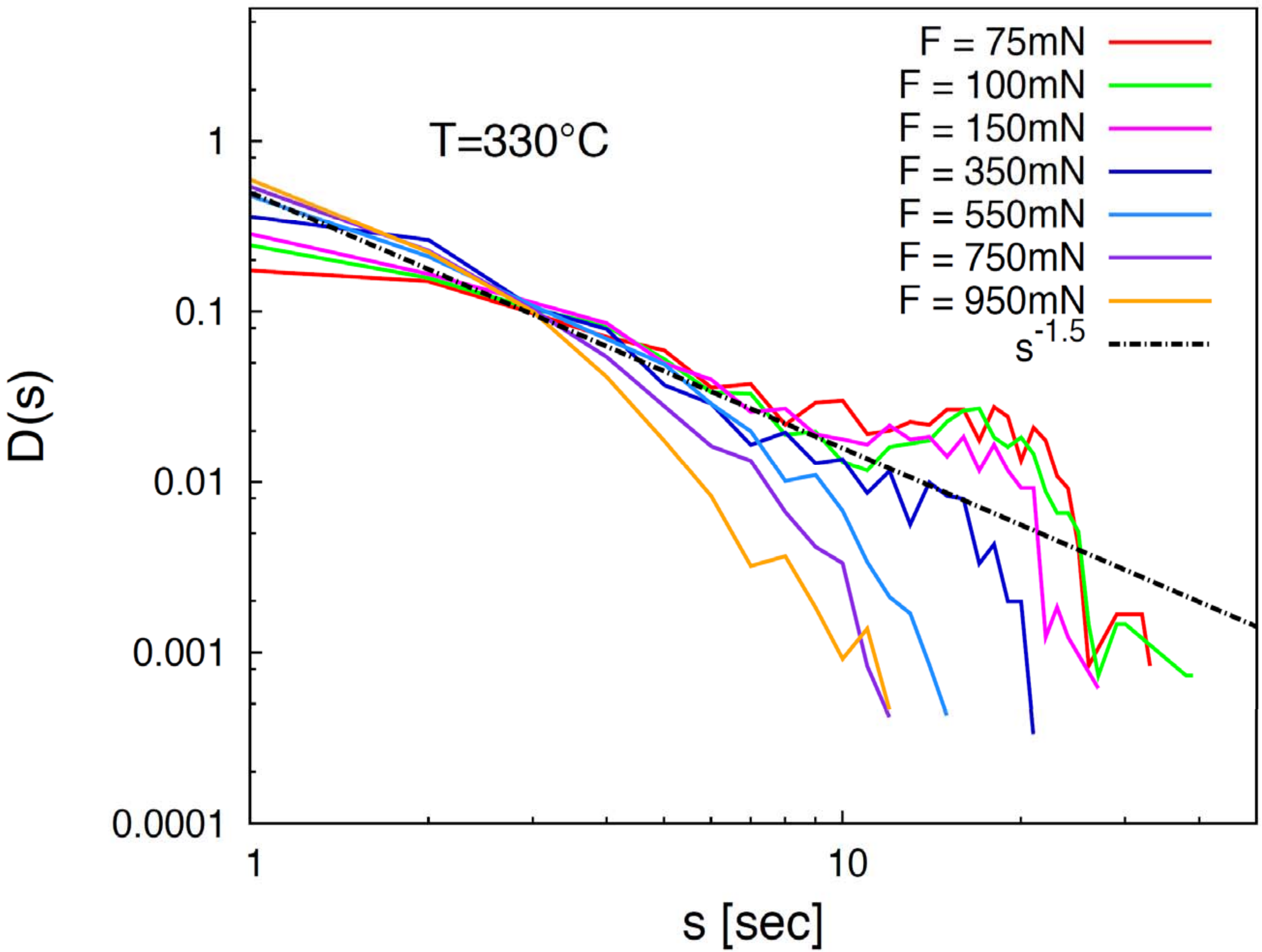
Avalanche size distribution:



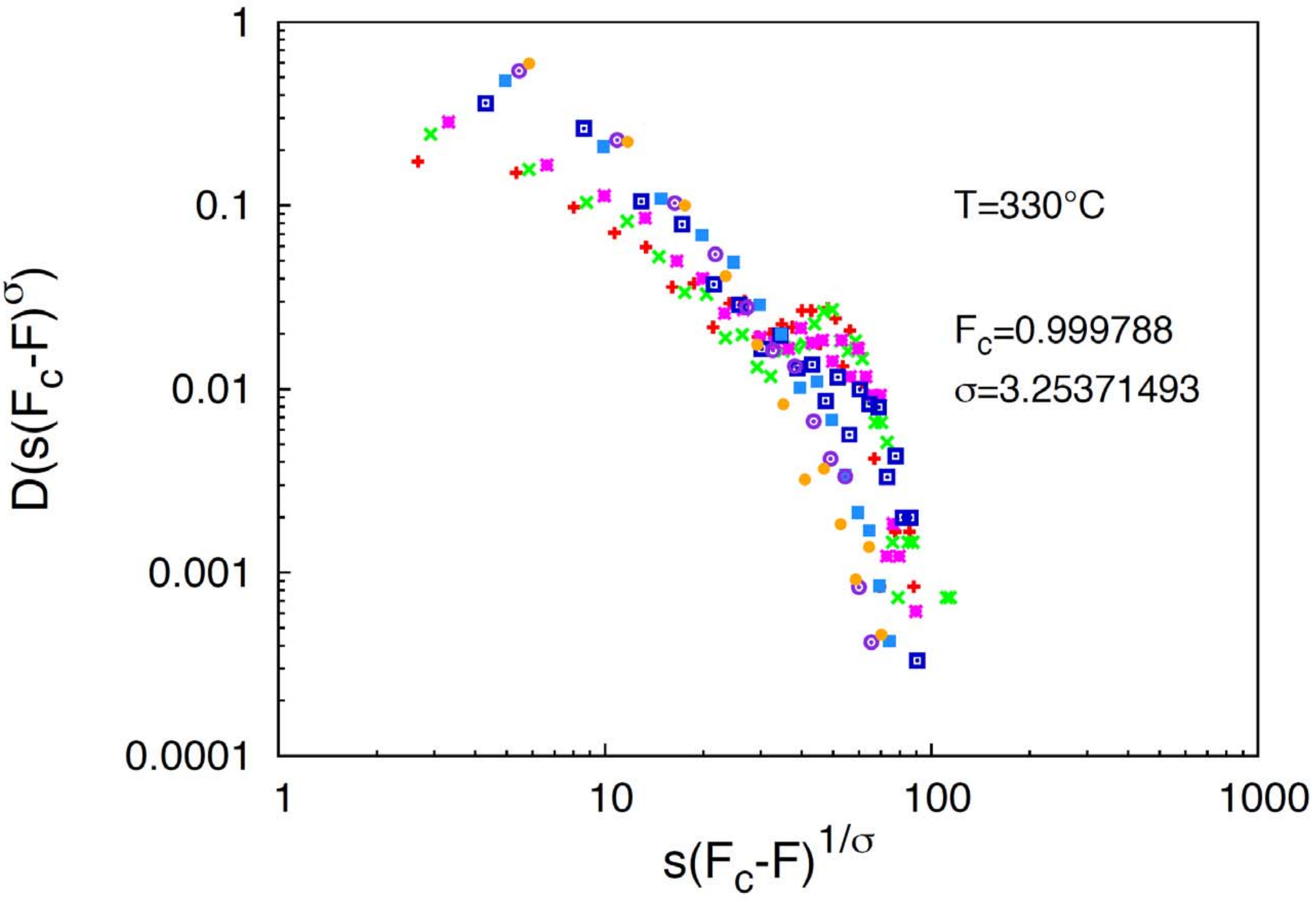
Power spectrum



Distribution of waiting time s for avalanches



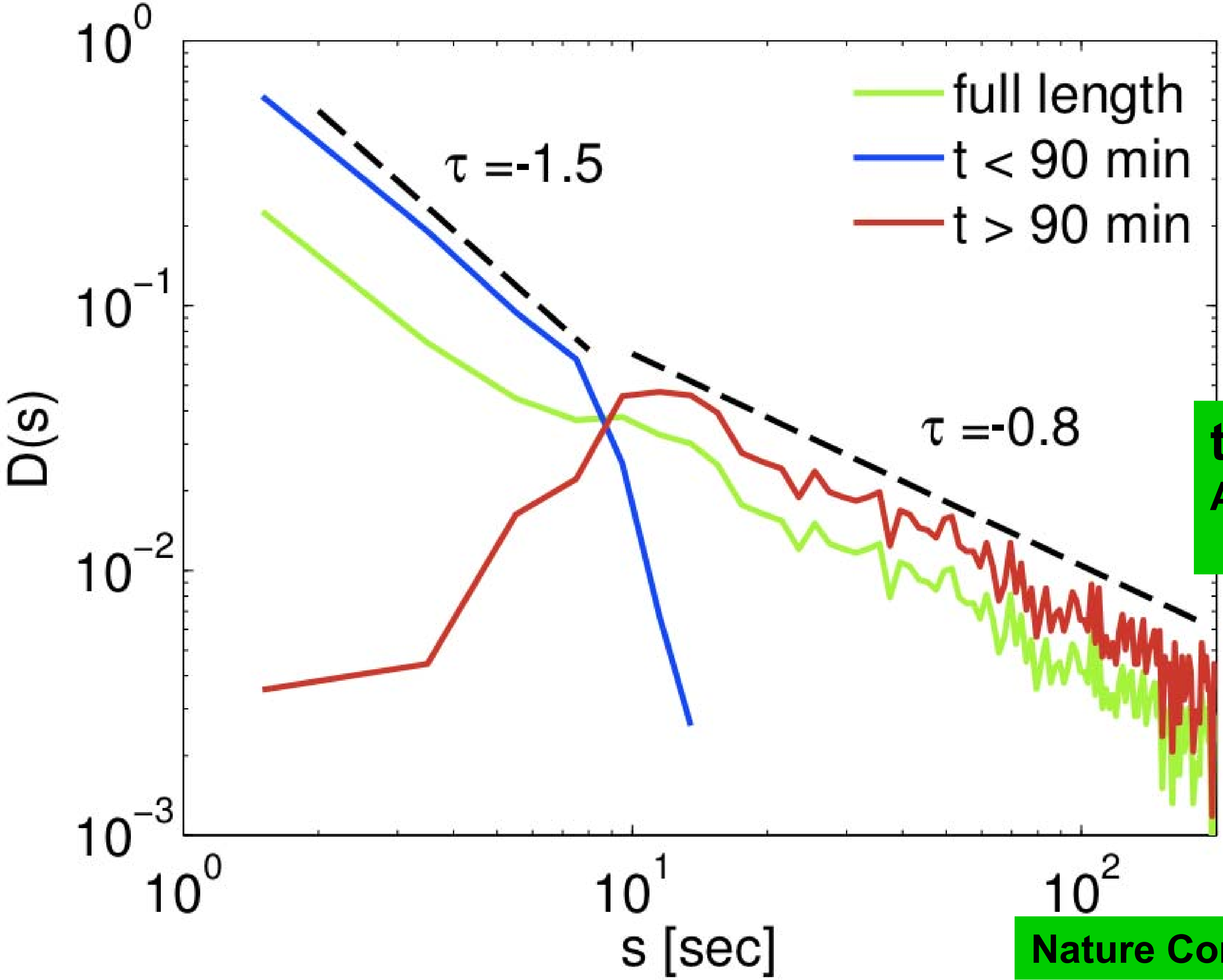
Scaling of waiting time distribution with applied stress at fixed temperature



$$D(s,F) \sim 1/s^{\tau} g[s \cdot (F_c - F)^{1/\sigma}],$$

with universal scaling exponents $\tau = 1.5$, $\sigma = 0.5$ and scaling function $g(x) \sim A\exp(-Bx)$,

Binning analysis for different time length s : single events versus coordinated avalanches?

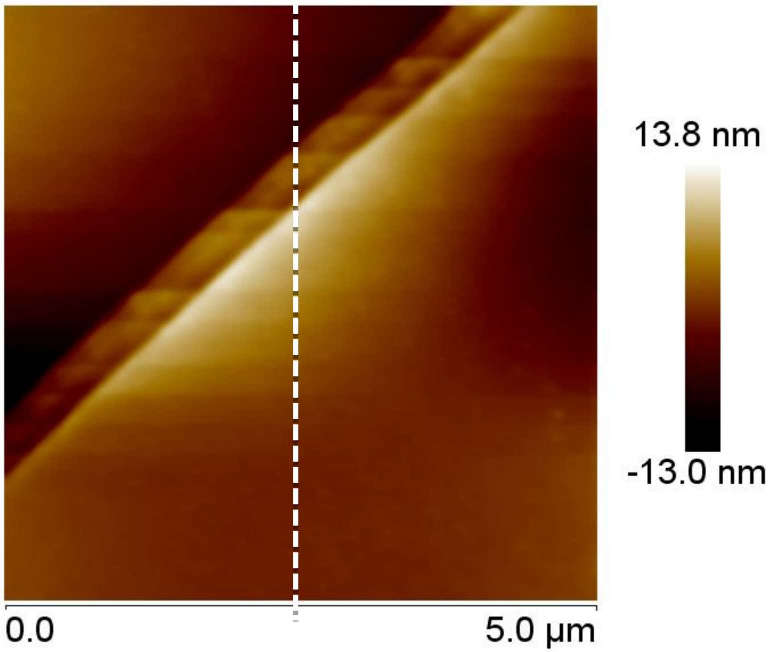


t ~ 0.8 from A.Lemaitre for plast. deformation

Nature Comm.5 (2014) 3616

Nano-shear bands

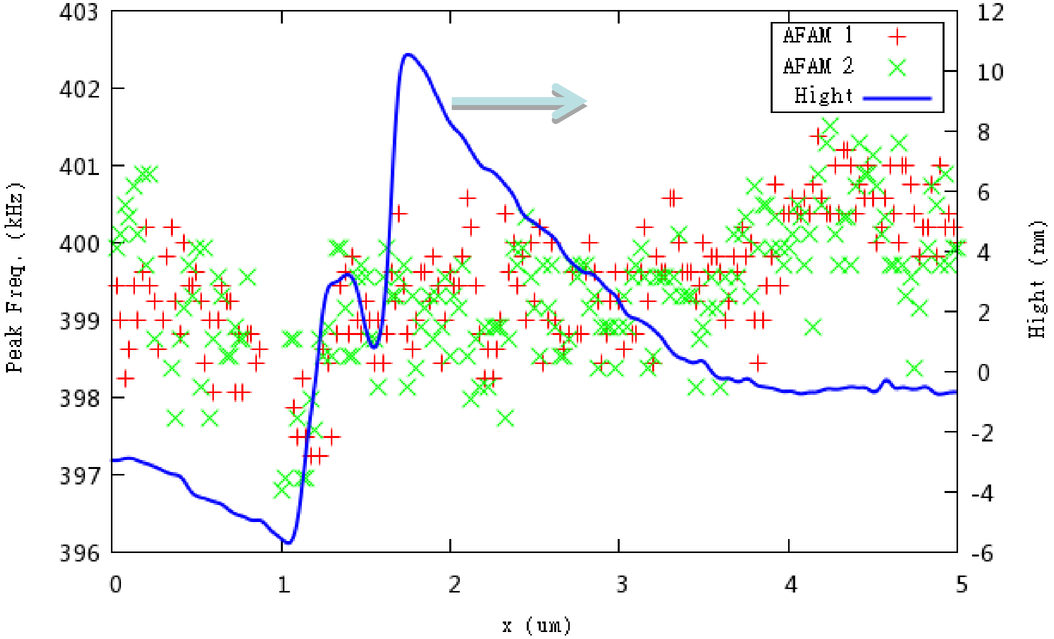
- Δl~ 15nm slip length of a 50µm thick sample under 45 degree assuming a STZ size of 3.5nm (1000 atoms) and critical strain of 2 % (~ 0.07nm):
- 20000 STZ x 0.07nm = 1.14 10^3 nm ~ 1µm offset of a macroscopic shear band
- 15nm offset about 1.5% ~ **300 STZ**
- Seen as offset in AFM and TEM work
- Upper limit –could be even smaller



Kc =0.85 N/m (determined from thermal tuning)

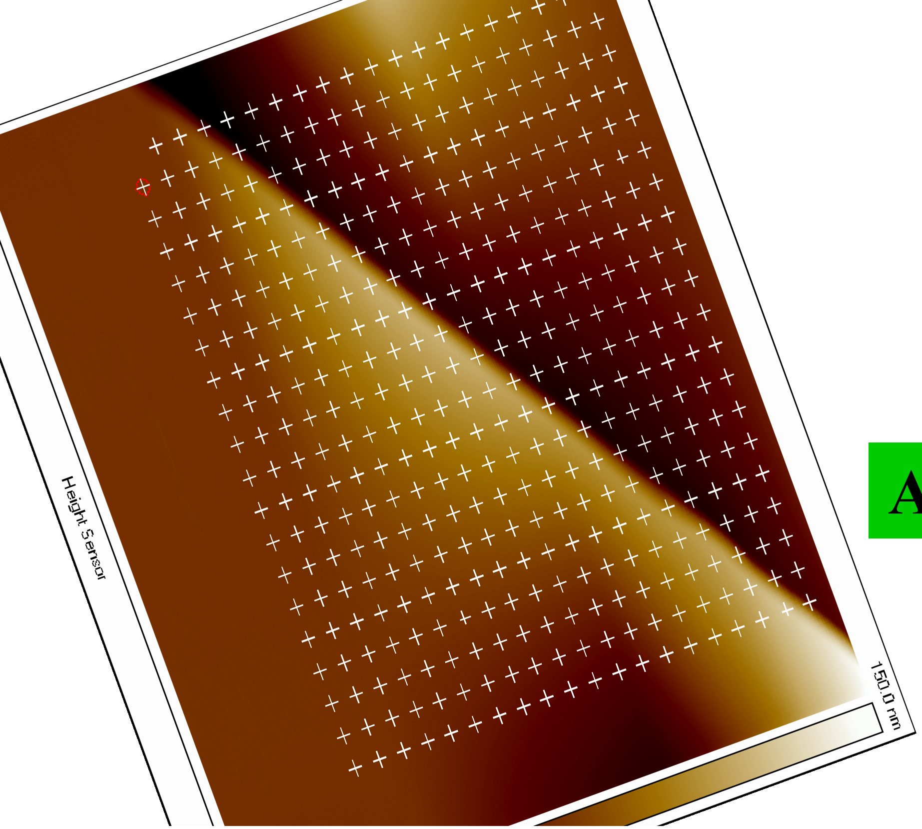
*Free resonance f*0 = 23.9 kHz

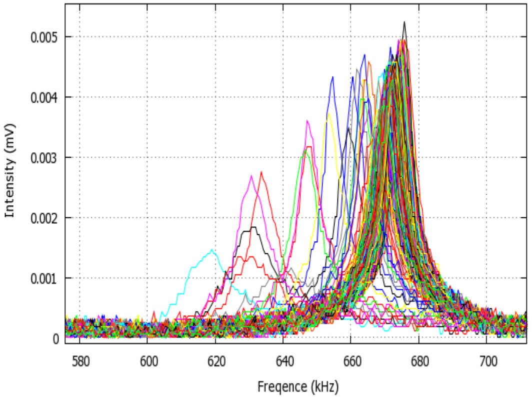
Static Force *F* = 17 nN



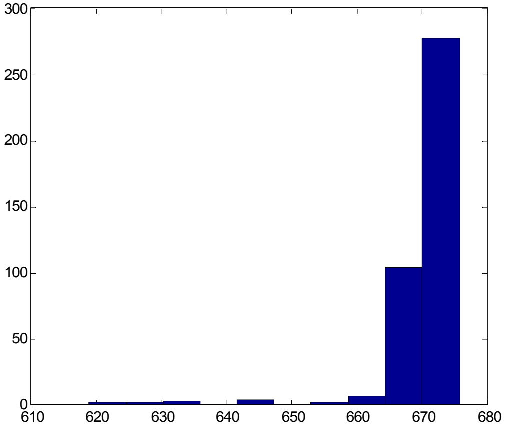
Shear offset = 16 nm

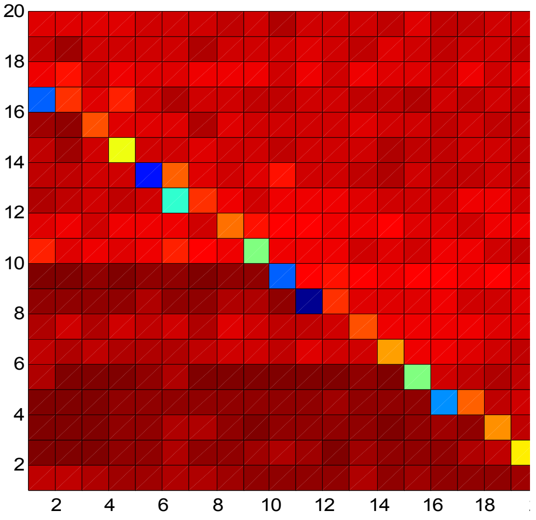
Hai Bin Yu, unpublished

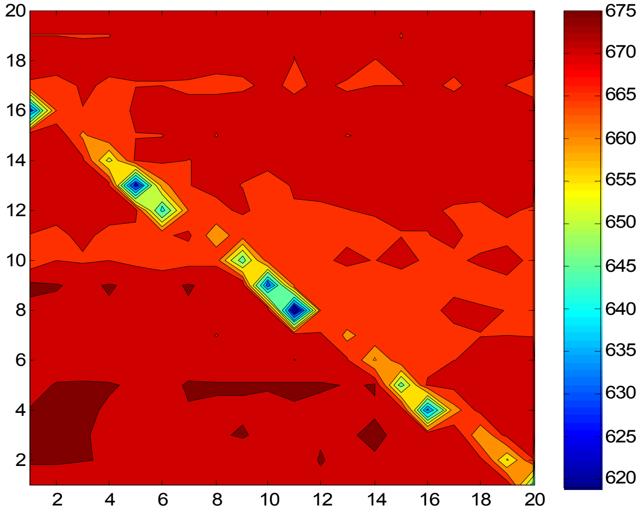




AFAM on shear bands







- The region near shear bands seems with low resonance frequency.
- However, the hight is large.

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A single shear band in a metallic glass: Local core and wide soft zone

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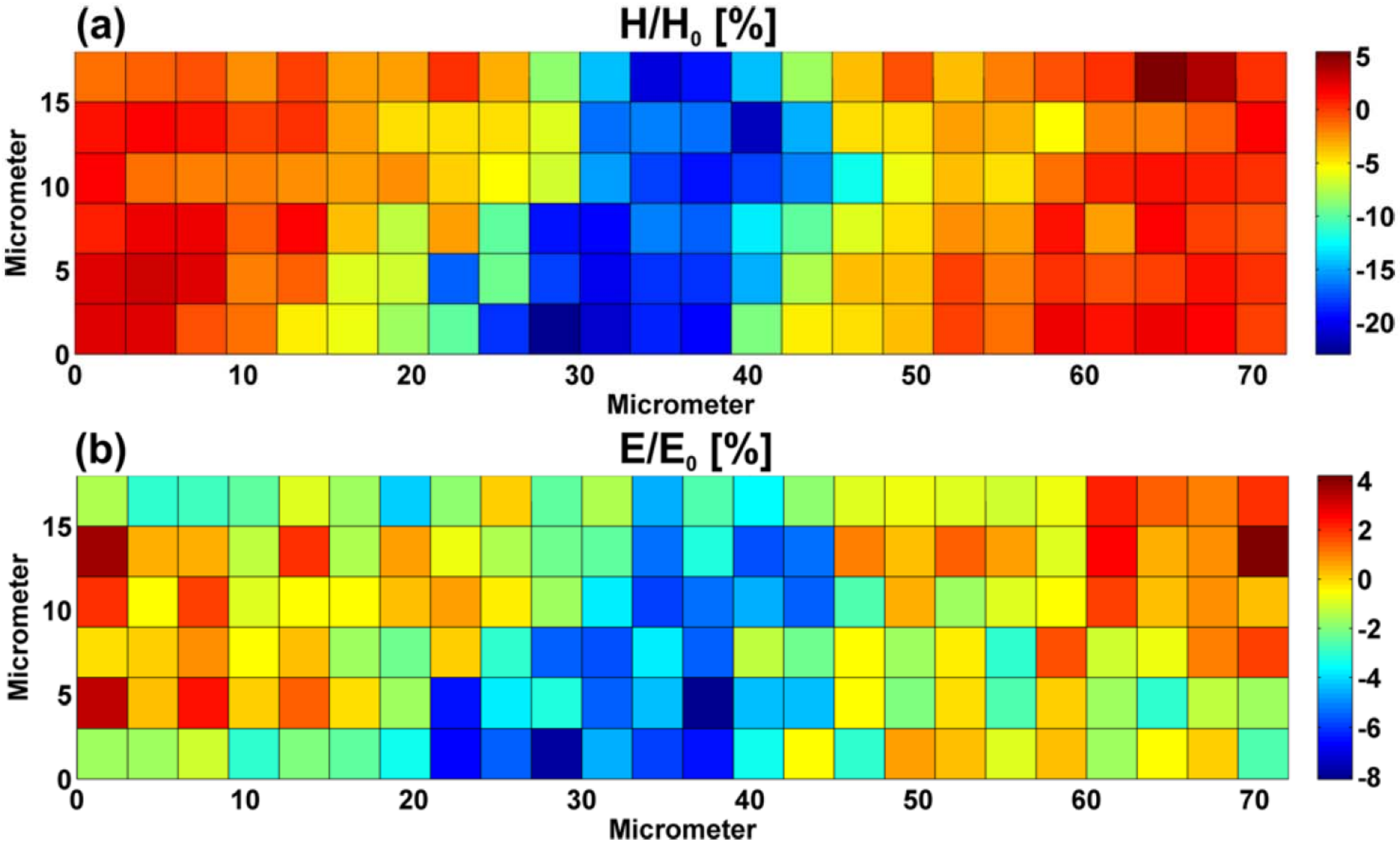
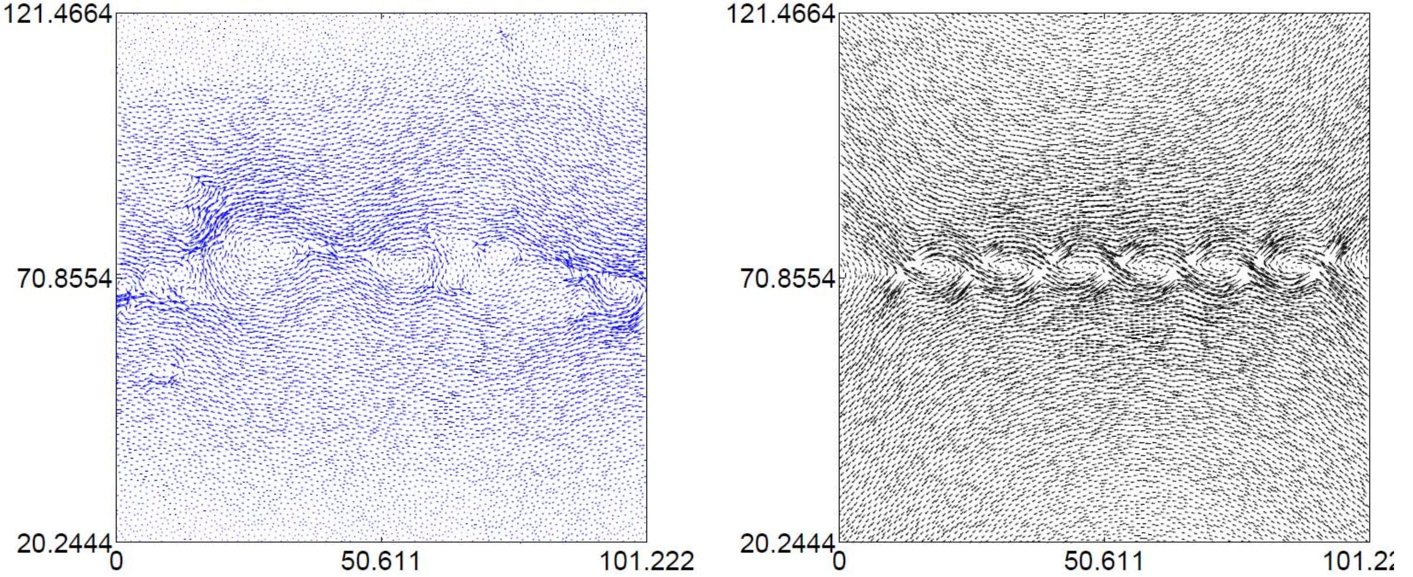


MD Simulation of STZ‘s (elastic quadrupoles) line up to form a nano SB



I.Procaccia et al. Phys.Rev E 2013

FIG. 4: (Color Online). Left panel: The nonaffine displacement field associated with a plastic instability that results in a shear band. Right panel: the displacement field associated with 7 Eshelby inclusions on a line with equal orientation. Note that in the left panel the quadrupoles are not precisely on a line as a result of the finite boundary conditions and the randomness. In the right panel the series of 7 Eshelby inclusions, each given by Eq. 8 and separated by a distance of 13.158, using the best fit parameters of Fig. 2, have been superimposed to generate the displacement field shown.

Summary

- beta relaxations are the fundamental excitations in a disordered system
- In BMG they form strings (**0.4 nm^3 ~ 20-30 atoms: factor 20 less than STZ size**)
- beta relaxations line up for diffusion of the small atoms far below the glass transition
- **above 2.5% pinning center** the beta relaxations are stopped
- Crackling noise analysis show powerlaw statistics common for small avalanches
- avalanches or nano shear bands form out of **300 STZ (1-D)**

For a review on beta relaxations see: HB Yu, WH Wang and K.S. Materials Today 2013