Double Dynamics for Design of New Responsive Polymer Networks and Gels

ESR12: Modelling the linear dynamics of Double Dynamics Polymer Networks

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1 **Personal information**

2 **Long-term work: ESR12**

1. Personal information

Educational Background

M.E. Degree in Materials Science and Engineering, Chongqing University, 09/2012- 06/2015

B.E. Degree in Material Forming and Control Engineering, Qingdao University of Technology, 09/2008-06/2012

Employment and Experience

Lab Technician (Supervised by Dr. Quan Chen), Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, 06/2017-05/2018

Technical Engineer, Shanghai Volkswagen Automotive Co., Ltd, 07/2015-07/2016

Intern, Gree Electric Appliances Co., Ltd-Chongqing Branch, 10/2012-01/2014

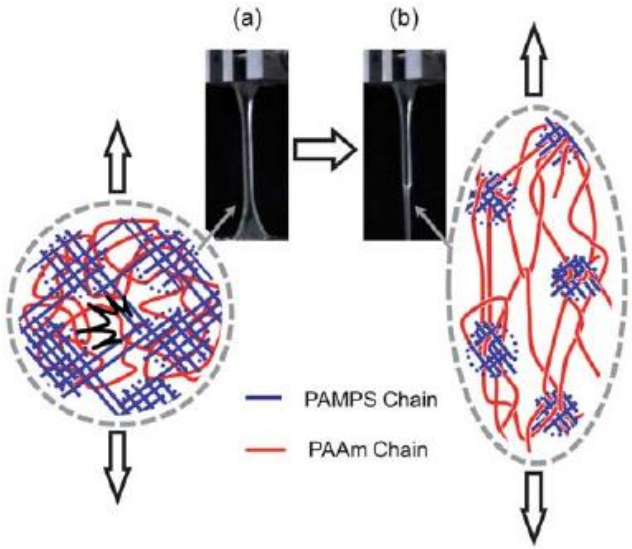
2. Long-term work: ESR12

Highly crosslinked and stretched

Plays the role of "Sacrificial minority network"

Second "Majority" network offers large deformability

Coherence of the overall structure



Major limitation

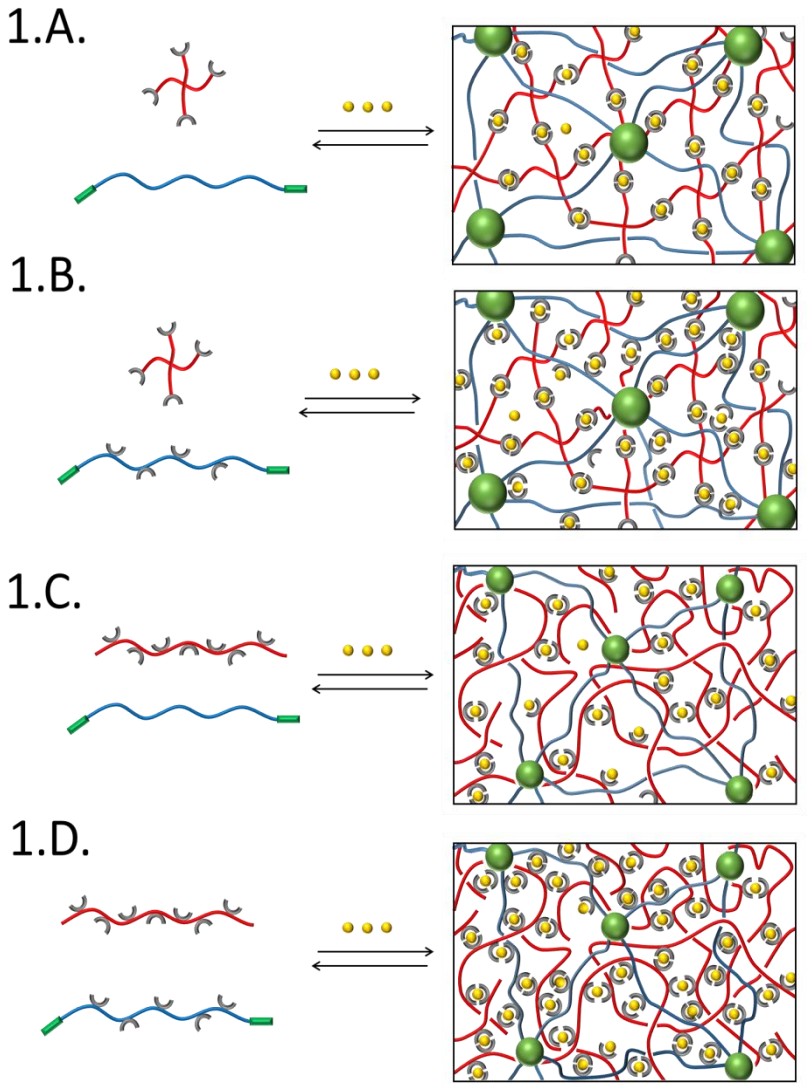
The first network is permanently damaged under external deformation field, due to irreversible scission of covalent crosslinks, which limits theirs improved stiffness to the first loading.

Replace the Covalent bonds of the stiff network by reversible bonds.

DDNs relies on a combination of metal-ligand interactions, phase separation and entanglements.

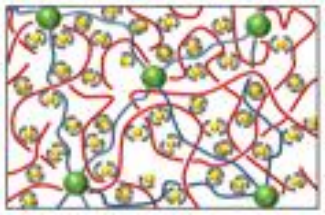
A first network, with short lifetime, will be composed of telechelic star polymers or long linear polymers bearing side groups (red chains in systems 1.A-D), crosslinked by metal-ligand interactions (symbol (•)).

The other network with long lifetime, will be based on the phase separation of ABA triblock copolymers (blue chains in systems 1.A-D). The outer (A) blocks of the triblocks will be chosen so as to ensure very strong and stable associations, whereas their middle block (B) will be very long (entangled) in order to provide a large extensibility.



Objective:

During the project, cooperating with other partners, I will investigate and model the linear dynamics of DDNs, in order to push this concept towards material design.



main characteristics

(1) composition and architecture of the building blocks

(2) lifetime of the interactions

(3) degree of interpenetration

(4) type of interactions between the sub-networks, etc.

Systematically varied to understand their influence on DDN structure and dynamics.

In order to model the viscoelastic behavior, I will **start from the tube model developed at UCL** to predict the properties of supramolecular entangled polymers. My main contribution will be to extend it to an entangled polymer network governed by two different supramolecular dynamics.

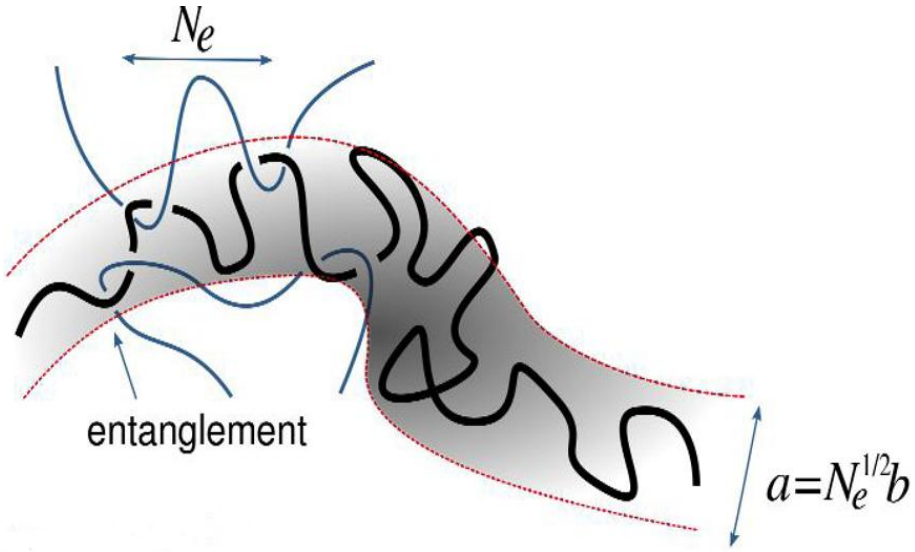
The beginning work plan:

1. Bibliographic research and elaboration of a tube model for describing the rheology of linear entangled polymers: A comprehensive literature review is required about the dynamics of entangled supramolecular polymers and about the properties of DDNs. Meanwhile, I will receive a training on tube models and will prepare my own code, based on the expertise of our group.

2. Rheometry: I will measure specific sets of samples, which will help understanding the influence of their composition parameters. Determining the statistical composition of the sticky chains.

3. Modelling: I will work on developing a model to determine the rheology of entangled sticky chains, and including the sticker dynamics in my tube model. Determining a strategy to describe my experimental data. If necessary, new samples will be designed in order to answer specific questions that need to be addressed for the modelling part.

Tube model



Polymer chain confined by entanglements to a tube-like region of diameter a, spanned by a random walk of entanglement length N_e.

Metallo-supramolecular polymers: Tube-based Time marching algorithm (TMA) model

Tube theory for classical polymers

- Rouse model to entangled chains
- Reptation mechanism of de Gennes
- Contour length fluctuation (CLF)
- Constraint release (CR)

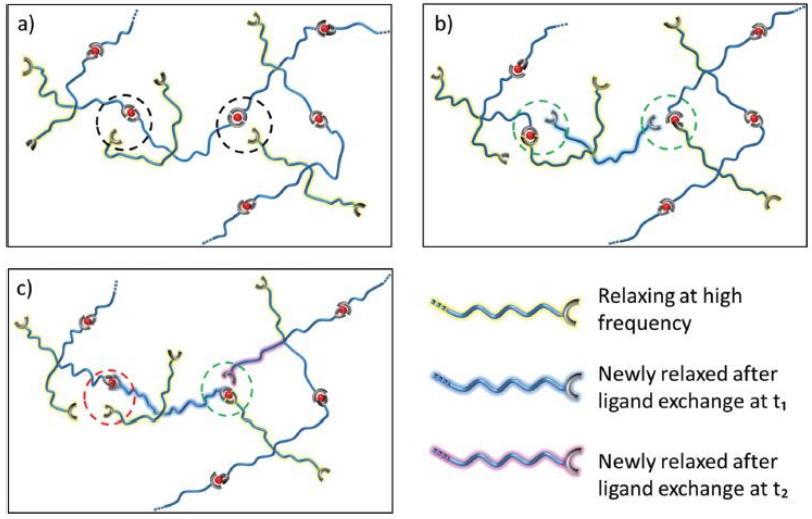


FIG. 4. Schematic representation of ligand exchange mechanism on telechelic star polymers (a) at $t=0$, (b) at $t=t_1$, and (c) at $t=t_2>t_1$.

Metallo-Supramolecular polymer

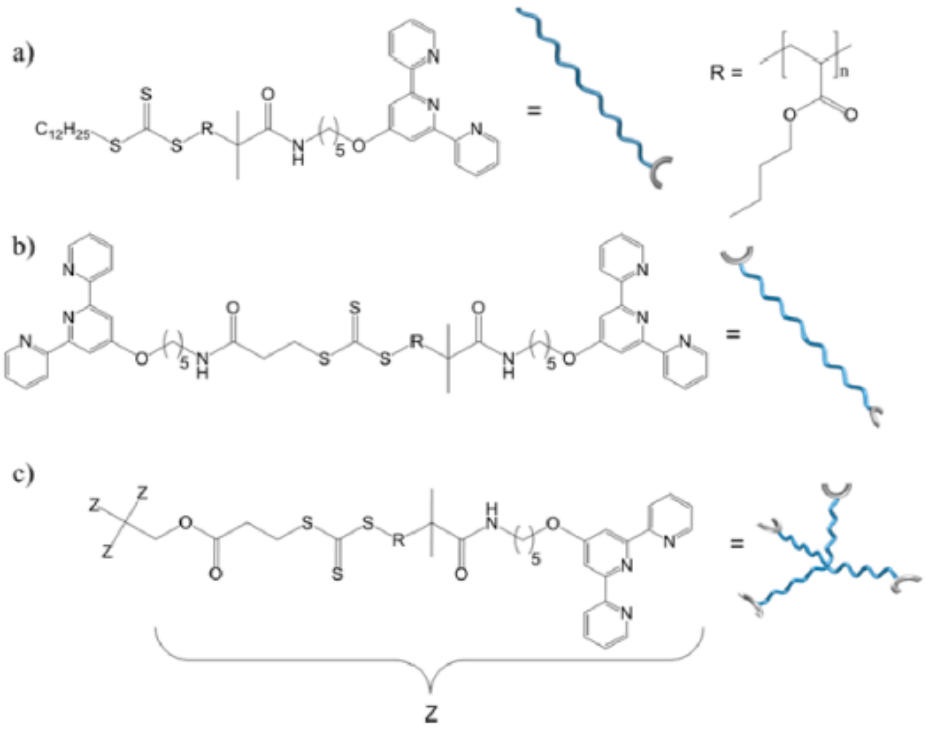


Figure 1. Chemical structures of (a) linear monofunctional P*n*BA end-functionalized with terpyridine (P*n*BA-tpy), (b) linear bifunctional P*n*BA-tpy$_2$, and (c) four-arm star P*n*BA-tpy$_4$.

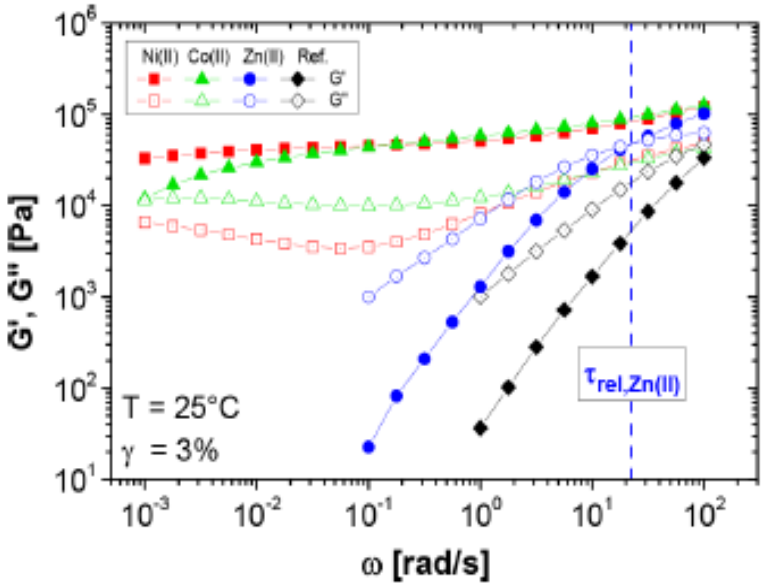
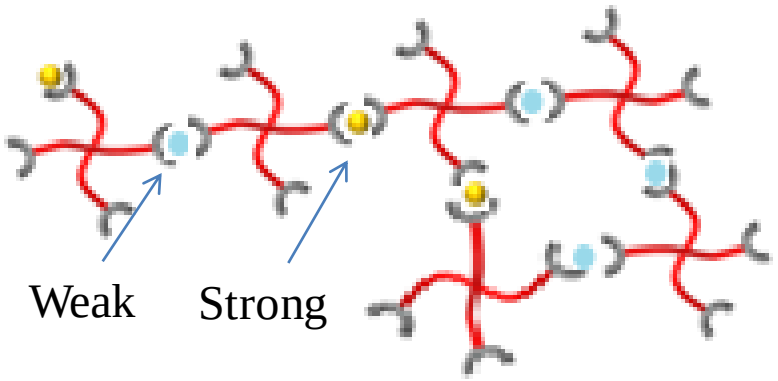
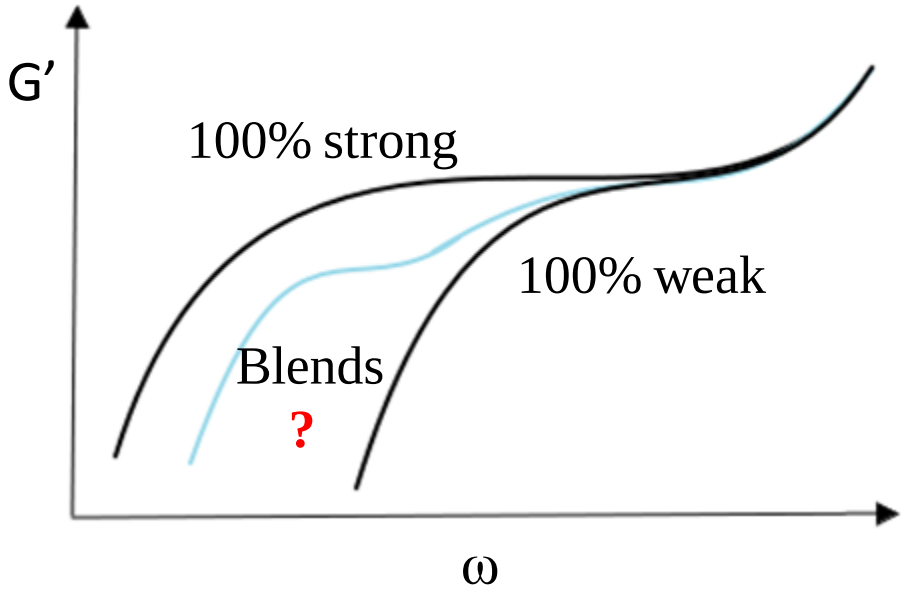


Figure 9. Linear rheology curves at 25 °C of four-arm star P*n*BA-tpy$_4$ (melts) with different transition metal ions. The diamonds correspond to the reference polymer without metal ions. The storage modulus G' is represented by filled symbols and the loss modulus G'' by unfilled symbols.

Different transition metal ions: Zn^{2+} , Cu^{2+} , Co^{2+} , Ni^{2+}

1. To blend two different ions in the same sample





Stability: $Zn^{2+} < Cu^{2+} < Co^{2+} < Ni^{2+}$

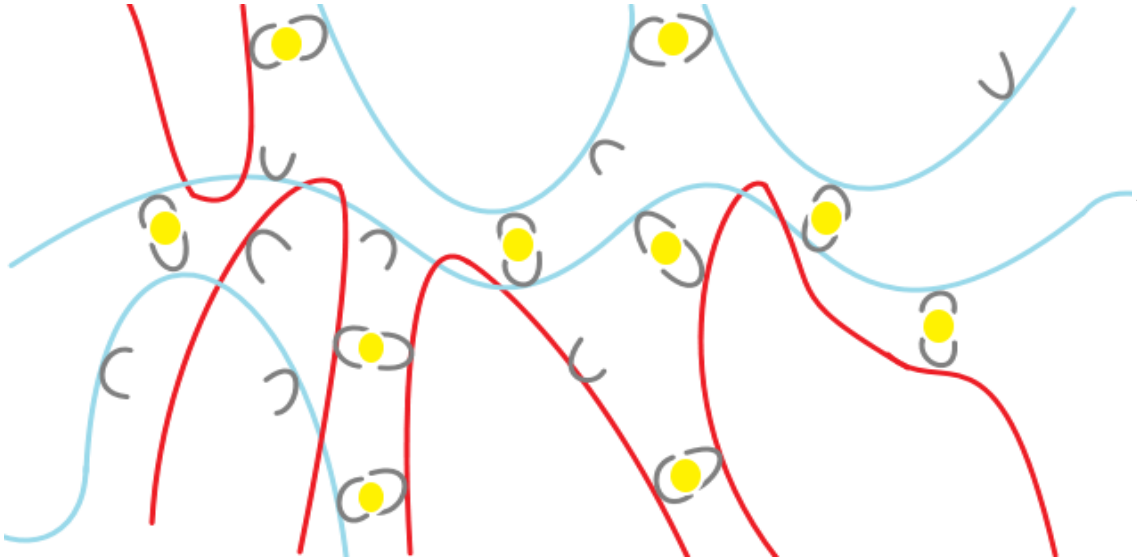
To investigate the influence of the blends with various ratios on the rheological behavior, and determine specific contribution to the viscoelastic properties.

To study the effect of external stimuli such as shear and temperature on the dynamic responses of the blends.

2. The linear sticky chains

A central idea in this project is chain entanglement dynamics:

Chain entanglement can couple two polymer networks and to bridge broken parts of a network. Moreover, these topological crosslinks allow maintaining elasticity even after the individual transient bonds along the chains are dissociated, and thus promote slow recovery, since the topological network still percolates the whole sample. This may strongly affect material extensibility and responsiveness.



To investigate the linear viscoelasticity of the linear sticky chains based on metallo-supramolecular networks.

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Thanks for your attention!