Relating activation of shear transformation zones to β-relaxations in metallic glasses

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Outline

I. Issues

II. Beta-relaxation in MGs

III. Activation energy of STZs in MGs

IV. Relation of β-relaxation & STZs

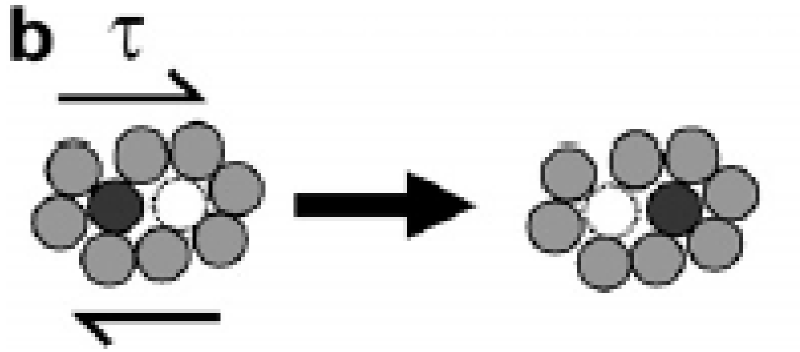
V. Summary

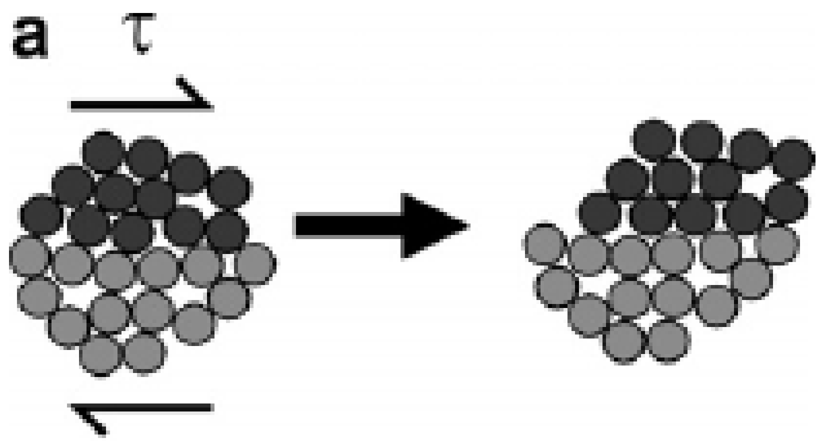
I. Issues

Issue 1. Plastic deformation mechanism of metallic glasses far below T_g

Free volume model **STZ model**

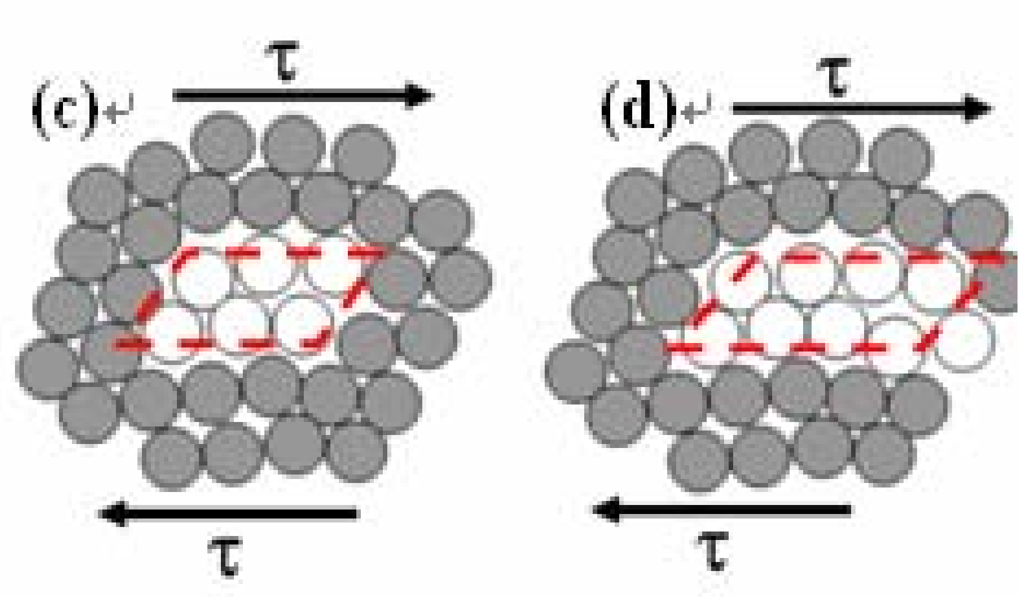
$$\eta = \eta_0 \exp[C(T)/k_B T]$$



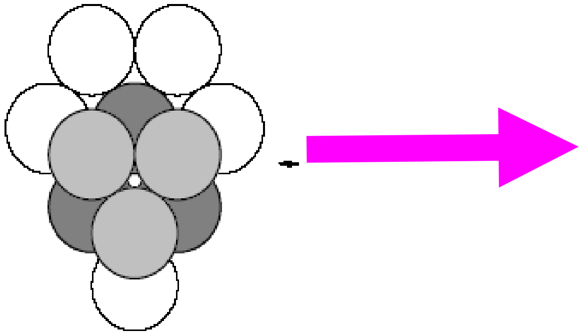


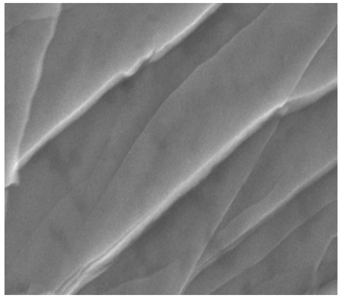
STZ model

The isolated STZ is elastically confined by elastic matrix



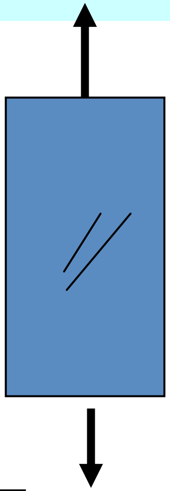
The self-assemble of STZs form shear bands



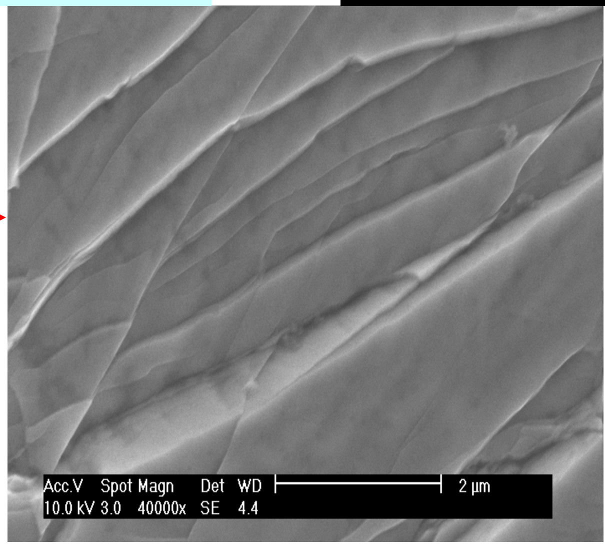


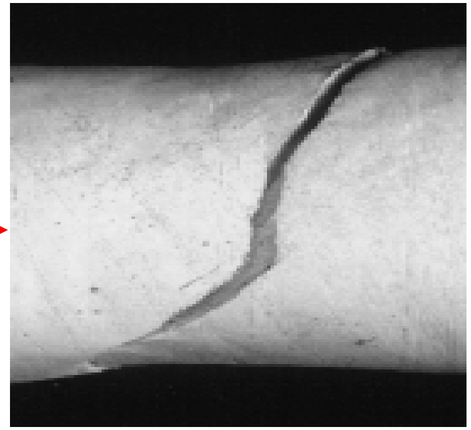
To understand STZs is important for overcoming brittleness and for understanding plastic deformation

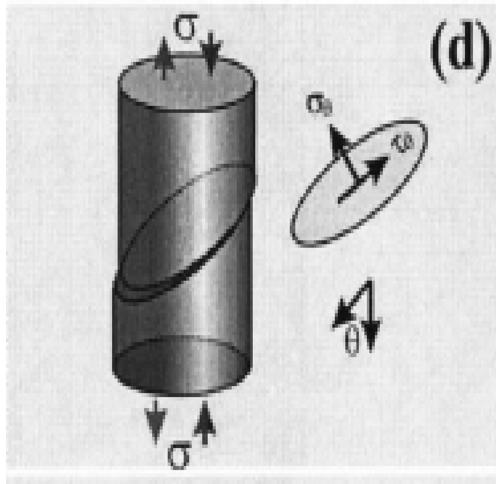
Inhomogeneous deformation → **Shear band** → **Brittleness**



Force



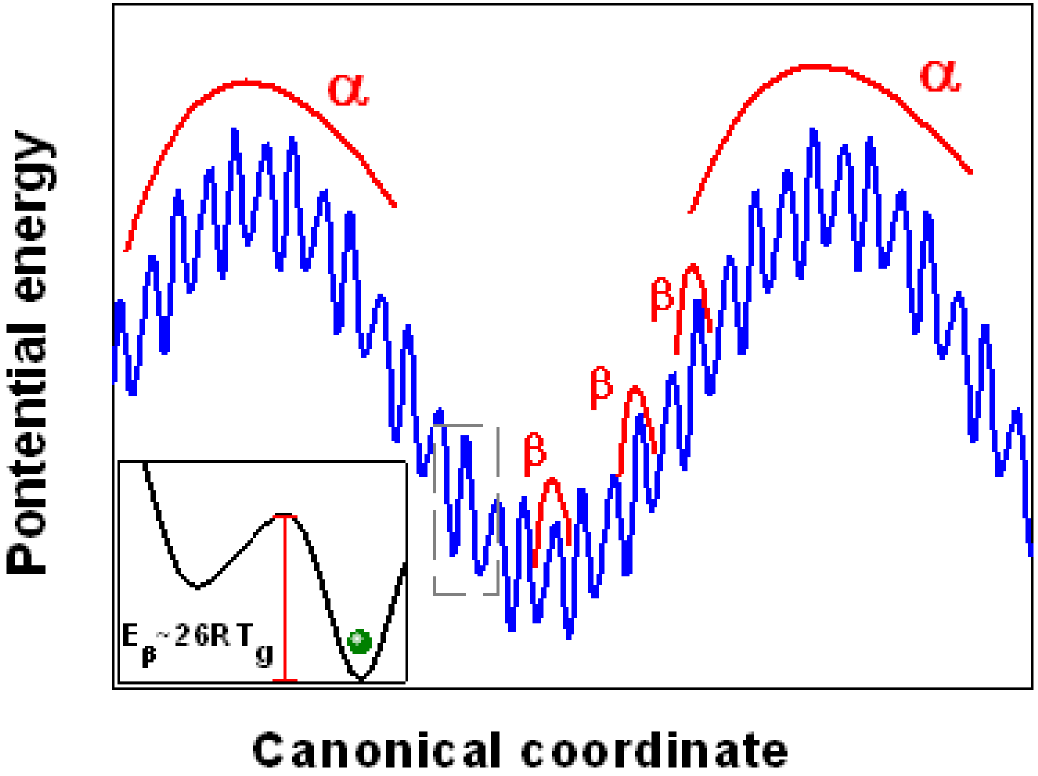




Brittleness is big problem for applications of MGs

Johnson & Samwer's CS Model PRL 2005

Based on assumption of β-relaxation relates with STZ



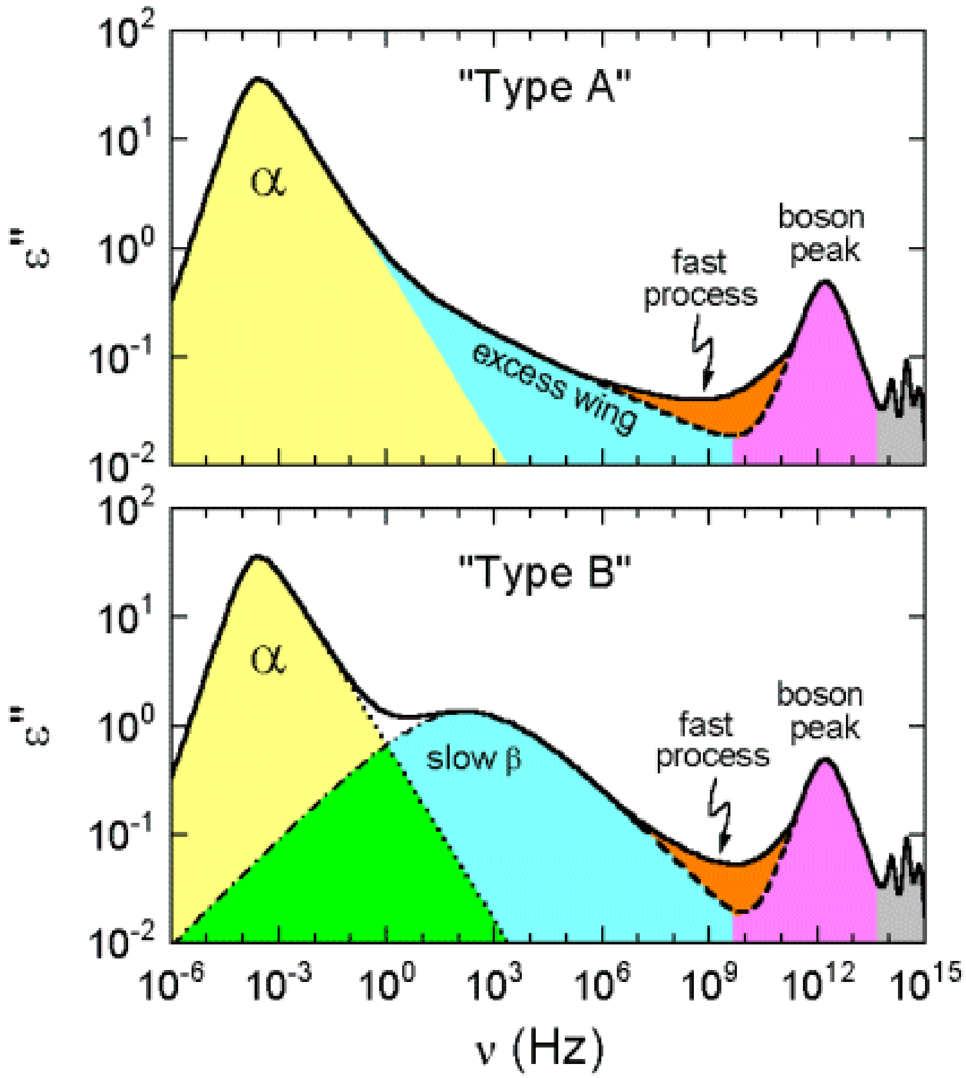
$$W = (8/\pi^2) G \gamma_c^2 \zeta \Omega,$$

Need experimental evidence for the assumption

Issues 2: β-relaxation

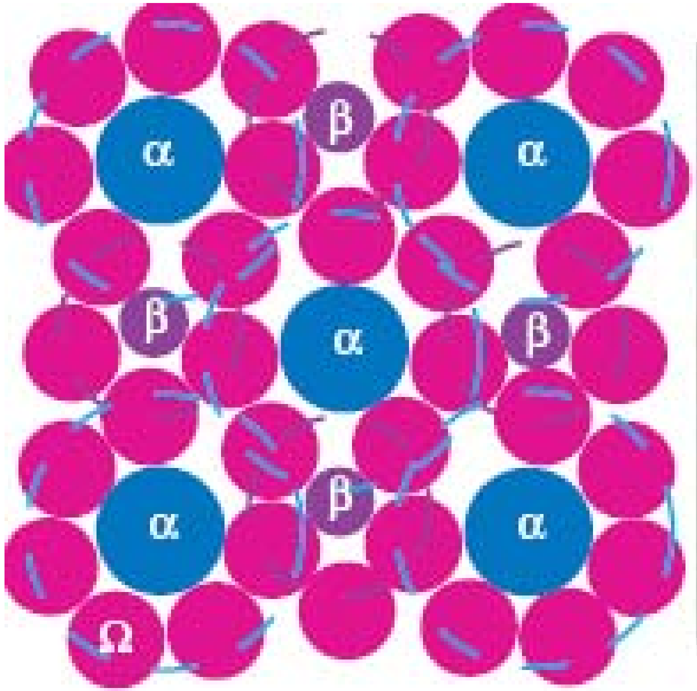
- ◆ Microstructural origin of the slow β-relaxation?
- ◆ The universality of β-relaxation in all glasses?

Organic glass-- slow β relaxation--motion of groups of atoms--J.Chem.Phys. 53, 2372, (1970)



Lunkenheimer diagram

Metallic supercooled liquids and glasses



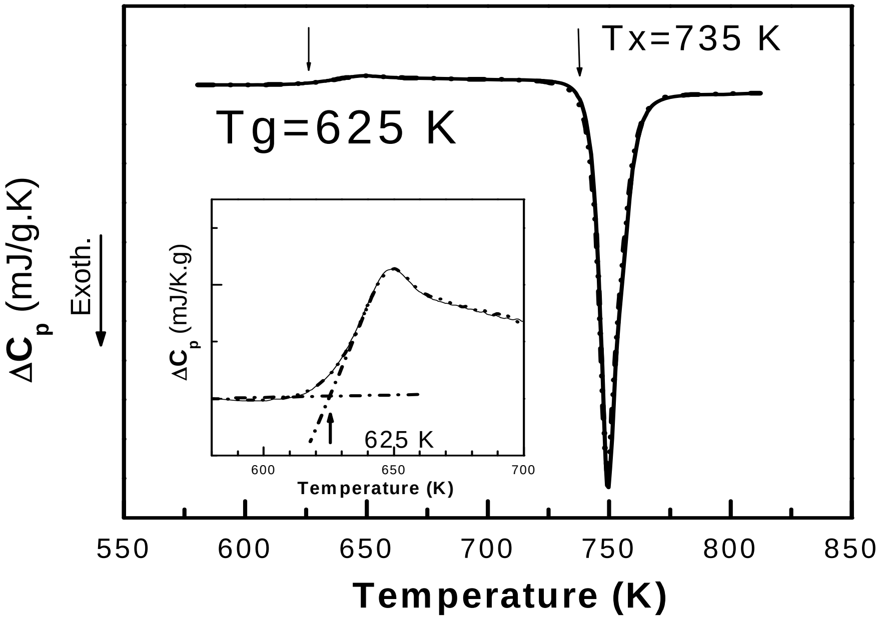
Miracle model

close to highly random packed atomic spheres

No complicated mobility forms occurring in non-metallic glasses such as intramolecular effect

MG is model system to clarify the structural origin

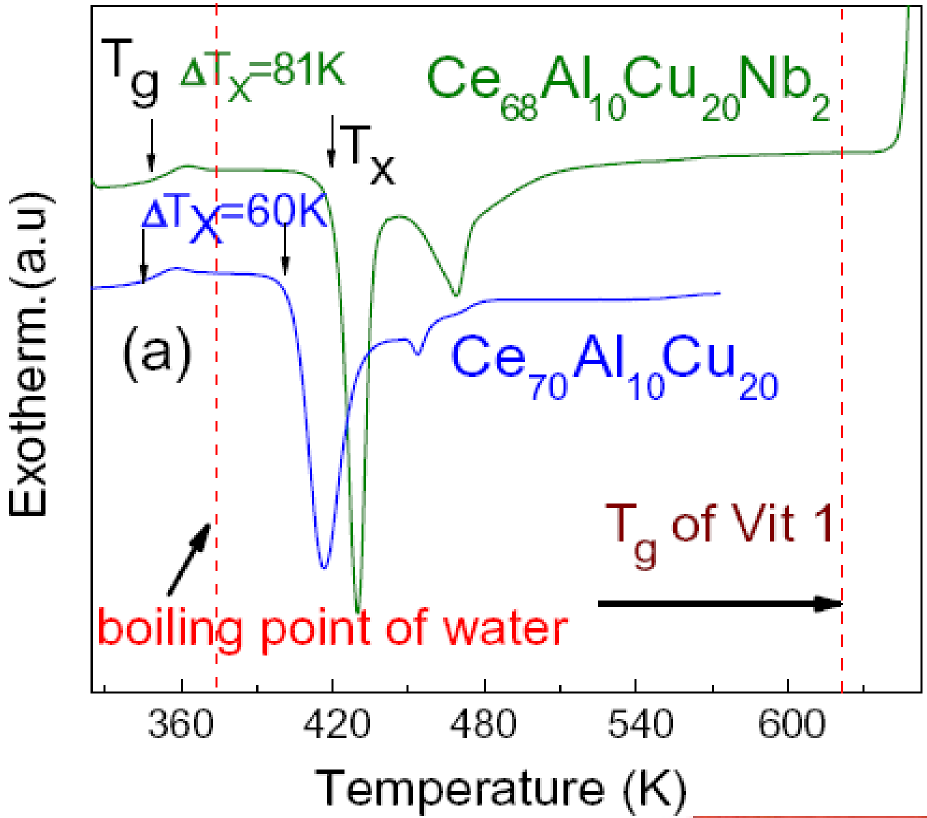
$Zr_{46.75}Ti_{8.25}Cu_{7.5}Ni_{10}Be_{27.5}$ (Vit4)

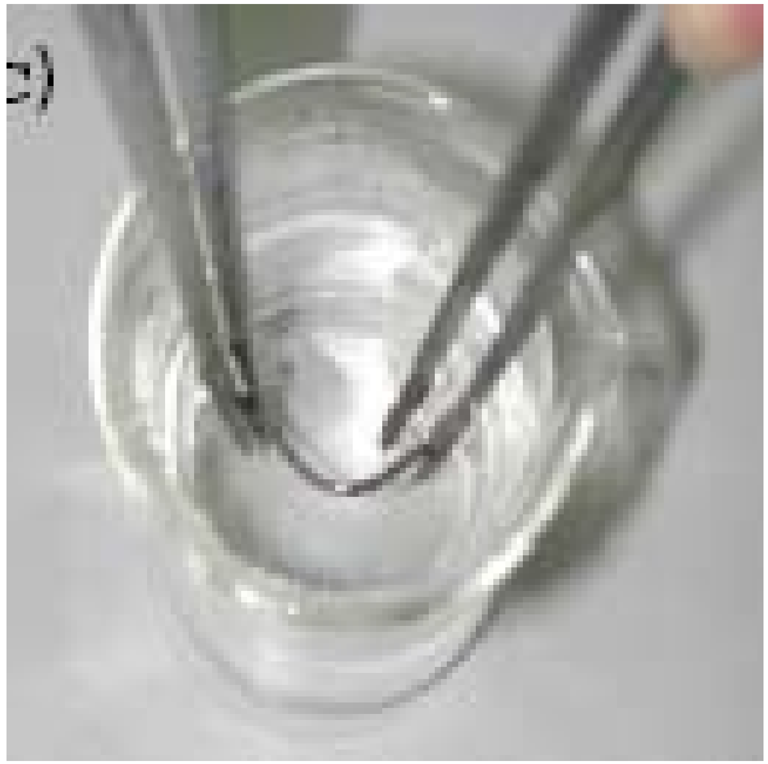


Bulk specimens allow effective physical properties measurements and stable supercooled liquid state

- **ΔT=110 K**
- **No phases separation**
- **High GFA**

β-relaxation is easier to be activated for low Tg MGs



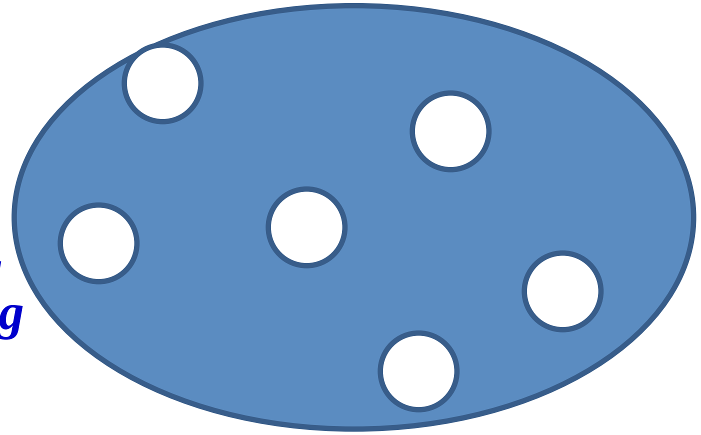


PRL 94, 205502(2005)

Issue 3: Relation between glass transition & plastic deformation in MGs

MG is homogeneous or inhomogeneous?

Topologically unstable even below T_g at certain sites: Liquid-like sites (Egami model)



Swiss cheese

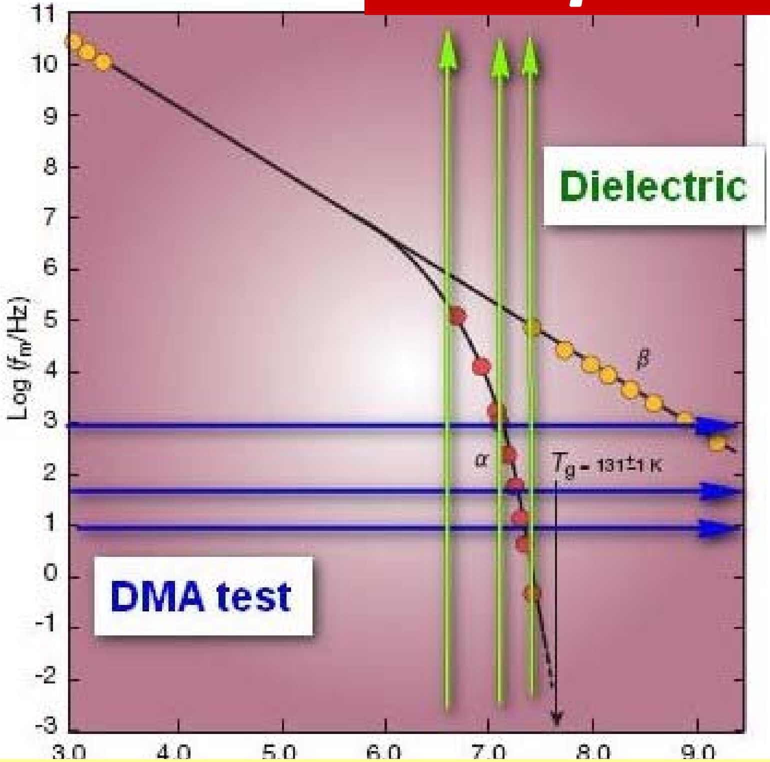
Glass transition occurs by percolation of liquid-like sites [Cohen & Grest, *PRB* 20, 1077 (1979)

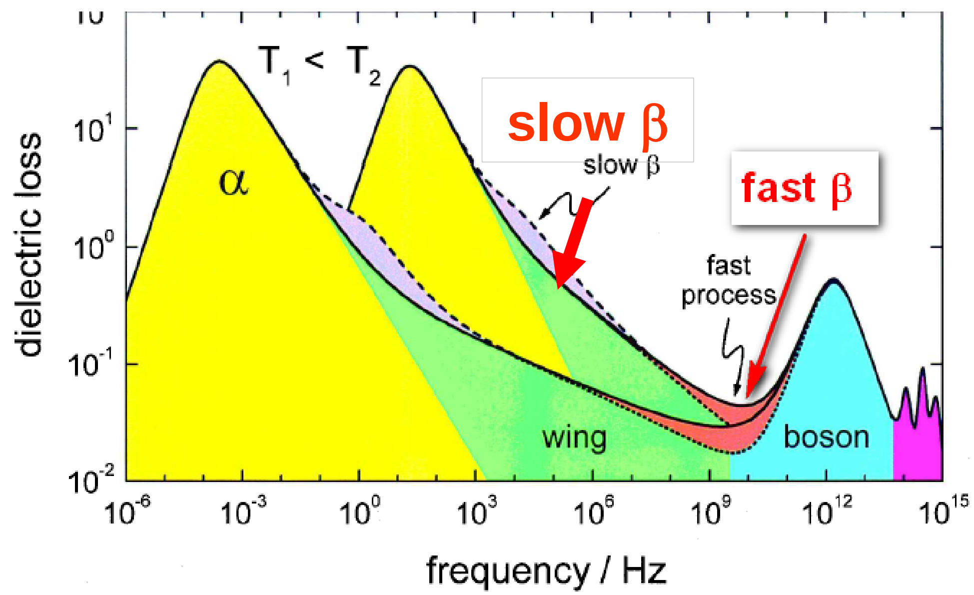
Liquid sites also initiates STZ

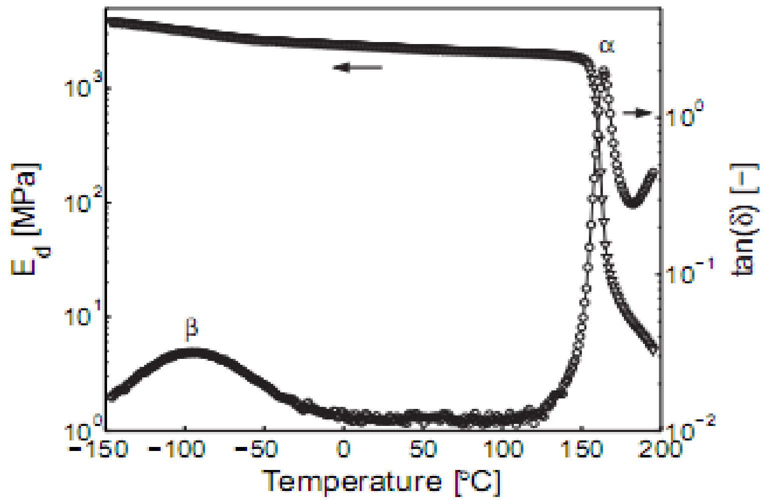
Need more experi. Evidence!

Glass transition & plastic deformation are equivalent?

II. β-relaxation in MGs





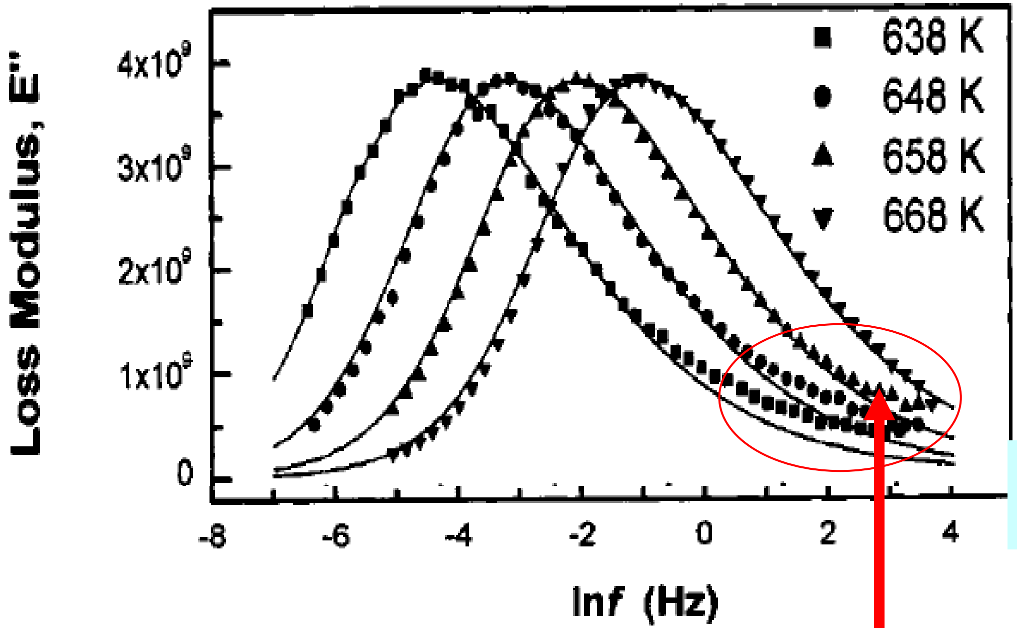


Dynamic mechanical analysis (DMA)

frequency *f* : 10^{-2} -- 1000 Hz

Complex elastic modulus, *G* = *G* ′ + *iG* ″

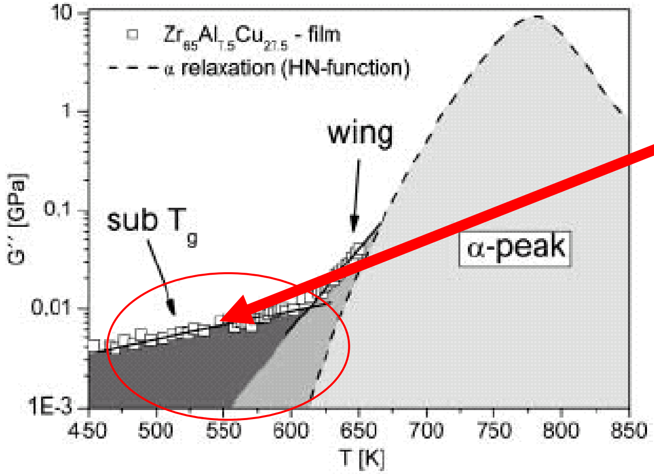
Appl. Phys Lett., 84, 2790(2004)



***f*-dependence of G` and G`` of vit4 supercooled liquid determined isothermally by DMA**

KWW fit: 0. 45 < β < 0.6

Excess wing

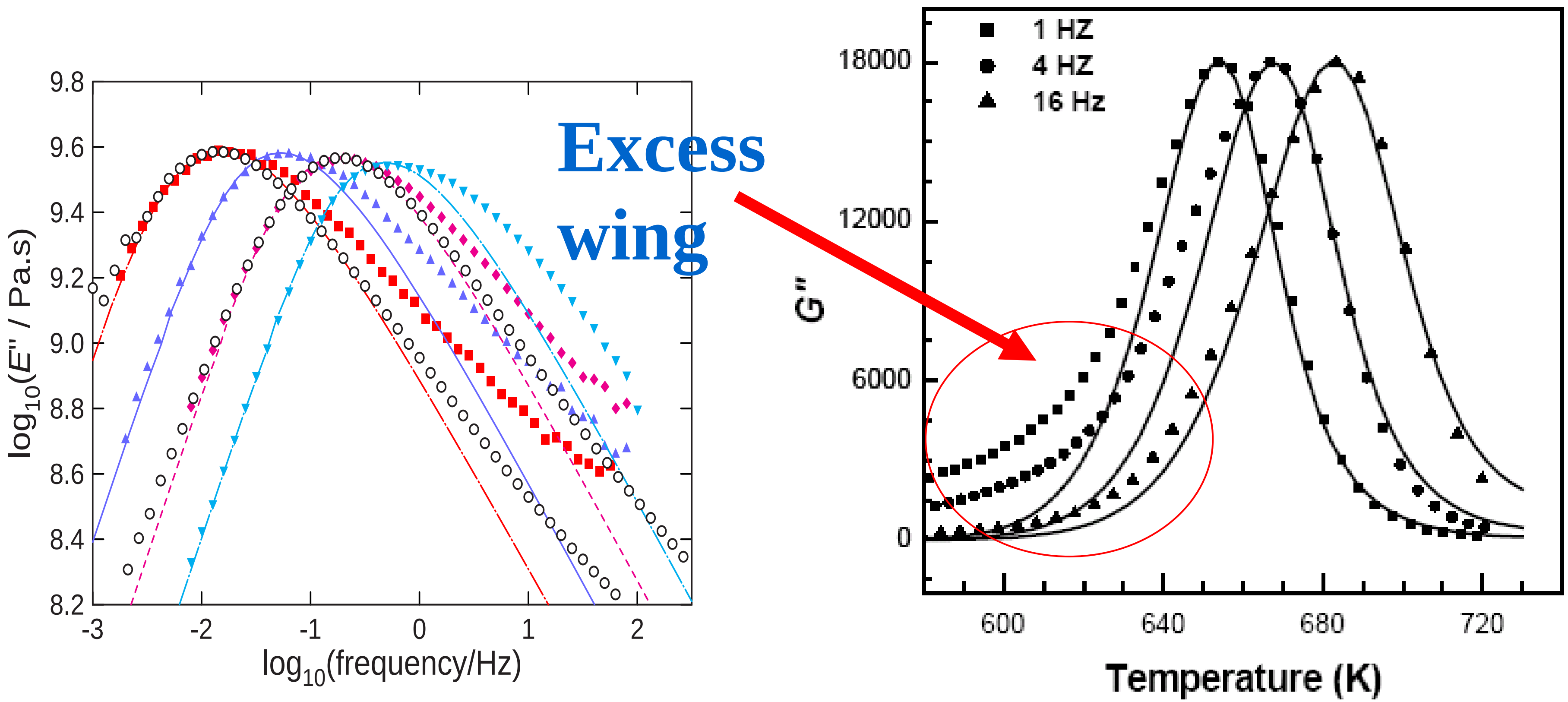


The solid lines are the KWW fits:

(KWW) form：F(t)=exp[-(t/τ)β] (β<1)

Samwer, Europhys. Lett. **68** , 226 (2004)

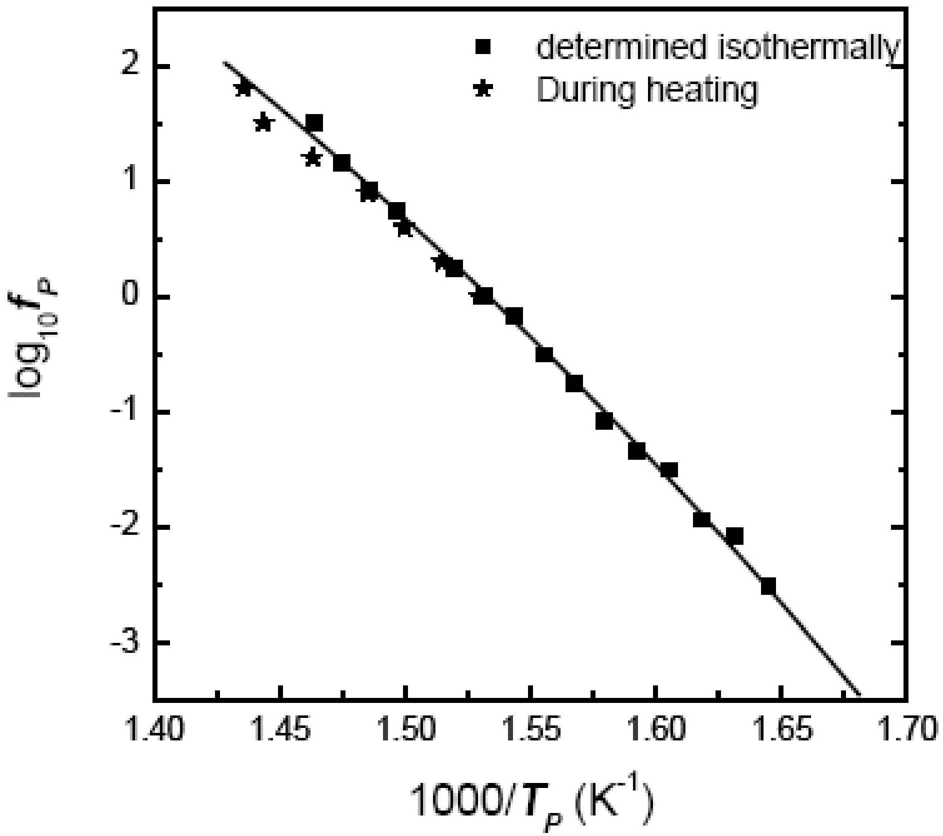
Double-paddle oscillator method



Comparison with dielectric relaxation loss data of a small molecule glass former

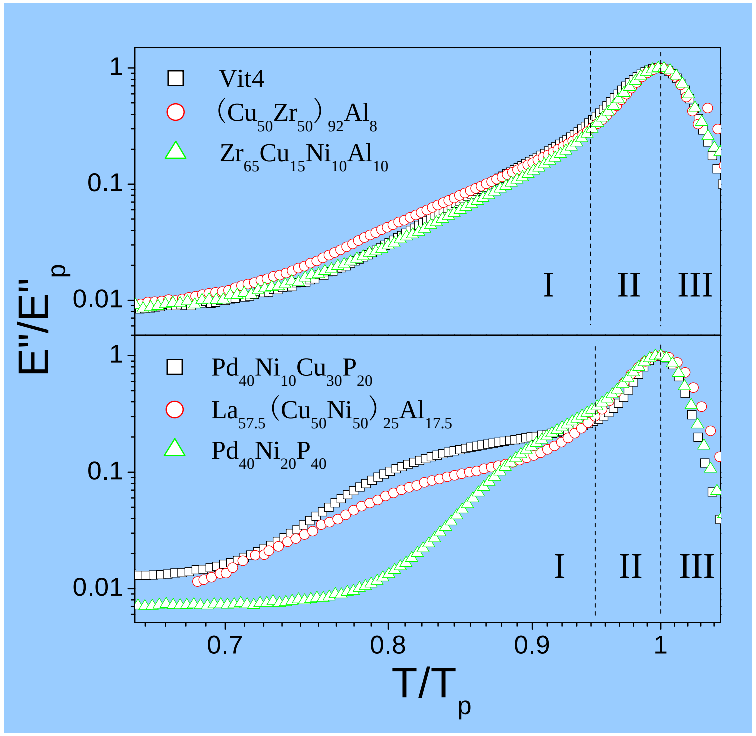
G''-curves of Vit4 SL determined in continuous heating processes at 1, 4 and 16 Hz respectively

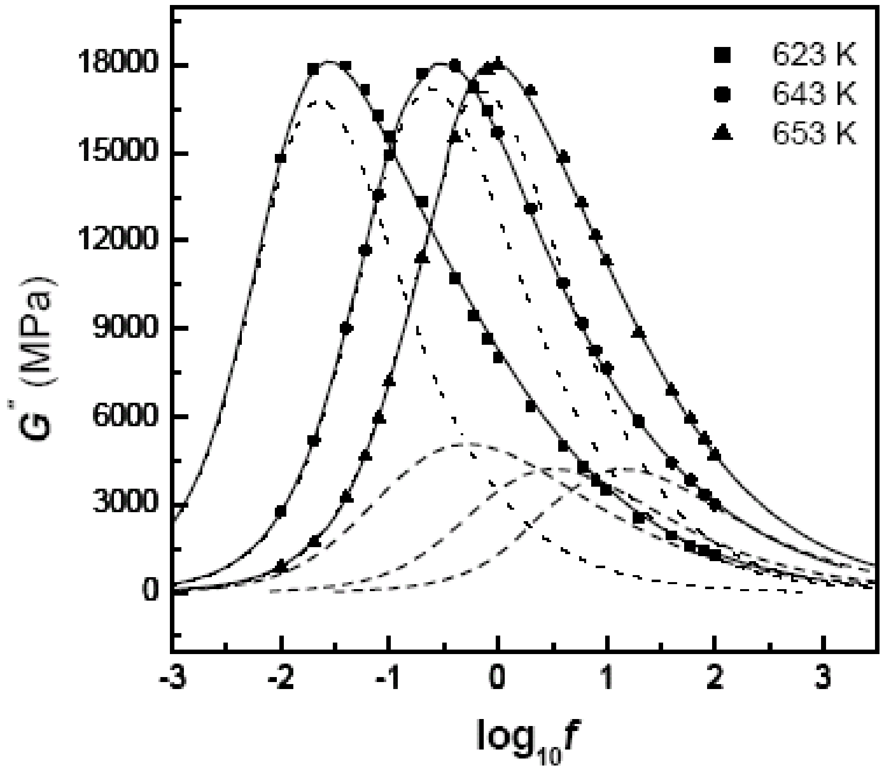
J Non-Cryst Solids 352 (2006) 5103



Plots of logf_P vs. 1000/T_p of G'' in isothermal and heating processes. The consistence affirms correlation between the two processes.

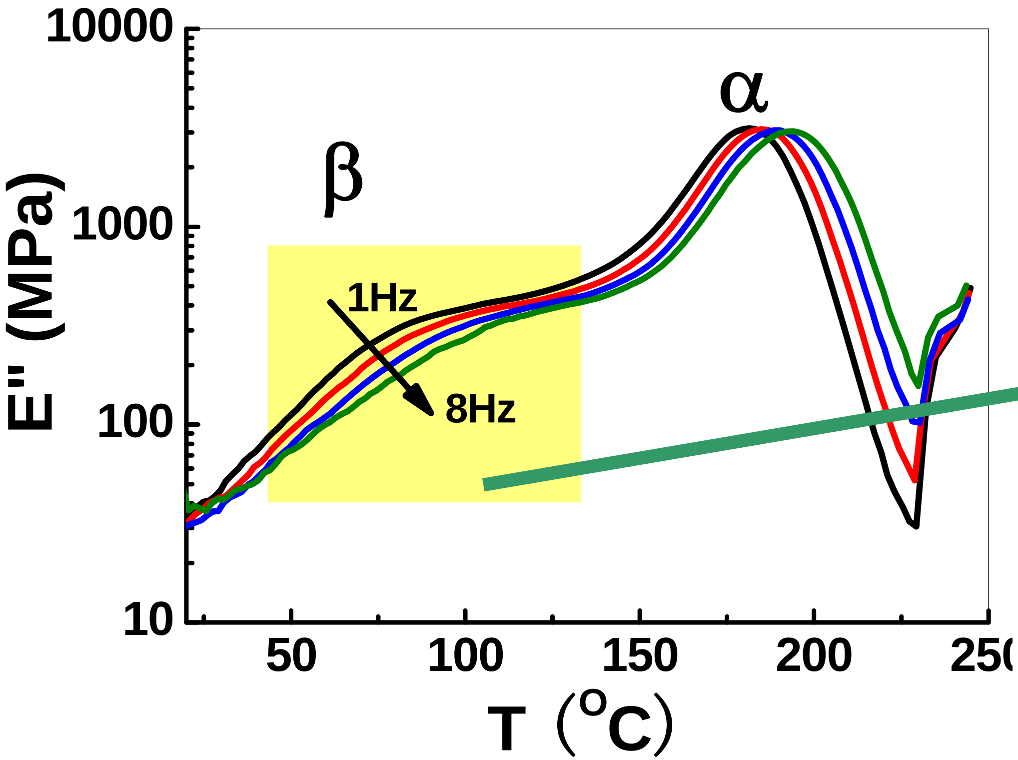
The existence of slow β-relaxation in metallic liquids

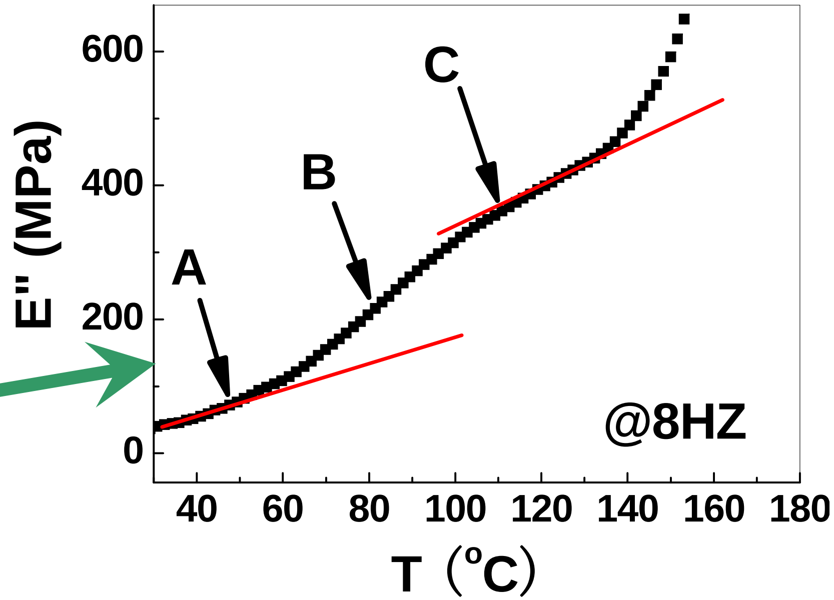


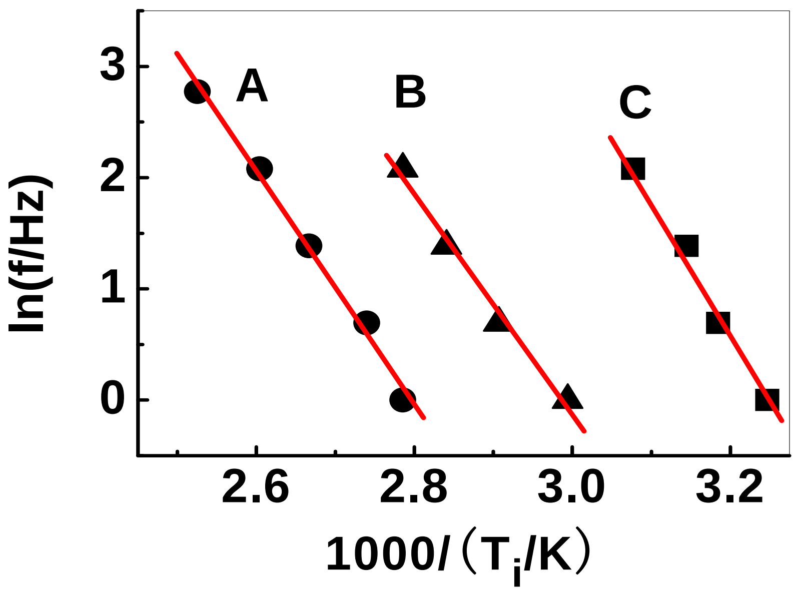


f-dependent G'' of vit4. The solid lines are the sum of two KWW form fits. The dash lines are fits for α-relaxation with β_{KWW} = 0.65. The dash dot lines are fits for β-relaxation.

Determine activation energy of Beta relaxation

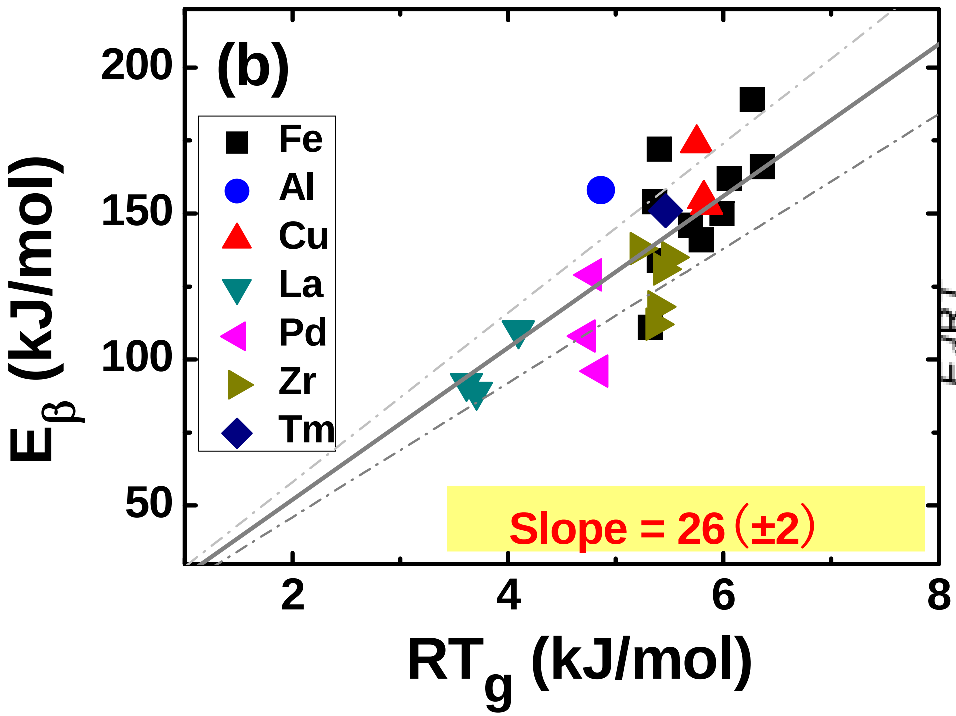


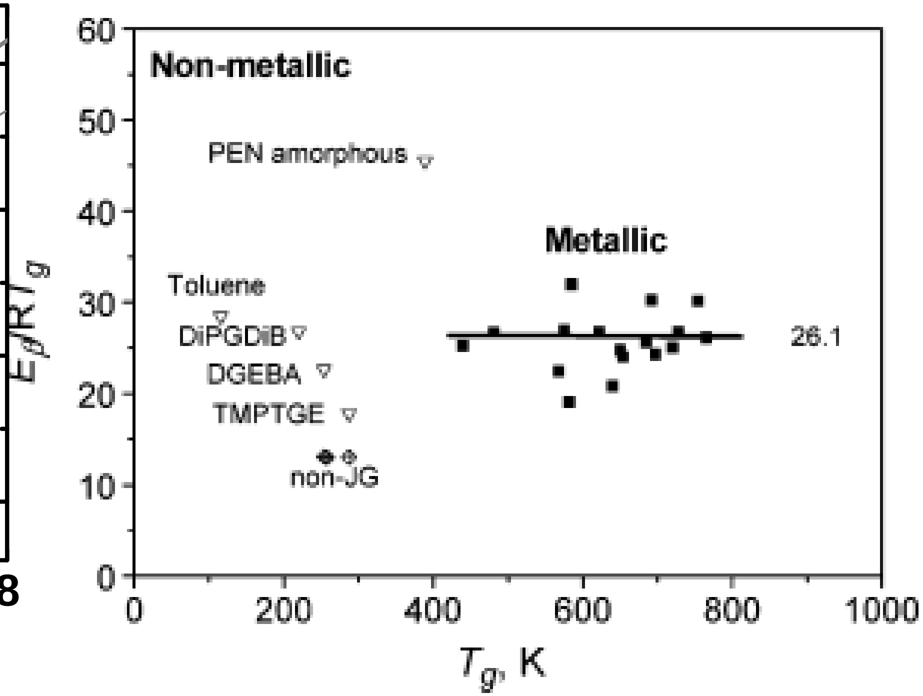




E_β **can be get from Arrhenius plot**

E_β in MGs: Scaling with Tg





J. Phys. Chem. C **2009**, *113*, 15001–15006

$$E_\beta = 26(\pm 2)\ RT_g$$

PRB 75, 174201 (2007)

E_β/RT_g = 26 is also consistent with that in non-metallic glasses (E_β/RT_g = 24)

III. Estimation of energy barrier of STZs

The W_{stz} values are complied from experimental measurements & simulation

M.W. Chen, PNAS 2008

Mayr, Phys. Rev. Lett. 97, 195501(2006)

$$W = (8/\pi^2)G\gamma_C\zeta\Omega$$

$$\Omega = nc_f V_a \quad V_a = M/(\rho N_0)$$

ζ~3 is a correction factor arising from matrix confinement of a STZ

$$\gamma_c \approx 0.027$$

n is atoms take part in an STZ events

$$W_{STZ} = N_0 W = (8/\pi^2)nG\gamma_c^2\zeta C_f V_m \approx 0.39GV_m, \text{ here } V_m = N_0 V_a$$

$$W_{SZT} \approx 0.39GV_m$$

IV. β-relaxation ~ STZ

The results indicate that:

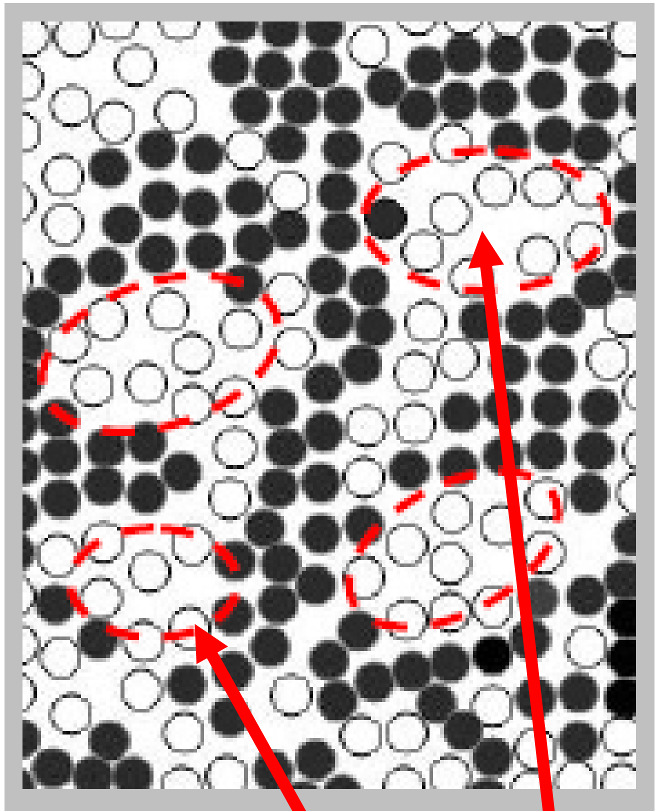
β-relaxation & STZs in MGs have common structural origin

The correlation is helpful for understanding the structural origin of β-relaxation in MG

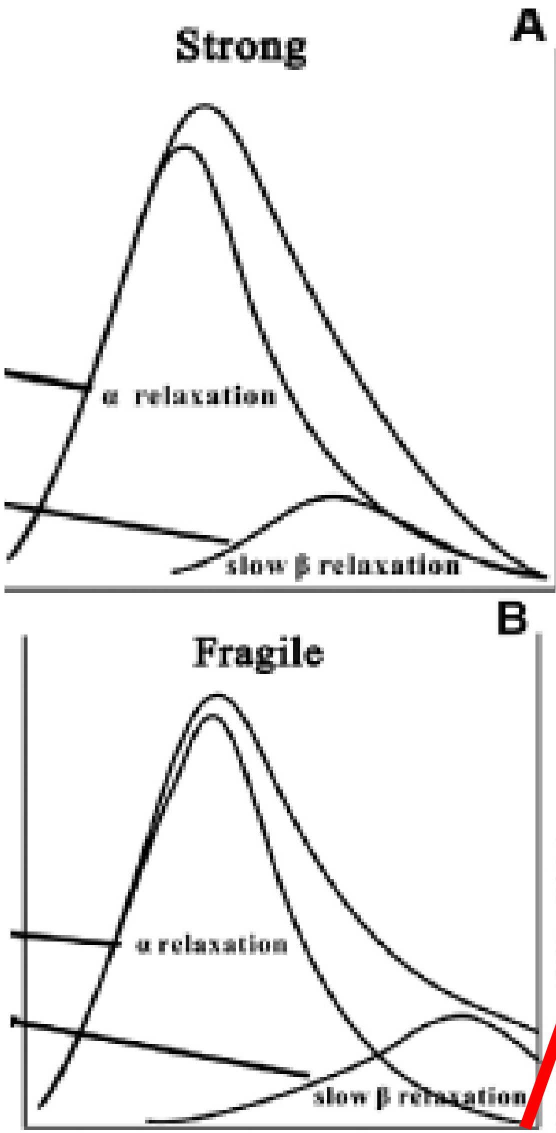
It is suggestive for understanding the relation of glass transition and plastic deformation

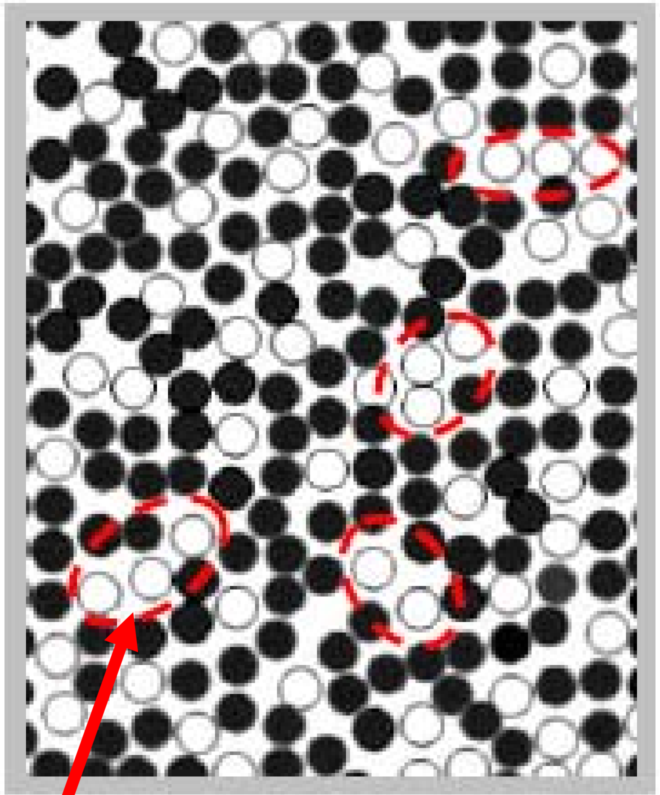
It is useful for understanding the plasticity in MGs and for developing of tough bulk MGs

Structural origin of β relaxation and STZs in BMGs



(a) Fragile glass. Larger Poisson ratio, fragility, and volume of potential STZs





(b) Strong glass. Smaller Poisson ratio, fragility, and volume of potential STZs

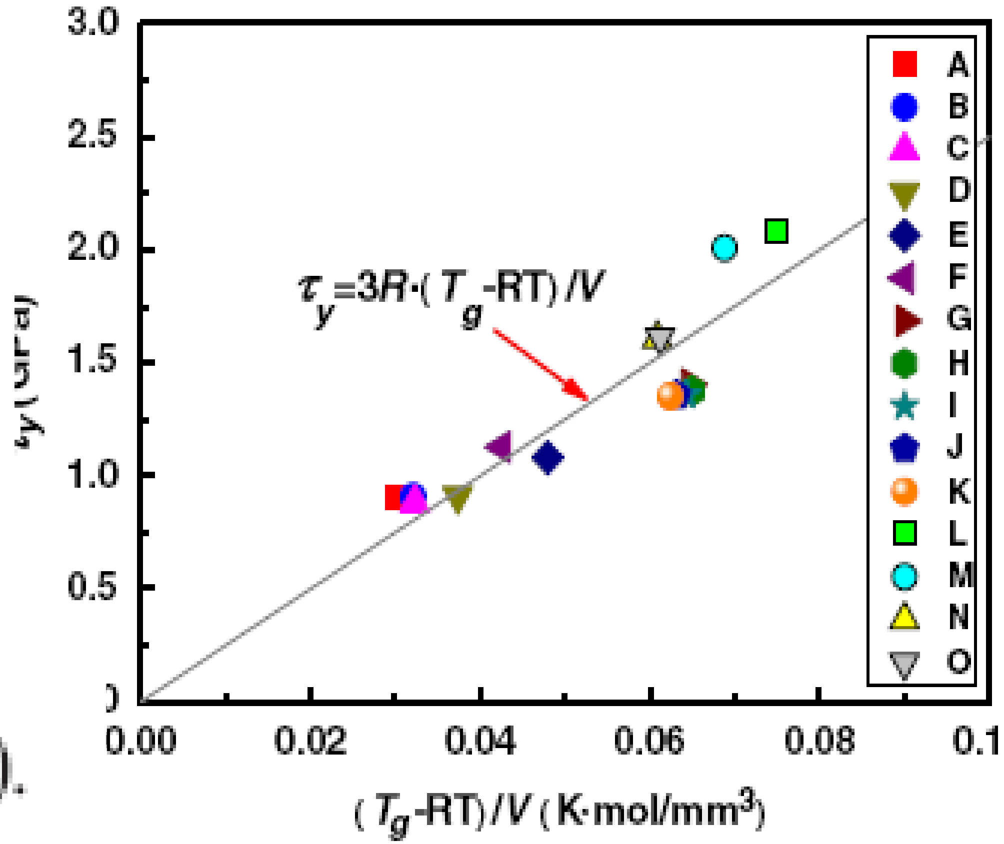
The nucleation sites of potential STZs ⇔ β-relaxations

Intrinsic inhomogeneity is a fundamental property of MGs

Relation between glass transition & plastic deformation in MGs

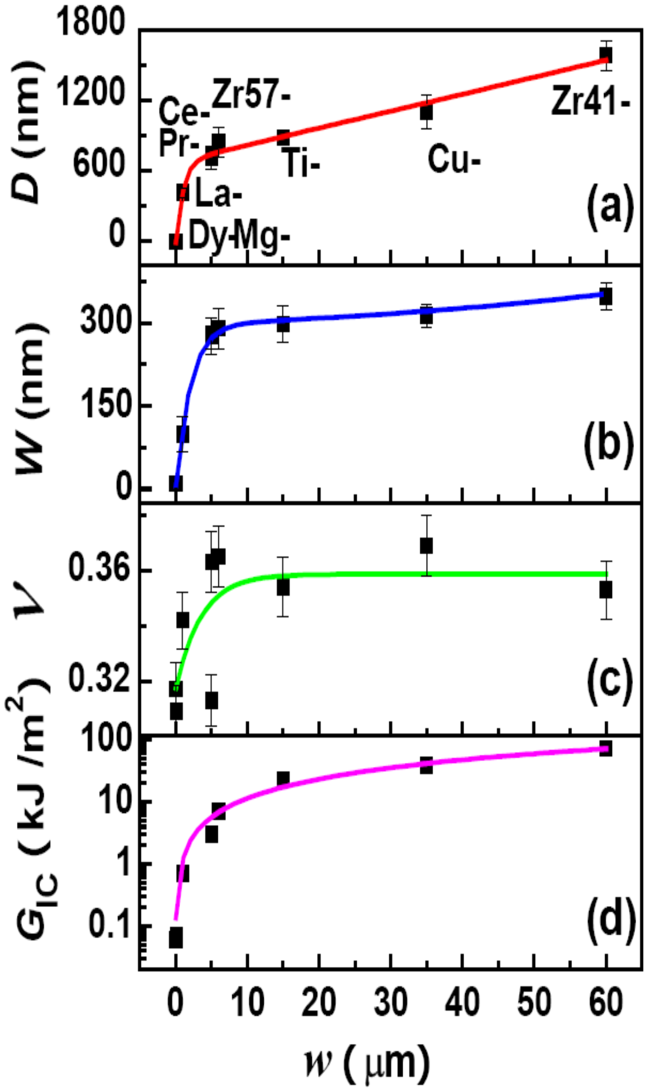
The linearity between yield strength and Tg unambiguously demonstrates that the plastic deformation of MGs driven by stress is equivalent to the glass transition induced by mechanical energy

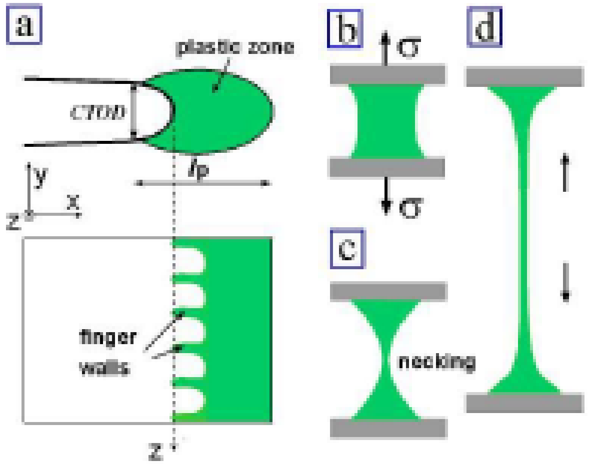
$$\tau_y = 3R(T_g\text{-RT})/(\gamma_0 V).$$

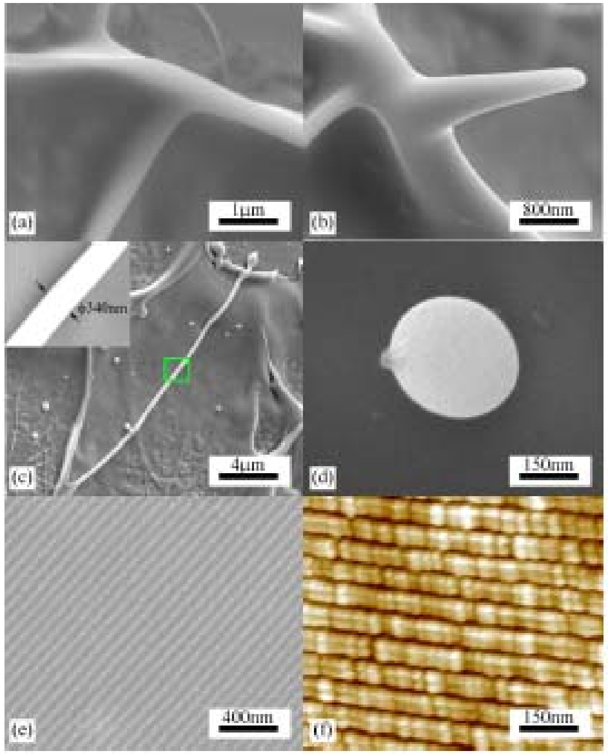


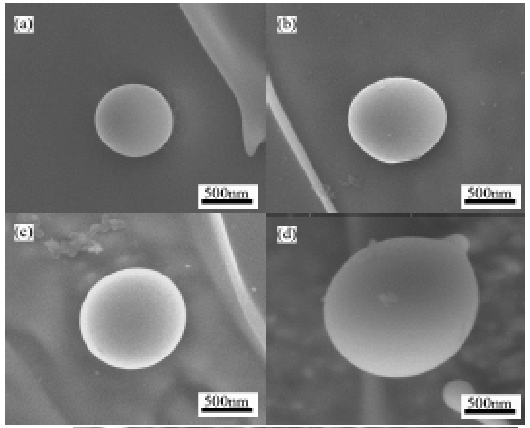
PRL 103, 065504 (2009)

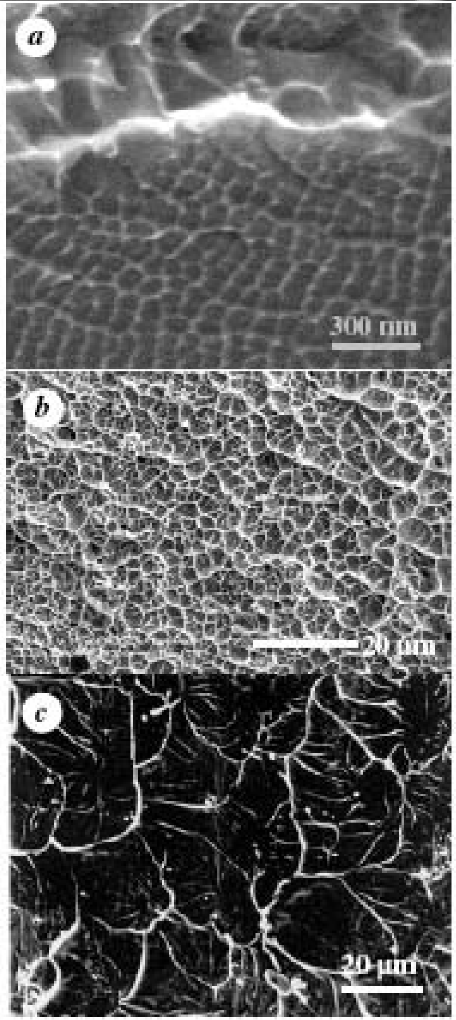
XX Xia, W.H. Wang, A.L. Greer, JMR, 2009



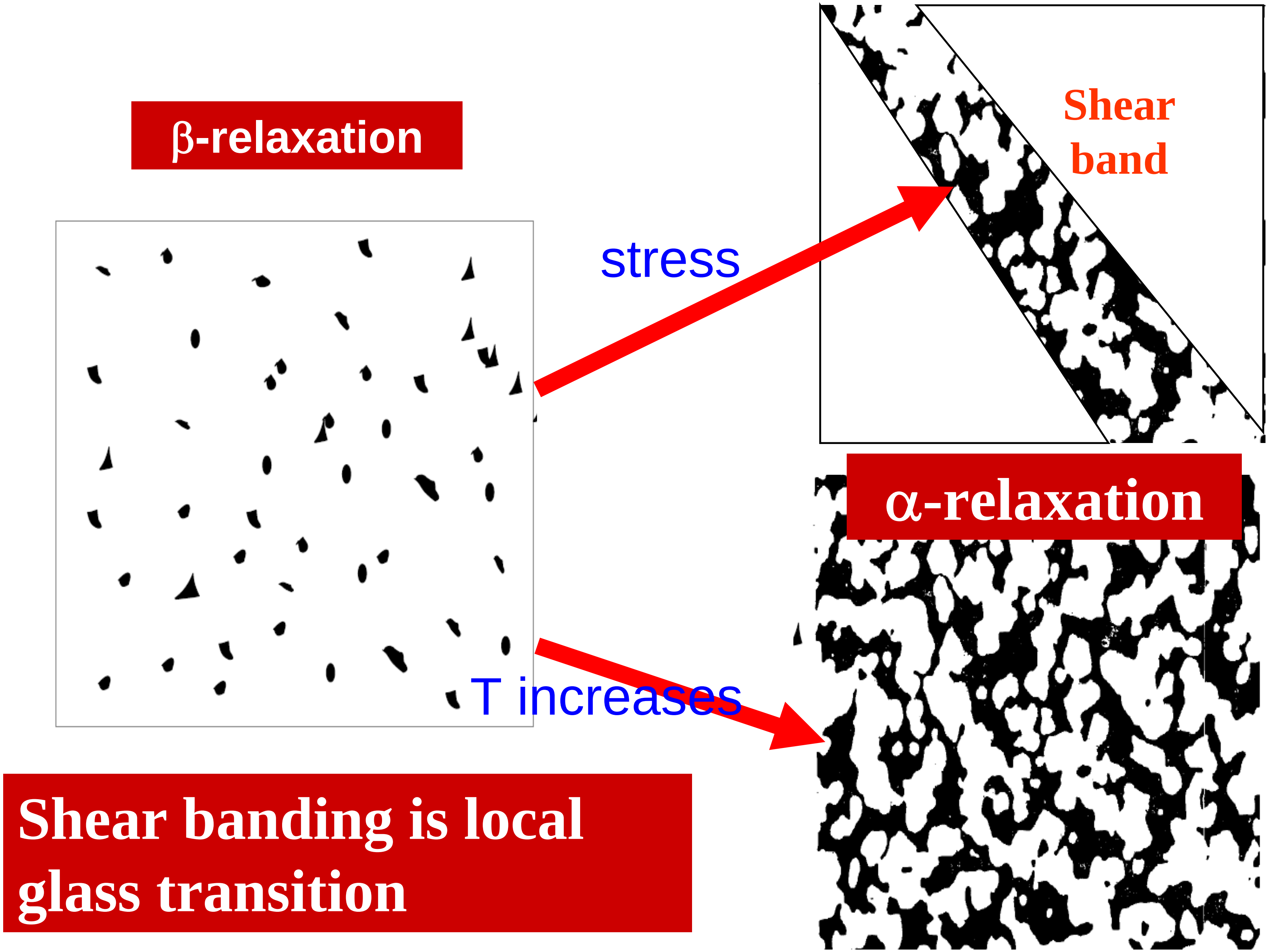




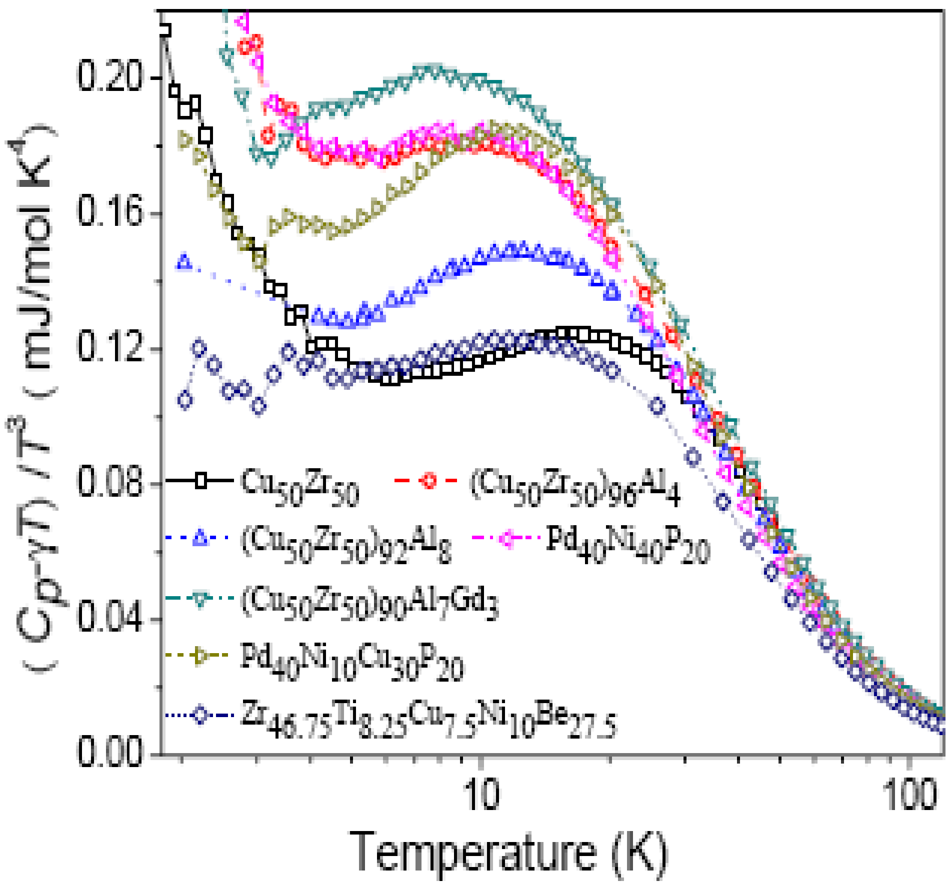


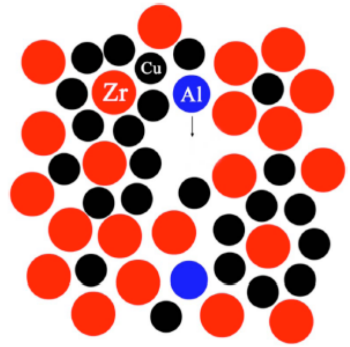


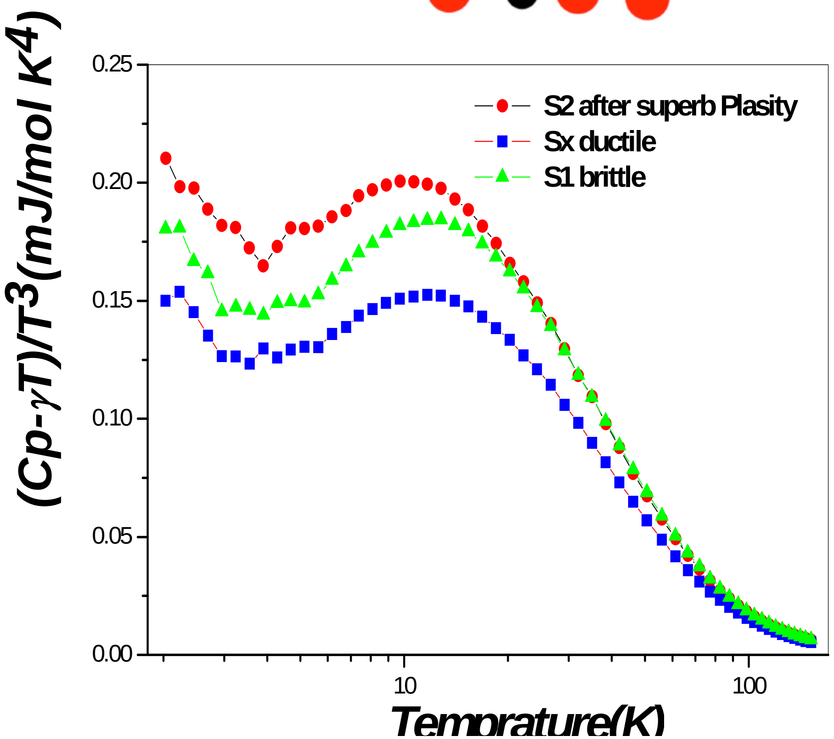
PRL. 94, 125510 (2005)


β-relaxation
stress
Shear
band
α-relaxation
T increases
Shear banding is local glass transition

Have implication for understanding Boson Peak





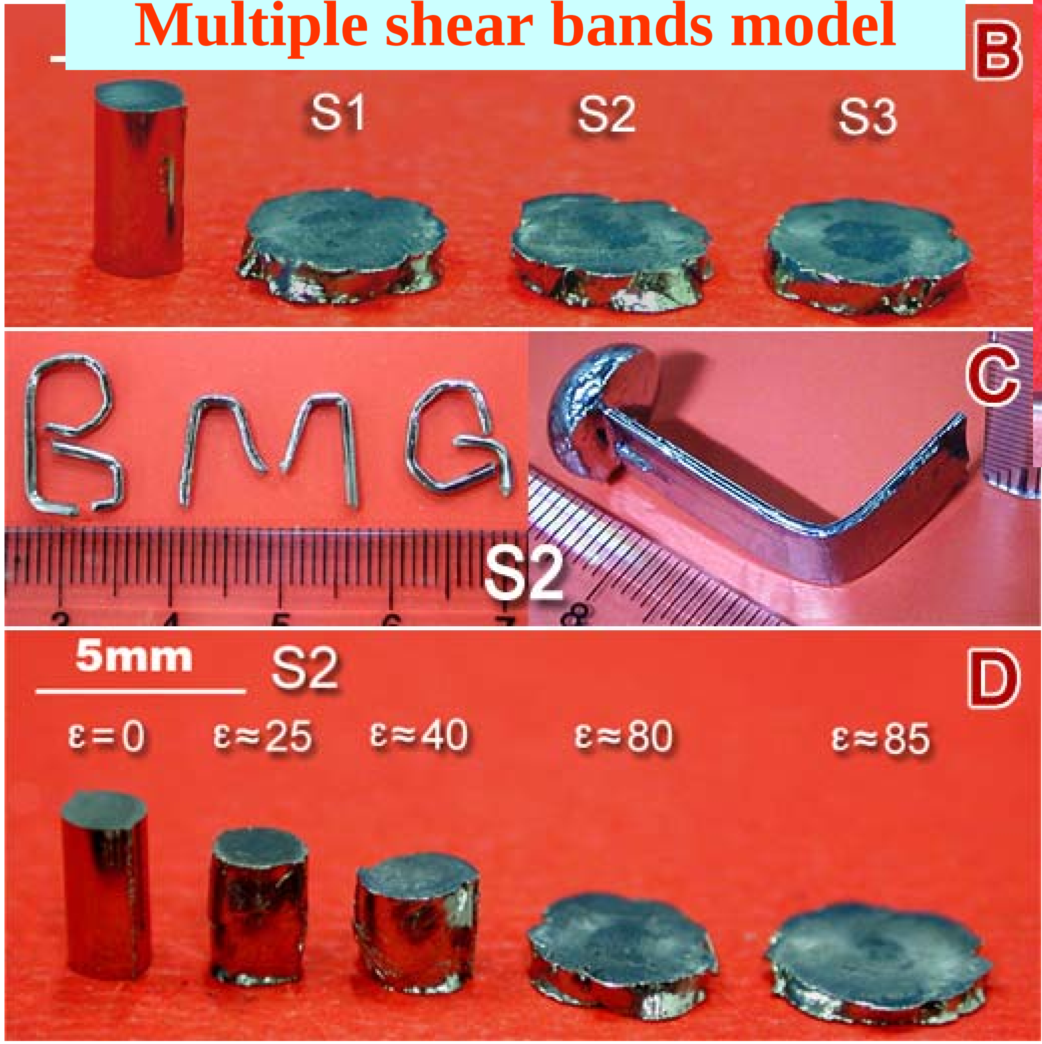


More pronounced boson peak indicates more loose atoms in fragile and ductile MGs

PHYSICAL REVIEW B 74, 052201 (2006)

The correlation between β-relaxation & STZs confirms: Inhomogeneity should related to plasticity

Multiple shear bands model



Cu50Zr50

PdSi

CuZrAl

CuZrAlNiSn

APL 92, 011915 (2008)

APL 91, 131901 2007

APL 93, 231912 2008

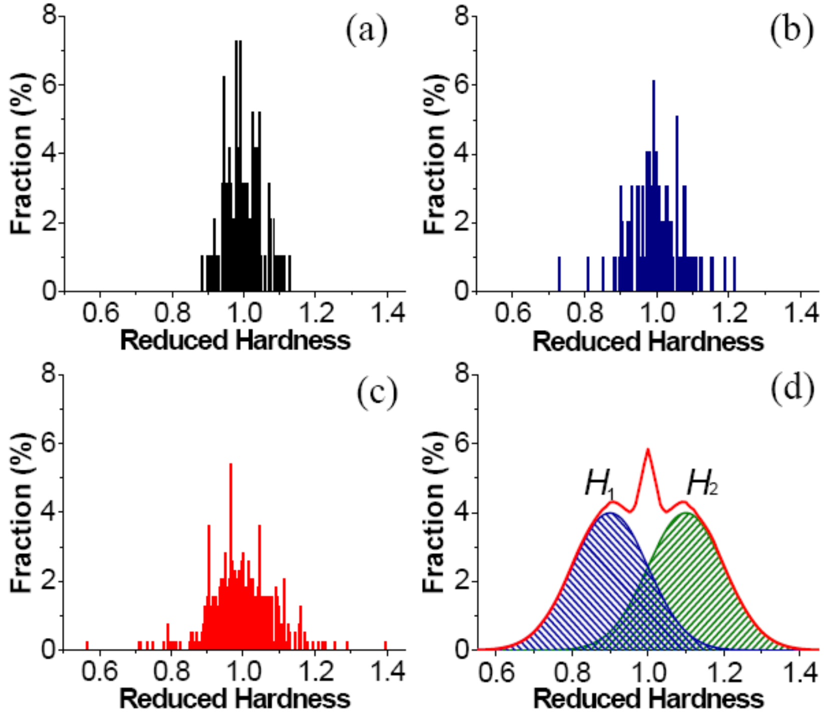
PRL 100, 075501 (2008)

JNCS 2008

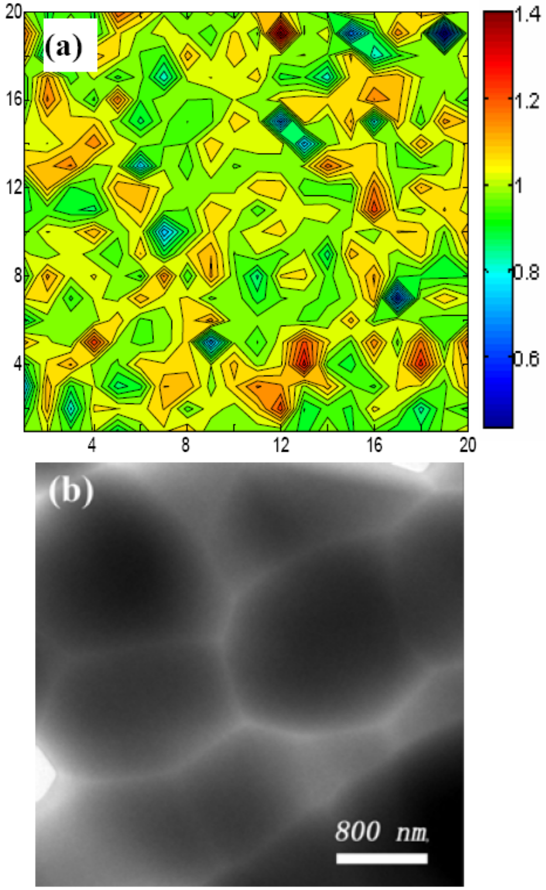
Phys. Stat Sol 3, 46 (2009)

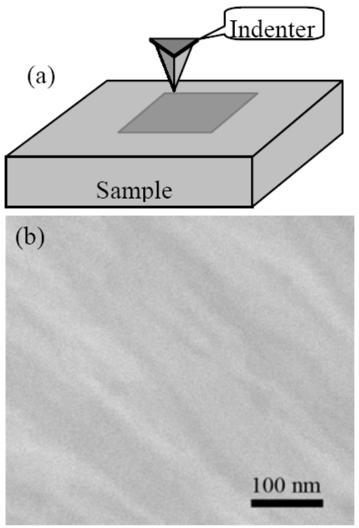
Science， 315, 1385(2007)

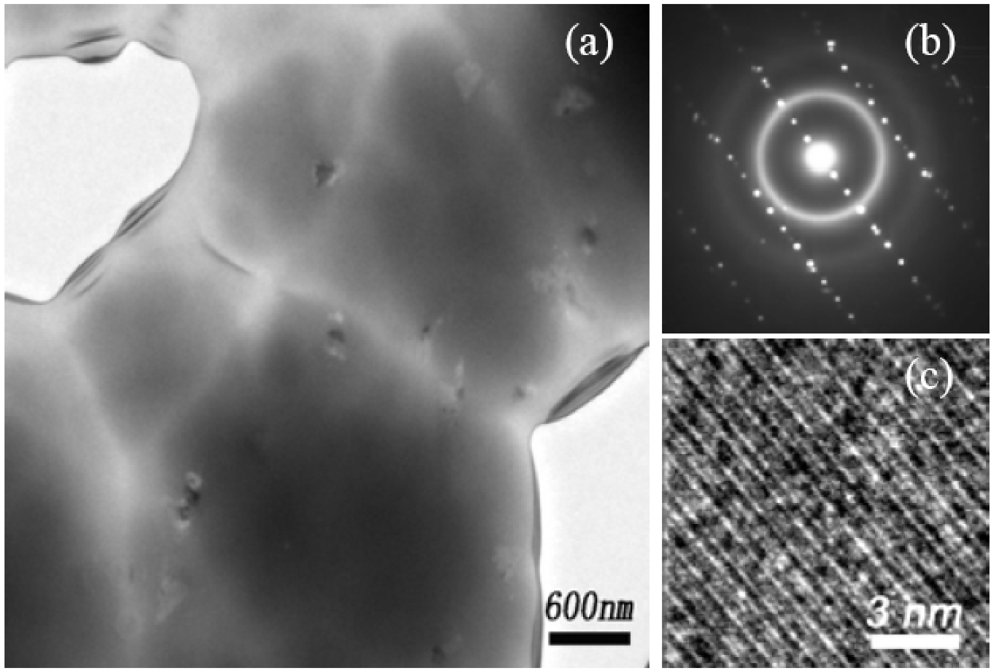
Existence of structural heterogeneity

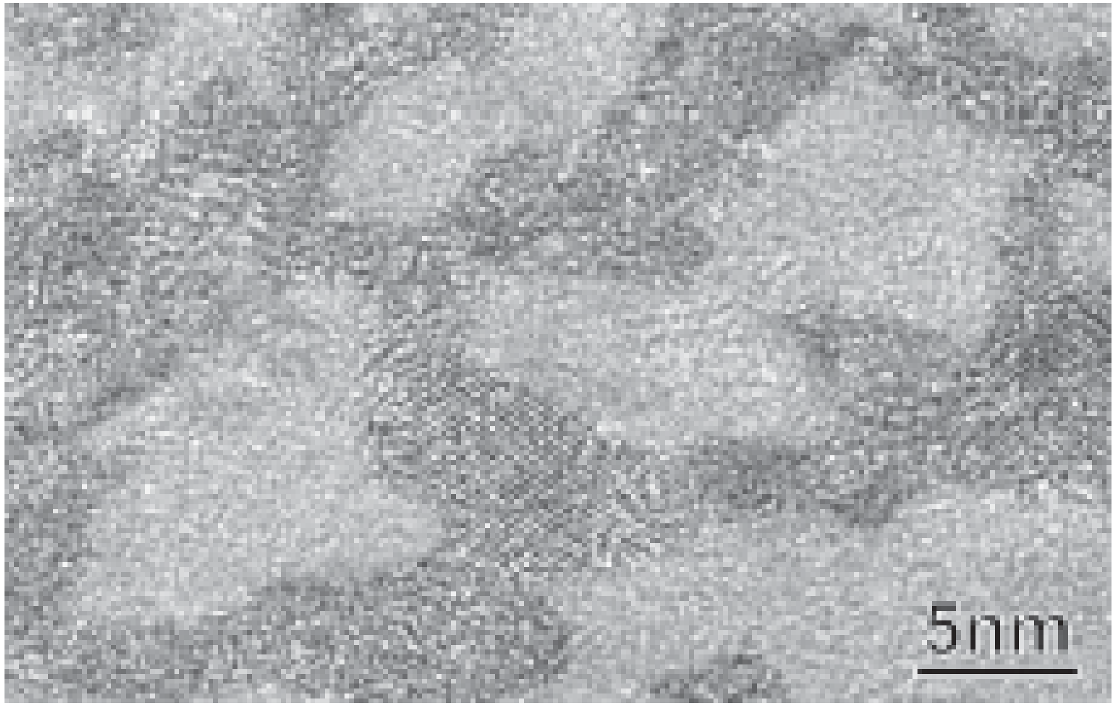


APL 2009





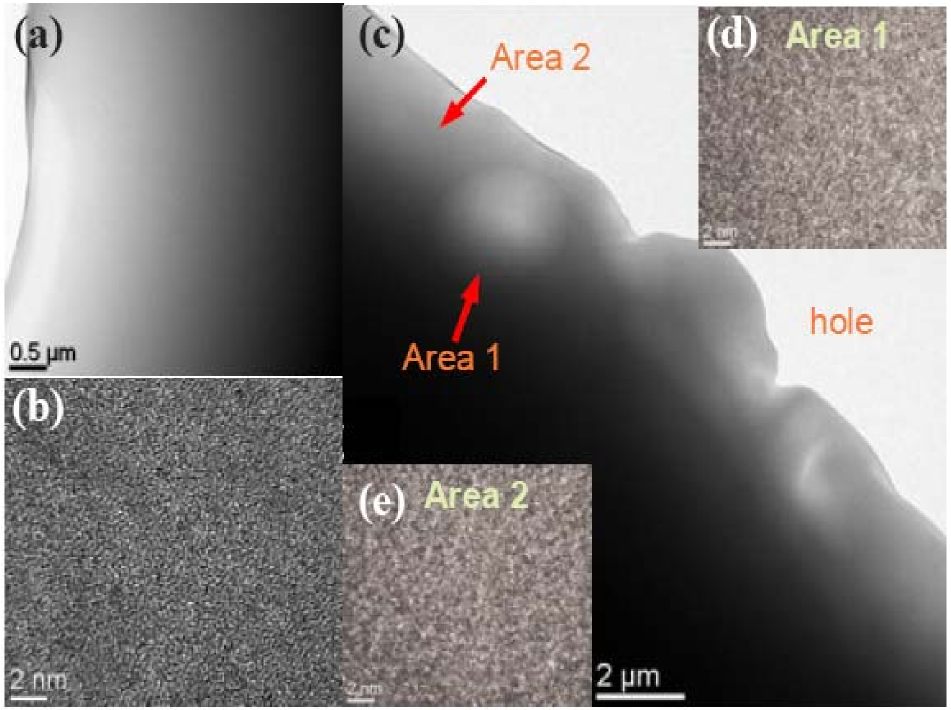




Ichitsubo et al.

PRL, 95, 245501 (2005)

Eckert Group

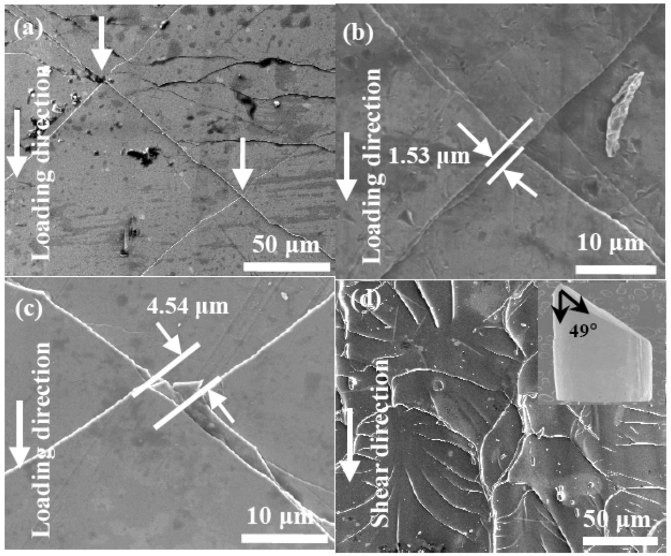


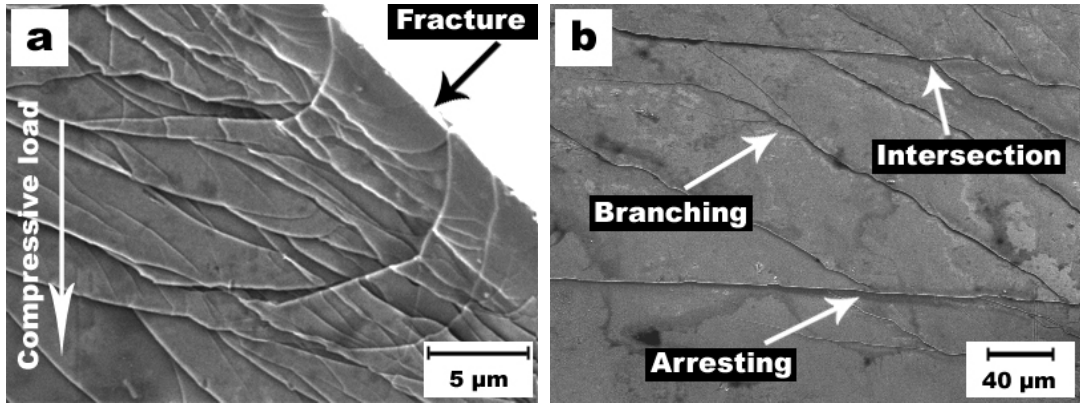
The mobility in soft regions is associated with β-relaxation

The soft regions benefit for multiple shear bands formation

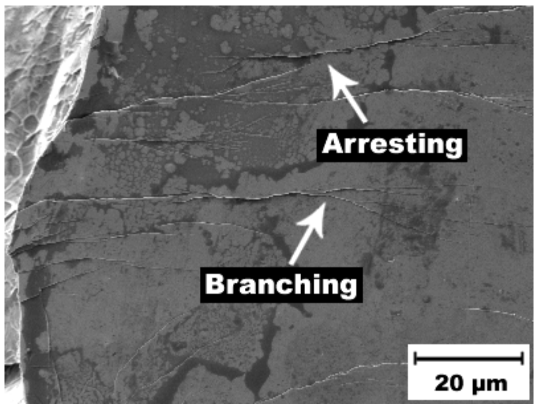
Multiply shear bands

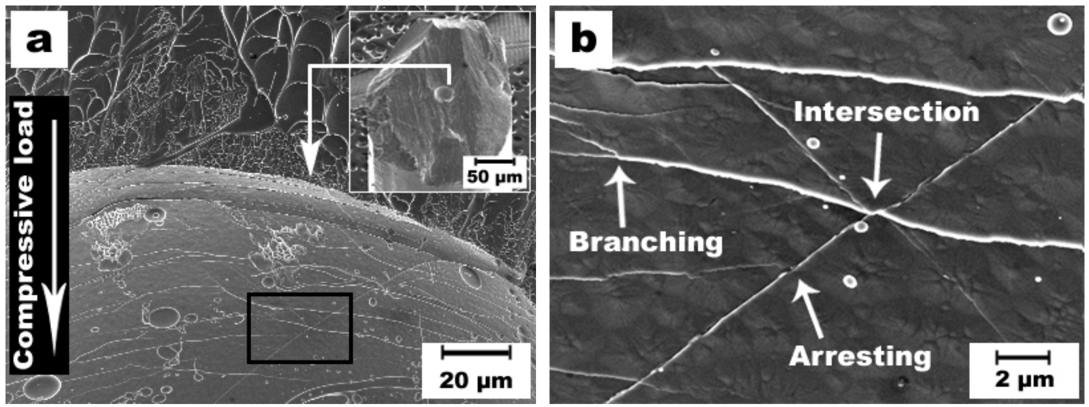
Interaction of shear bands



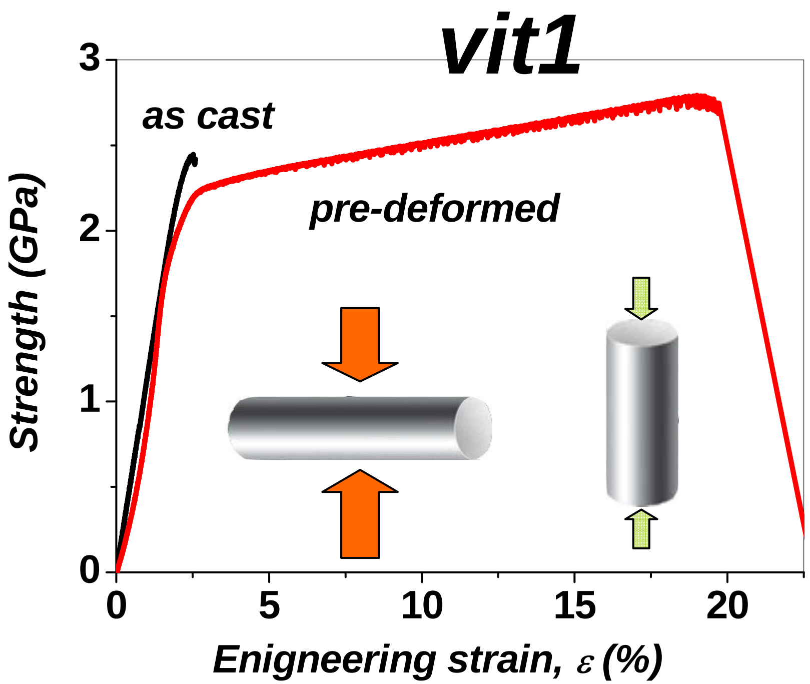


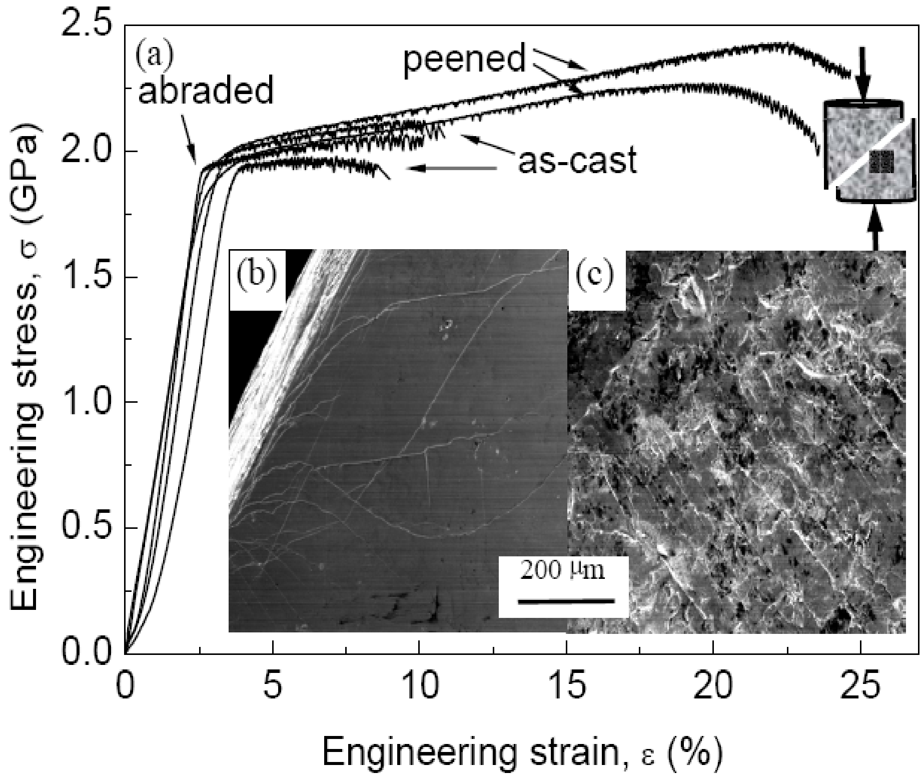
a) multiple shear band formation, b) arresting and branching of shear bands

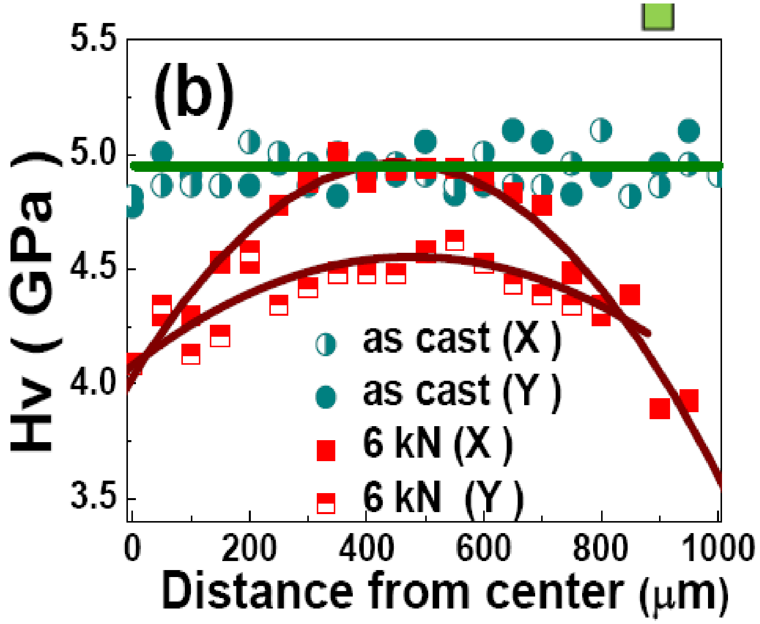




Formation of SBs inside the fractured Ni- BMG, a) overall image of a cavity in the fracture surface and b) magnification of area in a) illustrating the formation of SBs in different directions, the branching and arresting SBs are readily observed.







Scripta Mater , 2009

Shot peen induced pre-existing shear bands & stress can significantly improve plasticity of MGs

Nat. Mater 5, 857 (2006)

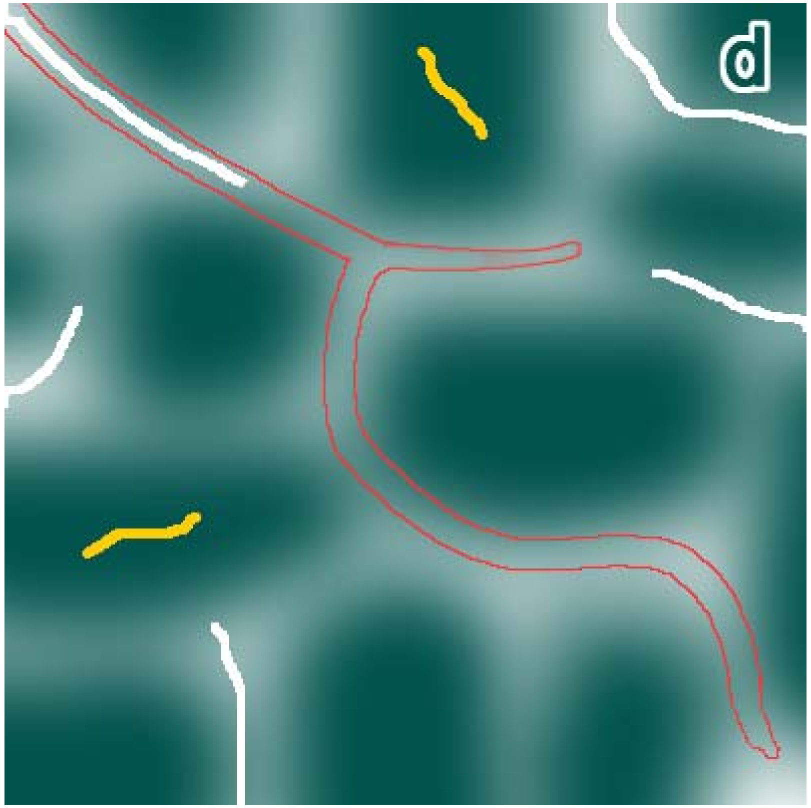
Structural inhomogeneity and plasticity

Soft（Low moduli, easy for STZ activation）

Nucleation of multiple SBs

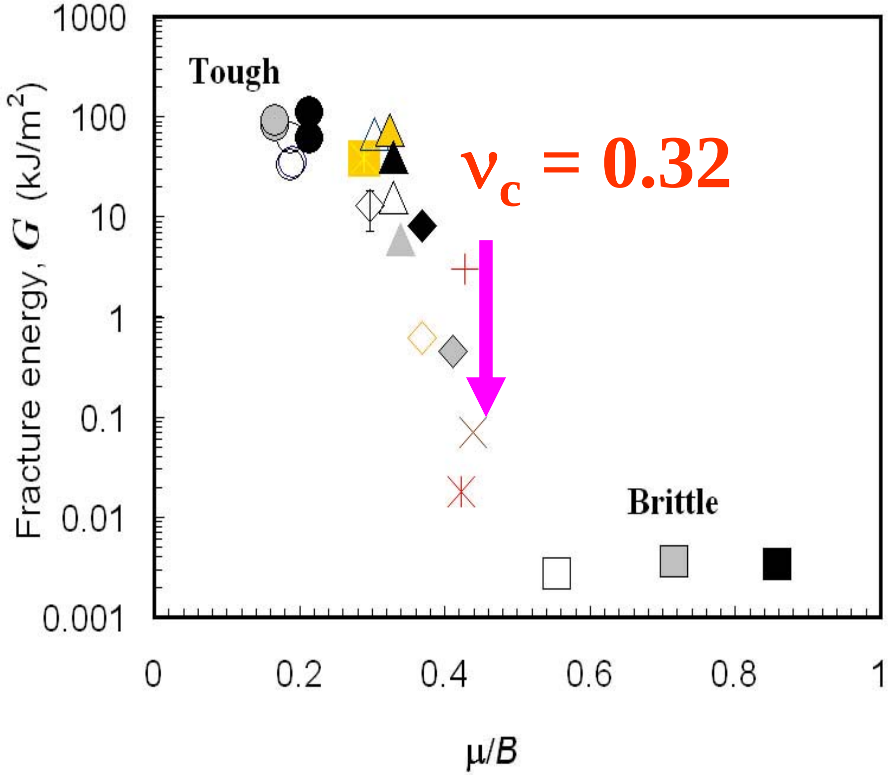
Hard（high moduli）

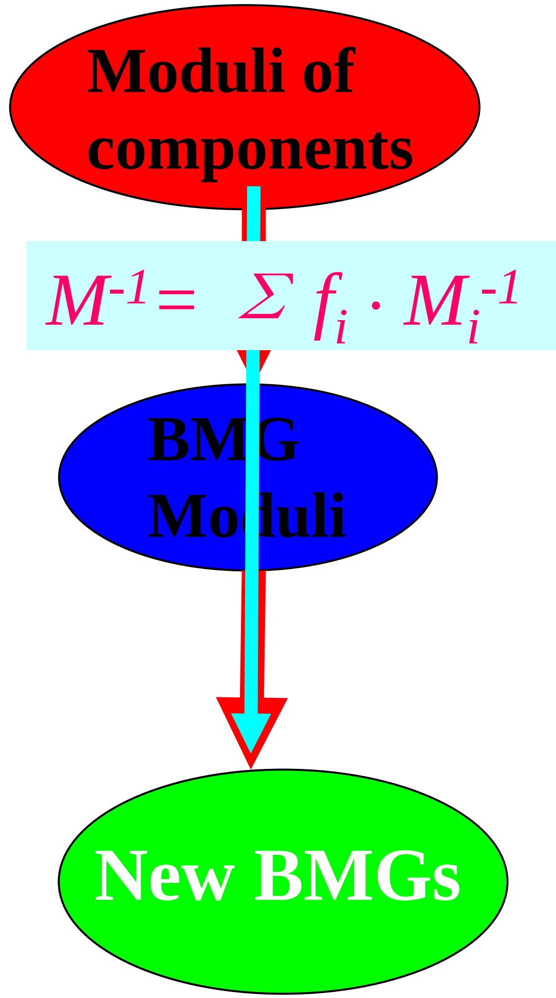
Block propagation of SBs



Soft/hard model

The correlation between β-relaxation and STZs is useful for understanding Poisson's ratio criterion





The larger Poisson ratio, the better the plasticity

BMGs with ν < 0.32–0.33 are brittle

Lewandowski, Wang, Greer, Philo Mag Let 85, 77(2005)

JAP, 99, 093506(2006)

The MG with larger ν has lower W_{STZ}, more inhomogeneous structure and larger plasticity

Lower W_{STZ} favors better ductility.

V. Summary

1. The existence structural or elastic heterogeneity in MGs have close relation with their plasticity

2. We find $E_{\beta} = W_{STZ}$.

3. β-relaxation and STZs in BMGs have a common microstructural origin

4. Our results are suggestive for understanding deformation mechanisms and origin of β-relaxation in MGs.

Thanks !