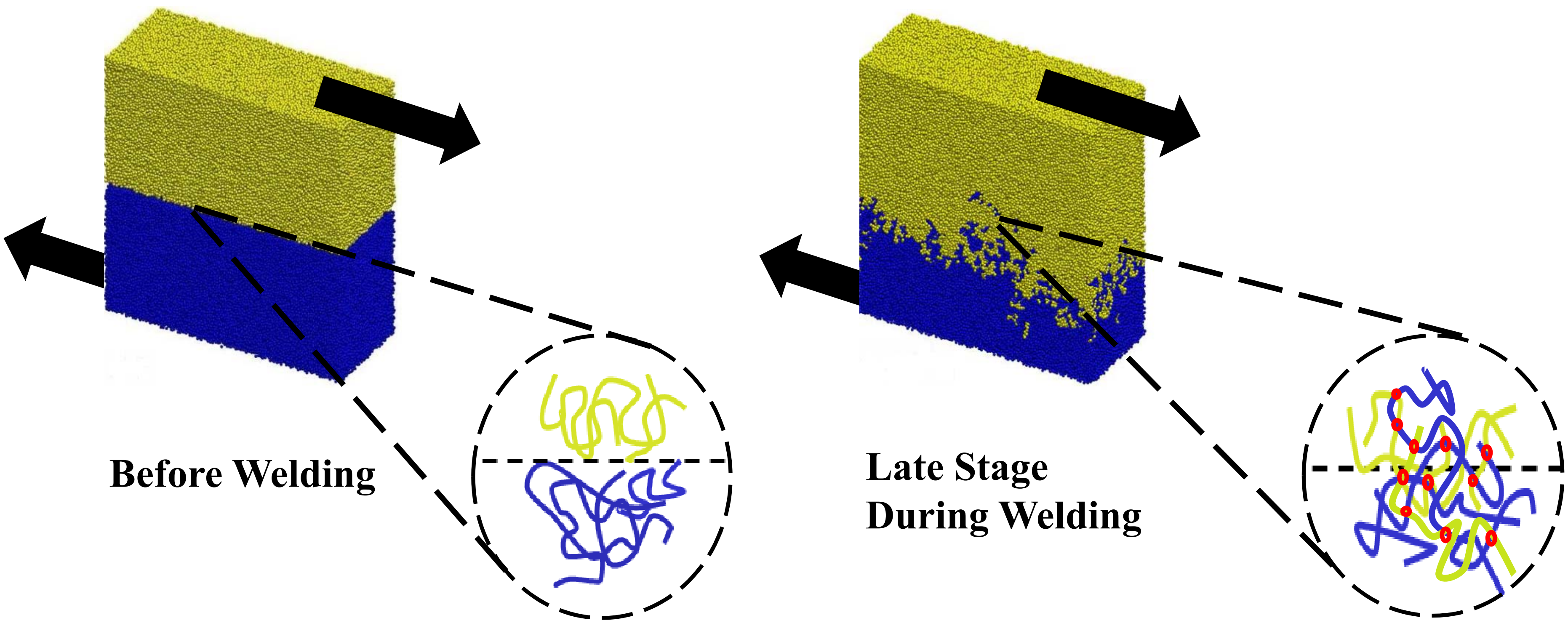
Shear Failure of Polymer Welds and Entanglements

How does interfacial strength develop during welding?
How does the development correlate with the evolution of interfacial structure?

T. Ge, M. O. Robbins, Johns Hopkins University
F. Pierce, G. S. Grest, Sandia National Laboratories
D. Perahia, Clemson University

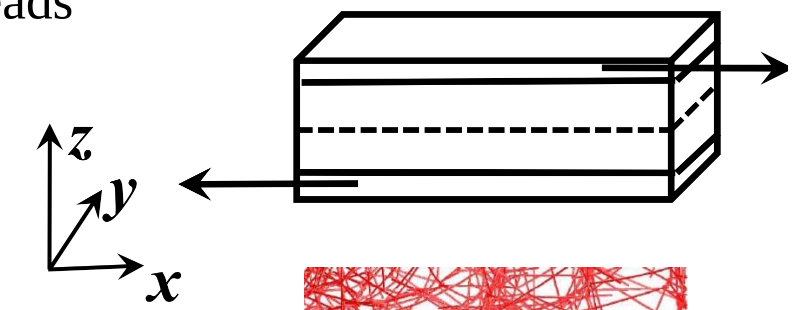
August 10, 2011

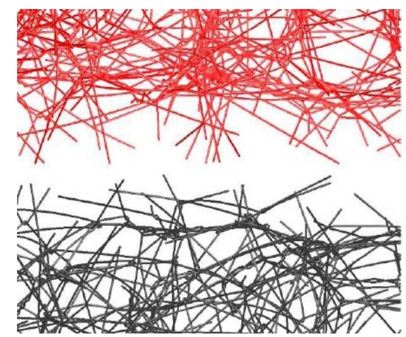


MD Simulation and PPA algorithm

Nonequilibrium molecular dynamics (MD) simulation

- Lennard-Jones potential between all spherical beads
  Breakable bond potential
  ratio of the forces at which the covalent and van der Waals bonds break ~ *100*
- Simple shear
  constant strain rate $d\gamma_{xz}/dt = 2\times10^{-4}$
  Periodic boundary conditions within the shear plane
  Temperature control

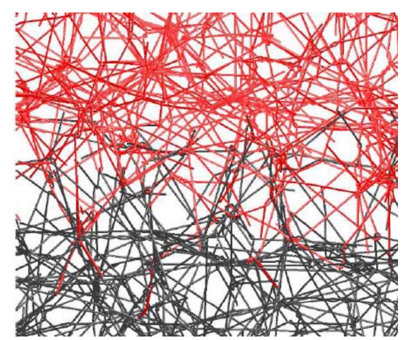




PPs before welding

Primitive Path Analysis (PPA)

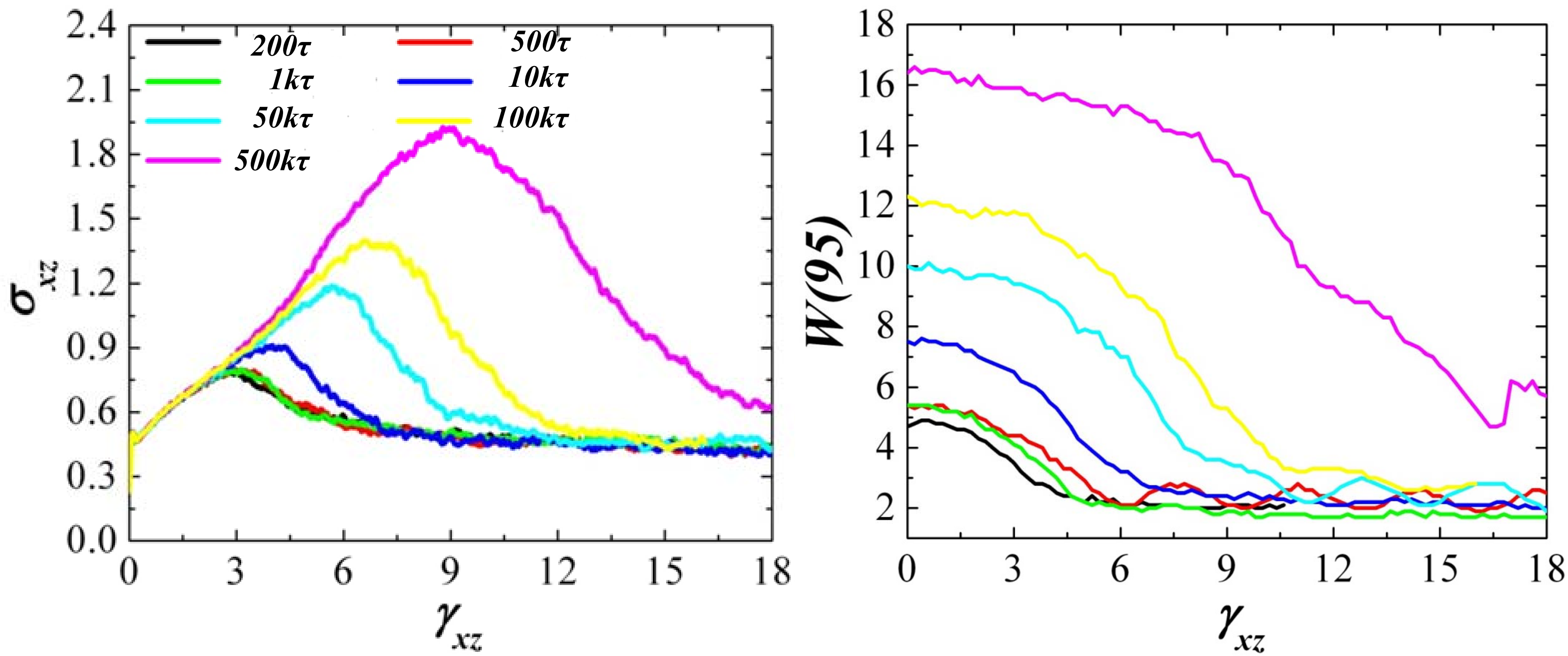
- Fix chain ends
  Deactivate intrachain excluded-volume interactions
  Retain interchain excluded-volume interactions
- **Minimize energy by cooling the system down to *T~0***
- Bond forces try to reduce the bond length to zero and pull chains taut
- Insert extra beads to reduce the effects due to chain thickness
- Contacts of Primitive Paths ⟺ Entanglements



PPs at late stage of welding

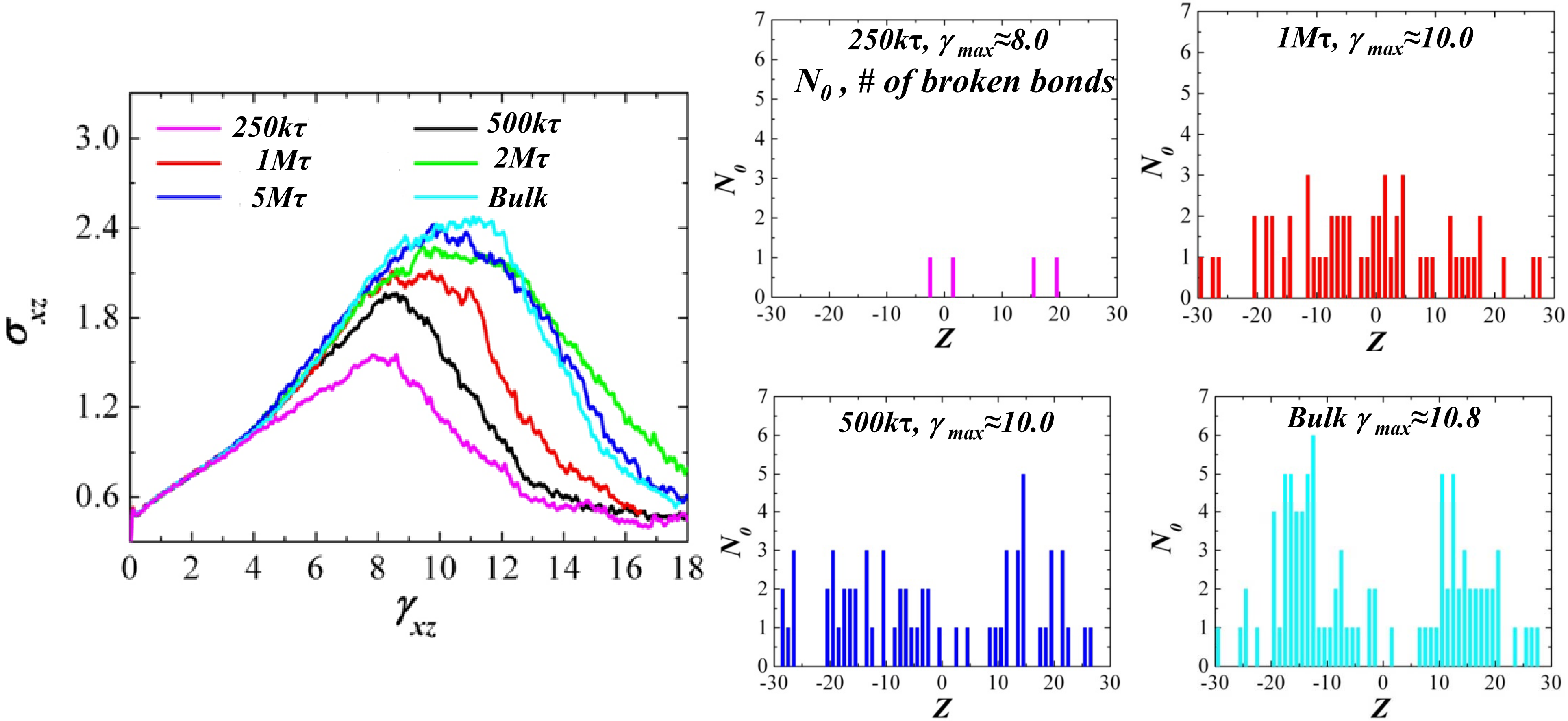
Interface fails by pure chain pullout at small *t*

- **Interfacial width decreases with shear strain**
  W(95), the distance between the planes where 95% atoms belong respectively to original upper and lower parts
- **At steady state , σ_{xz} is uniform along *Z***
  Strain hardening in the entangled regions away from the interface
  ➡ Strain localization near the interface
- **Universal final interfacial width and shear stress**



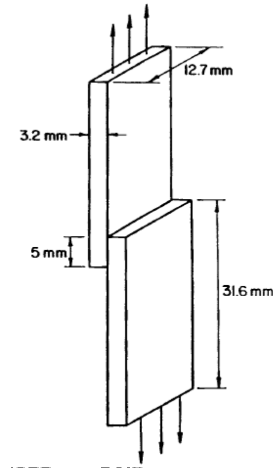
Interface fails by chain scission at large *t* and in bulk states

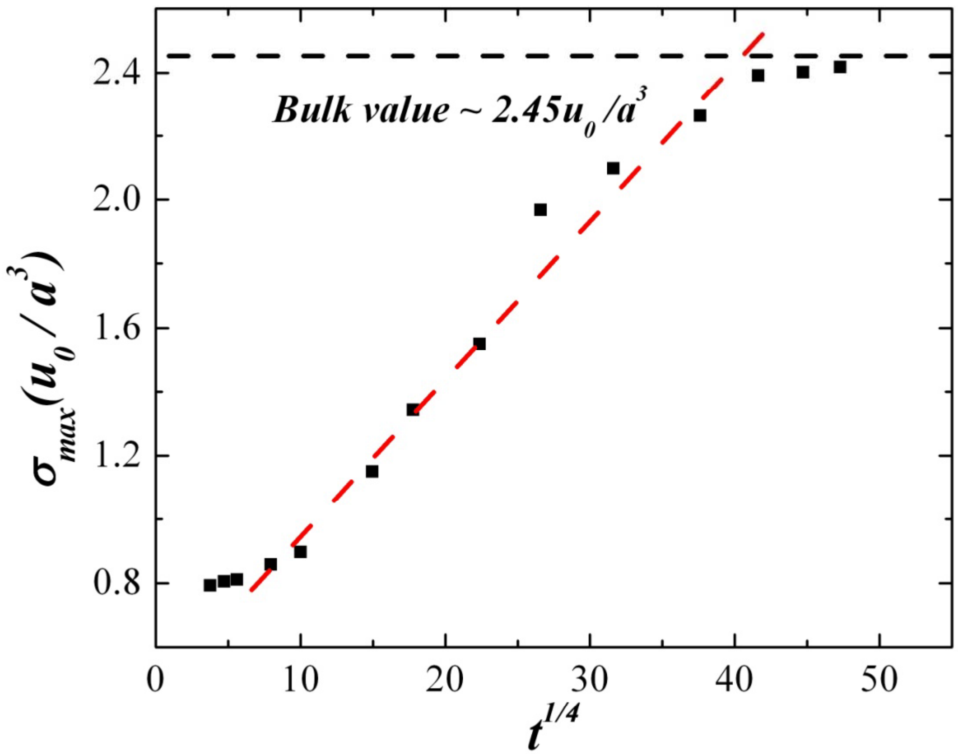
- **Broken bonds show up at large γ**
  Not only near the interface
- **After chain scission sets in, the stress-strain behavior starts to saturate towards the bulk result**

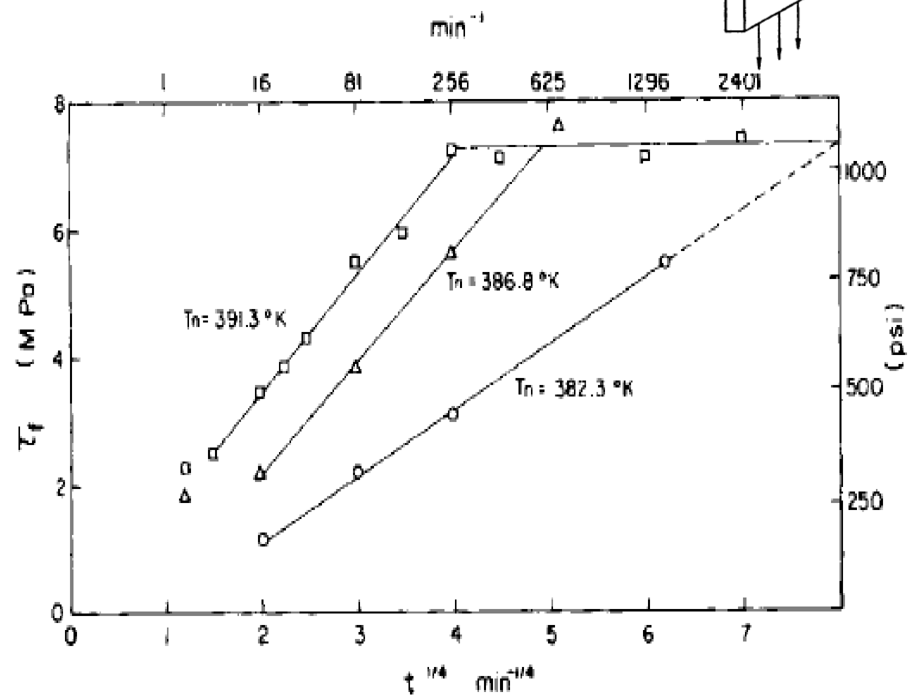


Time Dependence of the Maximum Shear Stress before Failure

- $t^{1/4}$ scaling law in the intermediate regime
- After chain scission sets in, σ_{max} saturates towards the bulk value
- Agree with the experimental results by the *Lap-Shear Joint Method*





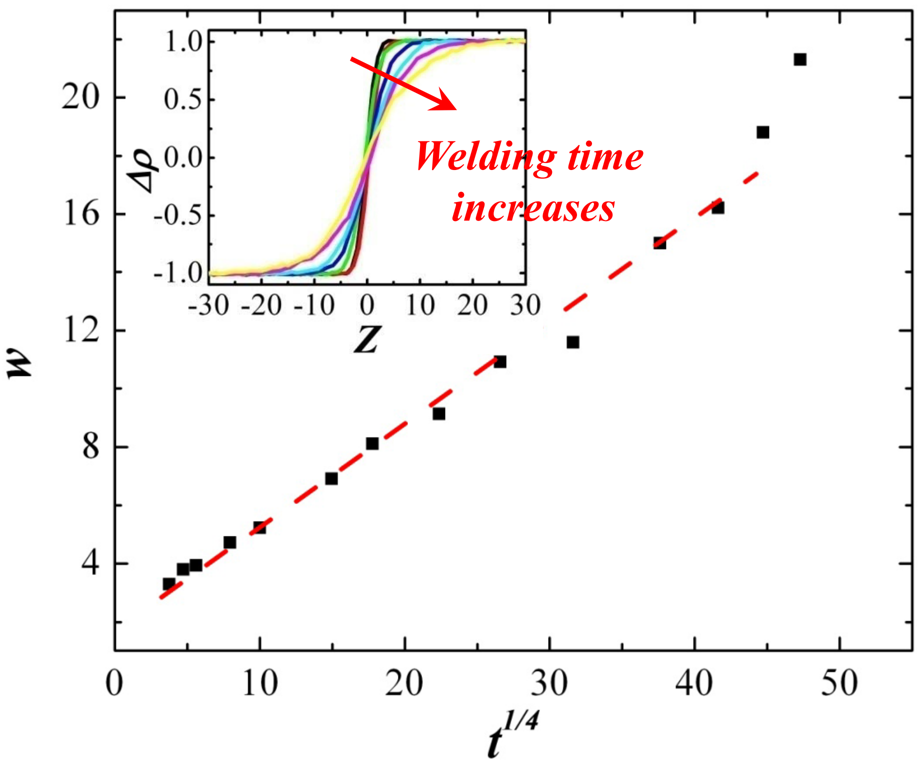


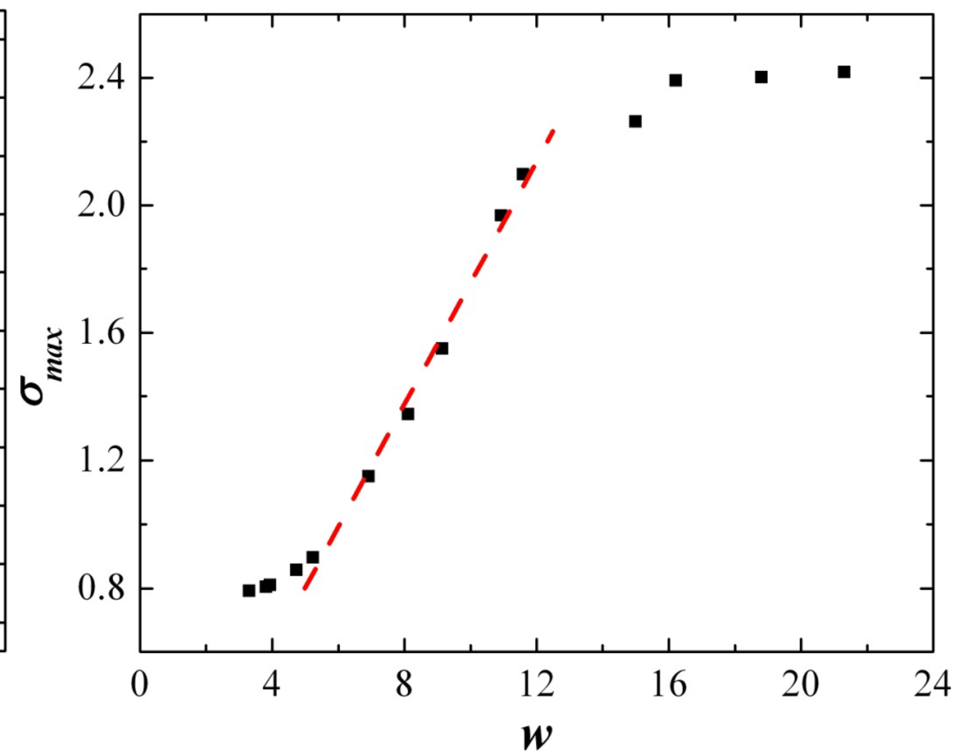
D.B.Kline & R.P.Wool (1988)

σ_{max} Correlates with Interfacial Width before Saturation

- **$t^{1/4}$ scaling law of the interfacial width w**
  w is obtained by fitting the initial density difference profiles using $tanh(2z/w)$
  Consistent with theoretical predictions based on reptation dynamics

- **Before saturation, σ_{max} correlates well with w**

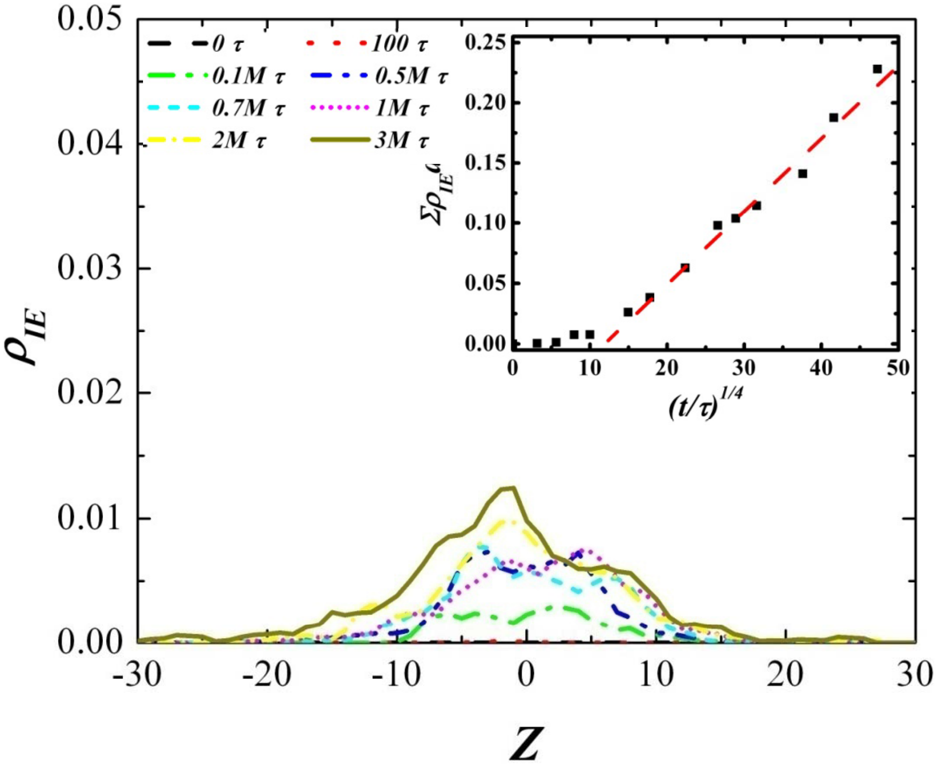




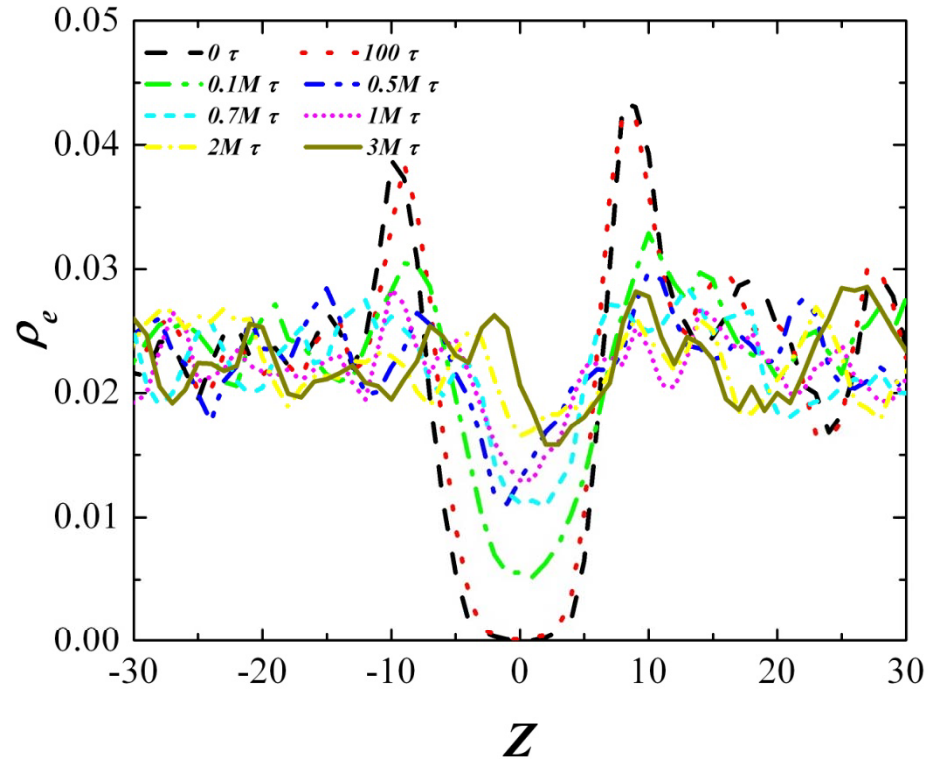
σ_{max} Correlates with Integrated Interfacial Entanglement Density Saturates as Entanglement Density Profile Approaches the Bulk Result

- **Interfacial Entanglements (IEs) form between chains from the opposite sides**
  $\Sigma\rho_{IE}$ obeys $t^{1/4}$ scaling law
- **Bulk shear strength is fully recovered when entanglement density ρ_e equals its bulk value**

Entanglements between chains from opposite sides



Entanglements between chains from any side



Conclusions

Power law dependence of interfacial shear strength on welding time

- σ_{max} rises with welding time as $t^{1/4}$, in agreement with experiment and theory of reptation dynamics.

- At small t , the interface fails via pullout of chain ends.
  At large t and for the bulk, shear failure is through chain scissions.

Correlation of interfacial strength with interfacial structure

- σ_{max} correlates with the interfacial width w and $\Sigma\rho_{IE}$ and both increase as $t^{1/4}$.

- The crossover to bulk strength coincides with the evolution of ρ_e to its bulk distribution.