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Resolving Properties of Polymers and Nanoparticle Assembly through Coarse-Grained Computational Studies

Gary S. Grest

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Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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Resolving Properties of Polymers and Nanoparticle Assembly through Coarse-Grained Computational Studies

Gary S. Grest
Center for Integrated Nanotechnologies
Sandia National Laboratories
P. O. Box 5800
Albuquerque, New Mexico 87185-MS1303

Abstract

Coupled length and time scales determine the dynamic behavior of polymers and polymer nanocomposites and underlie their unique properties. To resolve the properties over large time and length scales it is imperative to develop coarse grained models which retain the atomistic specificity. Here we probe the degree of coarse graining required to simultaneously retain significant atomistic details and access large length and time scales. The degree of coarse graining in turn sets the minimum length scale instrumental in defining polymer properties and dynamics. Using polyethylene as a model system, we probe how the coarse-graining scale affects the measured dynamics with different number methylene groups per coarse-grained beads. Using these models we simulate polyethylene melts for times over 500 μs to study the viscoelastic properties of well-entangled polymer melts and large nanoparticle assembly as the nanoparticles are driven close enough to form nanostructures.

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NOMENCLATURE

Abbreviation	Definition
CG	Coarse Grained
LAMMPS	Large Atomic Molecular Massive Parallel Simulator
MSD	Mean Squared Displacement
OPLS-AA	All Atom Optimized Potentials for Liquid Simulations
PE	Polyethylene
PDI	Polydispersity Index

1. INTRODUCTION

Polymer properties depend on a wide range of coupled length and time scales, with unique viscoelastic properties stemming from interactions at the atomistic level. The need to probe polymers across time and length scales to capture polymer behavior makes probing dynamics, and particularly computational modeling, inherently challenging. With increasing molecular weight, polymer melts become highly entangled and the long-time diffusive regime becomes computationally inaccessible using atomistic simulations with the time scale for a chain to move its own size becoming orders of magnitude greater the shortest time scales even for modest molecular weight polymers. While the largest length scales of polymer dynamics are controlled by entanglements, the shortest time and length scales required to resolve dynamic properties are not obvious. This knowledge is critical for developing models that can transpose atomistic details into the long time scales needed to model long, entangled polymer chains.

One path to overcoming the computational challenge of large time and length scales in polymers and polymer nanocomposites is to coarse grain (CG) the polymer, reducing the number of degrees of freedom and increasing the fundamental time scale. The effectiveness of this process depends on retaining the smallest length scale essential to capturing the polymer dynamics. The process of coarse graining amounts to combining groups of atoms into pseudoatom beads and determining the bead interaction potentials. Simple models like the bead-spring model[1-2] capture the main characteristics of polymers, but disregard atomistic details, they cannot quantitatively describe properties like structure, local dynamics, or densities. Numerous recent studies have worked to bridge the divide between atomistic and coarse models, developing new approaches to drive computational studies to larger length and time scales while maintaining relevant sub-nanometer details. However none of these studies have explored, as done here, the effect of varying the degree of coarse-graining on the properties of entangled polymer melts and polymer nanocomposites.

Here, using linear polyethylene as a model system, the effects of the degree of coarse-graining on macromolecular structure and dynamics were probed.[2-4] The backbone of polyethylene (PE) consists of -CH_2– methylene groups, which are a natural coarse-graining unit. Figure 1 illustrates how the CG models with λ=2-6 methylene groups per CG bead represent an underlying atomistic configuration. Though the chemical structure of PE is simple, it is a thermoplastic material useful in a large number of applications, with tunable mechanical properties determined by the degree of branching. Using these CG models, we are able to capture polymer chain dynamics for long entangled polymers for time scales greater 500 μs using models that accurately represent atomistic detail. Accessing these large length and time scales, which are simply not accessible using fully atomistic models, allows us to measure a wide range of properties from the single chain dynamics to the stress relaxation function and shear viscosity which depend on a hierarchy of length and time scale.

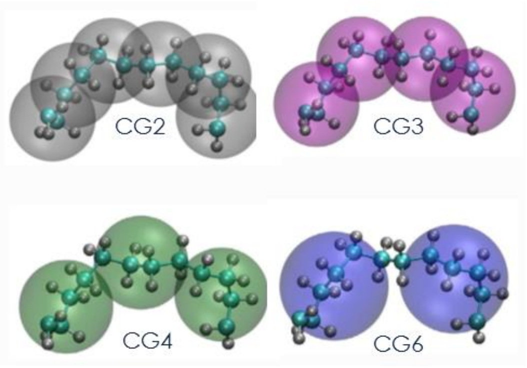

Figure 1. $C_{12}H_{24}$ segment of a PE chain represented with degree of coarse graining λ=2, 3, 4, and 6 methylene groups per CG bead. The bead diameter corresponds to the position of the minimum in the nonbonded interaction for each CG model.

2. MODEL AND METHODOLOGY

Each of the CG potentials was derived from a fully atomistic molecular dynamics simulation of a melt of C_nH_{2n+2} with n=96 at 400 or 500 K for λ=2, 4, 4 and 6 and n=95 for λ=5.[2-4] The atomistic simulations used the All Atom Optimized Potentials for Liquid Simulations (OPLS-AA) potential[5-6] with modified dihedral coefficients.[7] These modified OPLS-AA parameters reproduce the experimental static and dynamic chain properties for long alkanes better than the original OPLS-AA parameters. Tabulated CG angle and bond potentials were determined by Boltzmann inversion of the atomistic bond and angle distributions. Tabulated nonbonded potentials, shown in Figure 2, were determined by iterative Boltzmann inversion.[8] The intermolecular radial distribution function from the atomistic simulation was used as the target for iteration of the nonbonded potentials. The CG6 model has a surprisingly large equilibrium bond distance relative to the bead diameter. Therefore, a modified soft segmental repulsive potential[9] was added between CG beads to inhibit chain crossing for λ=6. Complete details of the model and methodology are given in Salerno et al.[2-3] and Peters et al.[4] along with plots of the two-body bond potentials, the three-body angle potentials and comparisons of the intermolecular radial distribution functions from the atomistic simulations and coarse grained simulations.

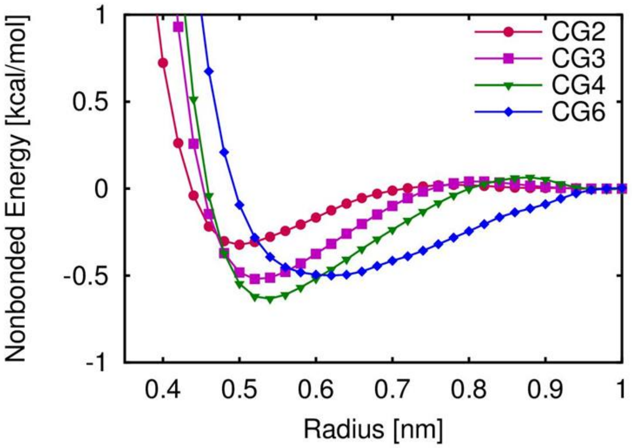

Figure 2. Potentials for nonbonded interactions for λ = 2-6.

One important feature of the CG models is that by eliminating the finest degrees of freedom, CG models allow a significantly larger time step than atomistic models. We found that one can use a time step δt = 20 fs for CG4, 5 and 6, 10 fs for CG3, and 2 fs for CG2, compared to 1 fs for the atomistic model. The reduction in the number of degrees of freedom in a system also creates a smoother free-energy landscape compared with fully atomistic simulation. We[2] have shown strong frictional and stochastic forces can be used to slow down the dynamics of the CG model to match those of the atomistic. Alternatively, one can take advantage of this increase in dynamics for the CG model to simulate effectively longer time scales.[10-11] While the former approach may be useful for coarse graining small molecules, for entangled polymers which already have inherently slow dynamics, this additional speed up for CG models is very advantageous. Combing the reduction in the number of atoms that one has to simulate, the significant larger simulation time steps and the increase in the dynamics from the smoother free energy surface, the effective simulation time is effectively increased by at least three orders of magnitude for $\lambda \geq 4$, allowing one to reach times scales not accessible using fully atomistic simulations.

All of the simulations were performed using the Large Atomic Molecular Massive Parallel Simulator (LAMMPS) molecular dynamics code developed at Sandia.[12-13]

3. RESULTS

3.1. Polymer Melts

In Salerno et al.,[2-3] we probed the dynamics of polymers as the number of atoms included in a CG bead is varied from λ=2 to 6. We found that independent of the degree of coarse graining, all static and dynamic properties are essentially the same once the dynamic scaling factor α and non-crossing constraint for λ=6 are included. Using these coarse grained models, we were able to reach times greater than 500 μs, allowing us to measure a number of quantities which can be compared directly to experiments, including the stress relaxation function, plateau modulus and shear viscosity. Here some examples of your results are presented to illustrate the power of the coarse graining methodology to example times and length scales not accessible by atomistic simulations while retaining chemical specificity. See Salerno et al.[2-3] and Peters et al.[4] for additional results. Some new results on modeling polydispersed melts will also be presented.

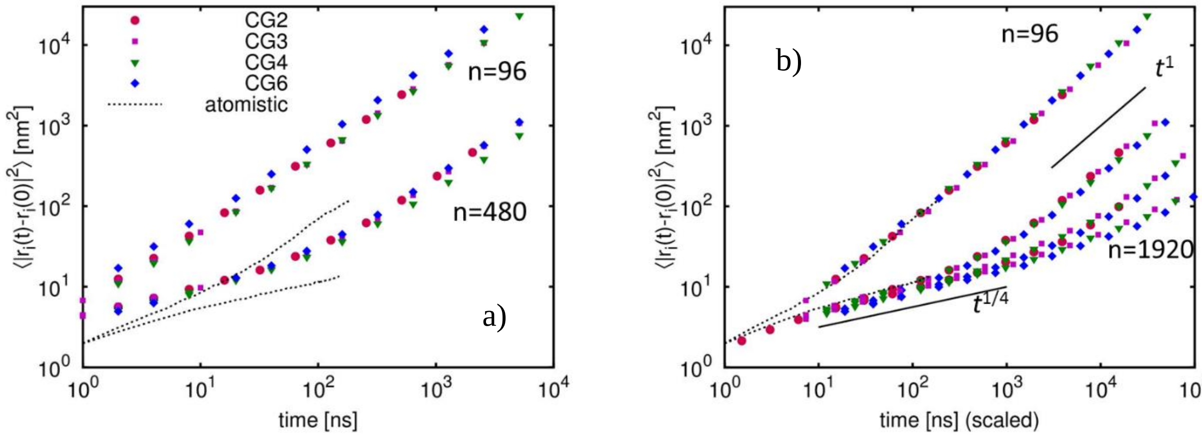

Figure. 3. (a) Mean squared displacement of the inner 24 -CH2- groups of each polymer chain at 500 K. (b) Same data as in (a), scaled by dynamic rescaling factor α. The solid lines represent the scaling predictions t^1 for the diffusive regime and $^{t1/4}$ for the reptation regime.

Coarse graining reduces the number of degrees of freedom in a system, creating a smoother free-energy landscape compared with fully atomistic simulations. This can be seen by measuring the mean squared displacement (MSD) for the atomistic model of PE with n=96 and 480 carbons to the equivalent CG model as shown in Figure 3(a). The mobility of the chains in the CG models is clearly larger than in atomistic simulations. By scaling the time for each of the CG models we create a single collapsed curve for each chain length for both the atomistic and CG data as shown in Figure 3(b). Notably, a single scaling factor α is required to collapse atomistic and CG data for each model, independent of chain length. For T = 500K, α varied from 6-9 for λ=2-6.[3] As seen in Fig. 3(b), the MSD has reached the diffusive regime where MSD $\sim t^1$ even for the longest chain length n = 1920. Over intermediate time scales, the chains show the expected $t^{1/4}$ scaling predicted theory.[14] These results demonstrate that one can capture long time and length scales with CG models while accounting for atomistic details. The MSD of the center of mass was then measured to test the scaling factor α. We[3] found that the MSD of the chain center of mass for chain lengths n = 96, 480, 960, and 1920 scaled by the same α as the monomer MSD, producing an excellent collapse. Not surprisingly, α is temperature-dependent.[4] For high T ≥ 500K, α is only weakly temperature-dependent but increases as temperature is reduced. For example for λ=4, α=6.2 for

T=500K and increases to ~12 at 400 K. This increase in α as t decreases is very advantageous in modeling entangled polymers near the glass transition, as the relaxation time diverges exponentially**.**

The stress response function after a small perturbation G(t) is one of the most important experimental measurements for polymers. For long entangled polymers, at short times G(t) decays as the chains locally relax in response to the perturbation like any fluid. However for intermediate times G(t) plateaus at G_O^N= ρRT/M_e where M_e is the entanglement molecular weight. This plateau region in G(t) occurs for intermediate times where the chains are assumed to move in a tube due to entanglements from the other chains. Only after the chains have reached the diffusive regime, does G(t) relax to zero. For polyethylene, the experimental values for G_O^N=1.6–2.5MPa, corresponding to Me of 1300–2000 g/mol.[15-16] The relaxation modulus for each of our CG models was measured for different chain lengths via equilibrium stress autocorrelations.[2-4] Figure 4 shows G(t) for n=1920 and 2560 for λ=4, where time has been scaled by the dynamic rescaling factor α. As clearly seen, the chains are long enough to show a clear plateau with a plateau modulus G_O^N ~ 2.4MPa, consistent with experiment. For comparison the longest chain systems we could study using fully atomistic simulations is n =480 which is not long enough to observe a plateau in G(t).

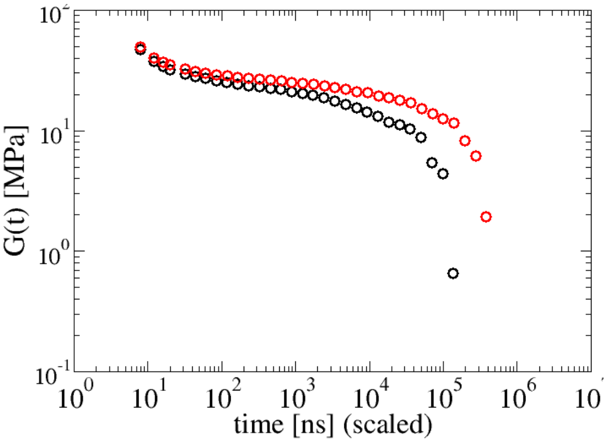

Figure 4. Stress autocorrelation function G(t) for λ = 4 at 500 K for n = 1920 (black) and 2560 (red).

Using non-equilibrium molecular dynamics simulations we measured the shear viscosity η as a function of shear rate over a wide range of shear rates from the shear independent regime at low shear rates to the shear thinning regime at high shear rates. Results for η versus scaled shear rate for n=96 to 1920 are presented in Salerno et al.[2] Our results for the zero shear rate viscosity η showed a crossover from a n^1 power law for small n to $n^{3.4}$ for large n at n_c ~ 250 or molecular weight ~ 3500 g/mol in excellent agreement with the experiment.[17-18]

While most studies of polymer melts model a homopolymer in which all the chains have the same length or at most a binary mixture of two lengths, experimental systems are never monodispersed. They are highly polydispersed with a range of chain lengths. The standard way to characterize polydispersity is the polydispersity index (PDI) defined PDI=M_w/M_n, where M_w is the weight average molecular weight and M_n is the number average molecular weight. M_n is more sensitive to molecules of low molecular mass, while M_w is more sensitive to molecules of high molecular mass. The best case experimentally for long polymers is PDI ~1.02 but in some cases PDI >2. Even for PDI ~ 1.02, the ratio of the largest to shortest chain is larger than 2. How polydispersity effects the chain mobility and viscoelastic response is difficult to predict theoretically and makes testing theoretical models, which are assume that the system is monodispersed, challenging.

Using our coarse grained model with λ=4, we have initiated a study of the effect of polydispersity on polymer chain mobility and viscoelastic properties. We built polydispersed systems of 2000 chains for PDI=1.02, 1.04 and 1.08 and 400 chains for PDI=1.16 for highly entangled chains of molecular weight Mw = 35,840 (n=2650 CH_2 monomers or 640 CG beads).

This chain length was chosen since it is long enough for the chains to be well entangled but short enough that the system fully relaxes on the time scales accessible to simulations (~500-600μs). Results for the mean squared displacement of the center monomers $g_1(t)$ and center of mass $g_3(t)$ for a monodispersed system (PDI=1.0) and three values of polydispersity PDI=1.04, 1.08 and 1.16 are shown in Figure 5. For short times the monomers in the center of the chain diffuse the same independent of the degree of polydispersity. However for longer times the MSD of the more polydispersed samples move faster. Unlike experiment, simulations can be used to extract more detailed information of how the various chain populations diffuse. For example the average diffusion constant of all of the chains as well as the shortest and longest can be readily determined as shown in Figure 6. As PDI the spread in the diffusion constant increases very rapidly with increasing PDI. While the diffusion constant for the longest chains decreases by a factor of 3 for PDI=1.16 compared to the monodispersed case PDI=1.0, the diffusion constant increases by a factor of 12 for the shortest chains. The average value of D increases by a factor of 2 over this range. By being able to follow chains of different individually we expect to be able to obtain new insight that is not accessible experimentally. The results of this study including data for the viscoelastic response G(t) are currently in preparation.

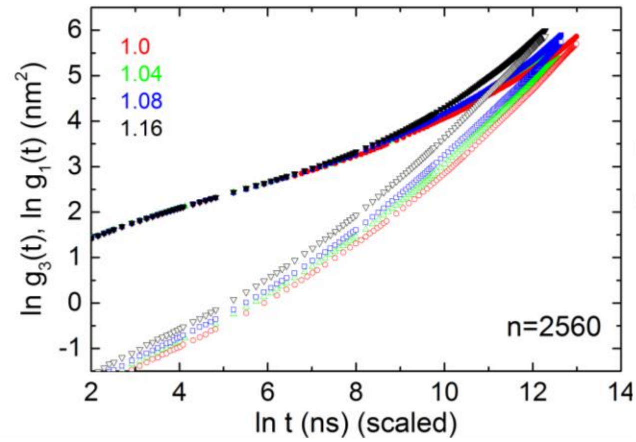

Figure 5. Mean squared displacement of the center 5 CG beads $g_1(t)$ (solid) and center of mass $g_3(t)$ (open) for 4 values of the polydispersity index (PDI) for n = 2560.

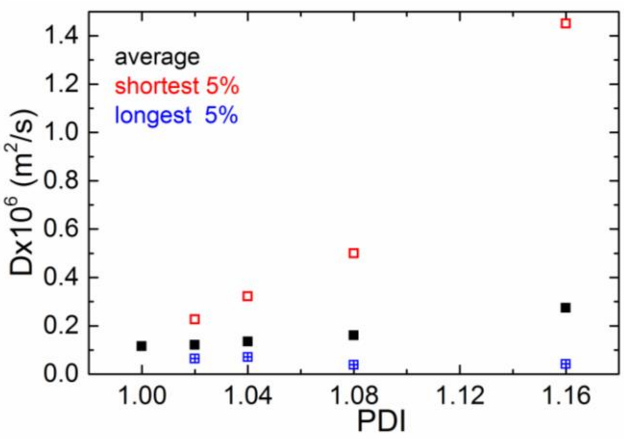

Figure 6. Diffusion constant D for polyethylene at 500K as function of PDI. Diffusion constant for the shortest 5% of the chains (red), longest 5% of the chains (blue) and average over all chains (black).

3.2. Nanoparticle Assembly

For long entangled polymers, it is clear from the results shown in previous section that one can incorporate a large number of atoms into a coarse grained bead and retain the chemical specificity of the polymer while modeling large systems for long times. However it is less clear what is the optimum length to model chains of length of tens carbons instead of hundreds or thousands as for entanglement polymers. One application in which is important is in modeling alkanethiol coated gold nanoparticles where the attached ligands are typically of order 10-18 carbons in length. These systems are of particular interest since alkanethiol coated nanoparticles, which self-assembly at room temperature into an ordered fcc lattice, at high, uniaxial strain, can be form gold nanowire or nanosheets.[19-21] However a number of question remain regarding how the formation of these nano structures depend on the nanoparticle size and shape and length and binding energy of the attached ligands.

Due to limitation on computational resources, fully atomistic simulations which are ideally suited to address these questions are too costly and time consuming, to span the wide range of relevant parameter space. It is currently possible to model only a few, selected systems atomistically. Hence the coarse graining approach outlined in the previous section is a promising approach since they are computationally much more efficient yet retain the chemical specificity of the system. Here we present some of our results for modeling alkanethiol coated nanoparticle assemblies.

We have built both fully atomistic and coarse grained models for 6 nm diameter gold nanoparticle with $HS(CH_2)_{11}CH_3$ attached. The details of the atomistic simulations can be found in Salerno et al.[22] The coarse grained systems are built in a similar manner except that the gold core is treated as a single large sphere and the ligand are modeled as in previous section with $\lambda=2$, 3 or 4 methylene groups per coarse grained bead. The nanoparticles are then assembled into an fcc array as illustrated in Figure 7 for the fully atomistic system and $\lambda=2$ and equilibrated at constant pressure for 10 ns. We then compressed the systems and measured the stress as a function of strain as shown in Figure 8.

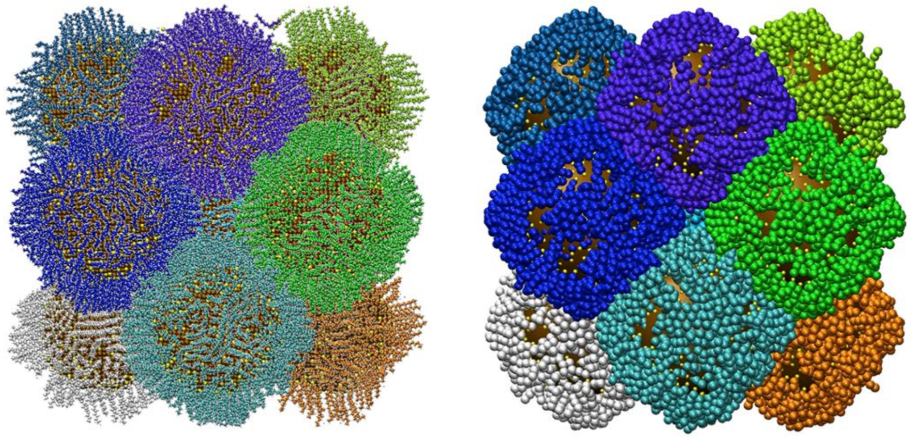

Figure 7. fcc array of 6 nm diameter alkanethiold gold nanoparticles with ligands of length 12 carbons for fully atomistic (left) and coarse grained model with $\lambda=2$ (right).

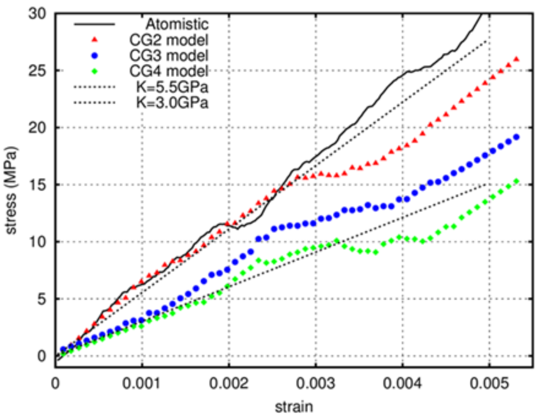

Figure 8. Comparison of stress strain for atomistic and CG models with $\lambda=2$, 3 and 4 at 1 atm. Dashed lines correspond to bulk modulus of 3.0 and 5.3 GPa.

As seen in Figure 8, the lowest degree of coarse graining reproduces the stress strain behavior of the fully atomistic system very well, while higher degrees of coarse graining under estimate the bulk modulus. The CG model with $\lambda=2$ agree well with the fully atomistic model for other properties including the lattice spacing versus pressure. We are currently applying the CG2 to study arrays of nanoparticles of diameter 4-12 nm for chain lengths of 12 and 18 carbons and comparing the results to experiment. Though for these systems we are restricted to a lower degree of coarse graining than for polymers, the computational speedup is of order 200 times that of the fully atomistic model.

4. CONCLUSIONS

Here we probed the structure and dynamics of polymers as the number of atoms included in a coarse grained bead. We have shown that for long, entangled polymers, independent of the degree of coarse graining, all static and dynamic properties are essentially the same once the dynamic scaling factor α and non-crossing constraint for λ=6 are included. Due to the larger time step and reduced number of degrees of freedom of the coarse grained model as well as the smoother free energy surface, the coarse grained simulations are effectively 3-4 orders of magnitude faster than the fully atomistic model, depending on the degree of coarse graining and the temperature.[2-4] Of the five models studies, λ=4 and 5 offer the optimum performance since larger degrees of coarse graining require an additional non-crossing constraint which negates the gain in effective speed due free pairwise interactions. The combination of increased time step, reduced number of degrees of freedom and dynamic scaling due to smoother free energy surface, translates to simulation times of hundreds to thousands of μs, which allows us to measure a number of quantities which can be compared directly to experiments, including the stress relaxation function, plateau modulus and shear viscosity. With this speedup, one can readily extend the present study to longer chains as well as including short and long chain branching in addition to the study of polydispersed systems.

For nanoparticle assemblies in which the attached ligands are much shorter, the optimum degree of coarse graining is λ=2. Larger degrees of coarse graining significantly underestimate the mechanical response of the system and overestimate the degree of compression as the pressure is increased. However even with λ=2, the increase of computational efficiency is significant, approximately 3 orders of magnitude compared to fully atomistic simulations, allowing us to explore a much large parameter space. Such coarse graining approaches are the only feasible way to study nanoparticles larger than 6-8 nm.

REFERENCES

1. Kremer, K.; Grest, G. S., Dynamics of entangled linear polymer melts: A molecular-dynamics simulation. *J. Chem. Phys.* **1990,** *92*, 5057-5086.

2. Salerno, K. M.; Agrawal, A.; Peters, B. L.; Perahia, D.; Grest, G. S., Dynamics in entangled polyethylene melts. *European Physical Journal Special Topics* **2016,** *225*, 1707-1722.

3. Salerno, K. M.; Agrawal, A.; Perahia, D.; Grest, G. S., Resolving Dynamic Properties of Polymers through Coarse-Grained Computational Studies. *Physical review letters* **2016,** *116*, 058302.

4. Peters, B. L.; Salerno, K. M.; Agrawal, A.; Perahia, D.; Grest, G. S., Coarse Grained Modeling of Polyethylene Melts: Effect on Dynamics. *Journal of Chemical Theory and Computation* **2017,** *13*, 2890-2896.

5. Jorgensen, W. L.; Madura, J. D.; Swenson, C. J., Optimized Intermolecular Potential Functions for Liquid Hydrocarbons. *Journal of the American Chemical Society* **1984,** *106*, 6638-6646.

6. Jorgensen, W. L.; Maxwell, D. S.; TiradoRives, J., Development and testing of the OPLS all-atom force field on conformational energetics and properties of organic liquids. *Journal of the American Chemical Society* **1996,** *118*, 11225-11236.

7. Siu, S. W.; Pluhackova, K.; Böckmann, R. A., Optimization of the OPLS-AA force field for long hydrocarbons. *Journal of Chemical Theory and Computation* **2012,** *8*, 1459-1470.

8. Müller-Plathe, F., Coarse-graining in polymer simulation: from the atomistic to the mesoscopic scale and back. *ChemPhysChem* **2002,** *3*, 754-769.

9. Sirk, T. W.; Slizoberg, Y. R.; Brennan, J. K.; Lisal, M.; Andzelm, J. W., An enhanced entangled polymer model for dissipative particle dynamics. *Journal of Chemical Physics* **2012,** *136*, 134903.

10. Harmandaris, V. A.; Kremer, K., Dynamics of Polystyrene Melts through Hierarchical Multiscale Simulations. *Macromolecules* **2009,** *42* (3), 791-802.

11. Fritz, D.; Koschke, K.; Harmandaris, V. A.; van der Vegt, N. F.; Kremer, K., Multiscale modeling of soft matter: scaling of dynamics. *Physical Chemistry Chemical Physics* **2011,** *13*, 10412-10420.

12. Plimpton, S., Fast parallel algorithms for short-range molecular dynamics. *J. Comp. Phys.* **1995,** *117*, 1-19.

13. LAMMPS molecular dynamics package. lammps.sandia.gov.

14. de Gennes, P.-G., Reptation of a polymer chain in the presence of fixed obstacles. *The Journal of chemical physics* **1971,** *55*, 572-579.

15. Raju, V.; Smith, G.; Marin, G.; Knox, J.; Graessley, W., Properties of amorphous and crystallizable hydrocarbon polymers. I. Melt rheology of fractions of linear polyethylene. *Journal of Polymer Science Part B: Polymer Physics* **1979,** *17*, 1183-1195.

16. Fetters, L. J.; Lohse, D. J.; Milner, S. T.; Graessley, W. W., Packing length influence in linear polymer melts on the entanglement, critical, and reptation molecular weights. *Macromolecules* **1999,** *32*, 6847-6851.

17. Ferry, J. D., *Viscoelastic properties of polymers*. John Wiley: 1980.

18. Graessley, W.; Edwards, S., Entanglement interactions in polymers and the chain contour concentration. *Polymer* **1981,** *22*, 1329-1334.

19. Wu, H.; Bai, F.; Sun, Z.; Haddad, R. E.; Boye, D. M.; Wang, Z.; Huang, J. Y.; Fan, H., Nanostructured Gold Architectures Formed through High Pressure-Driven Sintering of Spherical Nanoparticle Arrays. *J. Am. Chem. Soc.* **2010,** *132*, 12826-12828.

20. Wu, H.; Bai, F.; Sun, Z.; Haddad, R. E.; Boye, D. M.; Wang, Z.; Fan, H., Pressure-Driven Assembly of Spherical Nanoparticles and Formation of 1D-Nanostructure Arrays. *Angew. Chem. Int. Ed.* **2010,** *49*, 8431-8434.

21. Li, B.; Bian, K.; Lane, J. M. D.; Salerno, K. M.; Grest, G. S.; Ao, T.; Hickman, R.; Wise, J.; Wang, Z.; Fan, H., Superfast assembly and synthesis of gold nanostructures using nanosecond low-temperature compression via magnetic pulsed power. *Nature communications* **2017,** *8*, 14778.

22. Salerno, K. M.; Bolintineanu, D. S.; Lane, J. M. D.; Grest, G. S., Ligand structure and mechanical properties of single-nanoparticle-thick membranes. *Physical Review E* **2015,** *91*, 062403.

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