

CURRICULUM VITAE

Arindam Kundagrami

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DOB: March 31, 1973.

EDUCATION AND PROFESSIONAL EXPERIENCE

UNIVERSITY OF MASSACHUSETTS, Amherst, MA, USA

Postdoctoral Fellow (*Concentration: Theoretical Polymer Physics*) 2004-Present

Research Advisor: Murugappan Muthukumar

CHARGED POLYMERS - EQUILIBRIUM:

- Used equilibrium statistical mechanics to derive analytically the effective charge, and calculate numerically the phase boundaries and critical point of the first-order coil-to-globule transition of an isolated polyelectrolyte chain in poor solvent conditions. Used the concept to provide the underlying principle of solvent induced collapse (Experimental Collaborator: Manfred Schmidt's Lab., University of Mainz, Germany).
- Calculated using Edwards' variational theory the counterion distribution and chain configuration of flexible polyelectrolytes in presence of divalent salts. Demonstrated occurrence of charge reversal and first-order chain collapse due to multivalent ion-bridging.
- Studied the equilibrium properties (phase behaviors) of polyelectrolyte (synthetic and biopolymer) gels, their volume phase transitions in poor solvents or in the presence of multivalent salt ions.
- Established by numerical solution the validity of Edwards' variational theory as compared to the first principle self-consistent field theory (SCFT) of polymer solutions.

CHARGED POLYMERS - KINETICS:

- Studied solvent diffusion in polyelectrolyte gel swelling, and the time-dependence of reaction-diffusion fronts in model photoresists. In relation, studied the constitutive equation of stress relaxation and displacement vector diffusion in non-reactive polar solvents (Experimental Collaborator: Vivek Prabhu's Lab., NIST, USA).
- Developed numerical programs involving moving boundary conditions in non-trivial geometries to calculate temperature diffusion and related volume changes in polymeric materials.

POLYMER CRYSTALLIZATION:

- Proposed a continuum kinetic model of an entropic barrier recovering rate-limiting features of both nucleation and diffusion control for polymer crystal growth in both melts and solutions.

UNIVERSITY OF PENNSYLVANIA, Philadelphia, PA, USA

Ph.D in Physics (Concentration: *Theoretical Soft-matter Physics*)

1997-2003

Ph.D Advisor: Tom Lubensky

THESIS: Structure of TGB_C phases near the upper critical twist k_{c2}

- Calculated using generalized Abrikosov vortex lattice theory the detailed nature of smectic and director ordering in twist-grain-boundary-C (TGB_C) phases in liquid crystals, and the nature of transitions to them from the cholesteric phase. [<http://theory.pse.umass.edu/members.html#Arindam>]

INDIAN INSTITUTE OF SCIENCE, Bangalore, India

M.S in Physics (Concentration: *Non-equilibrium Statistical Physics*)

1994-1997

M.S Advisor: Chandan Dasgupta

THESIS: Generic Scale Invariance and Multiscaling

- Demonstrated using computer simulations the presence of extended self-similarity (ESS) and multi-exponent scaling (“multiscaling”) in height fluctuations in atomistic surface growth models.

PRESIDENCY COLLEGE (CALCUTTA UNIVERSITY), Kolkata (Calcutta), India

B.Sc (Honours) in Physics

1991-1994

- Pass subjects: Mathematics and Chemistry.

PUBLICATIONS

In preparation:

- **Arindam Kundagrami** and M. Muthukumar. “Super-diffusion in a model of polymer photoresist swelling”, *in preparation*.
- Jing Hua, **Arindam Kundagrami** and M. Muthukumar. “Polyelectrolyte gel collapse by divalent counterions”, *in preparation*.
- **Arindam Kundagrami** and M. Muthukumar. “Kinetics of osmotic-stress relaxation in polyelectrolyte gels: role of counterions in elasticity”. *in preparation*.

Communicated:

- Jing Hua, **Arindam Kundagrami** and M. Muthukumar. “Charge regularization in phase separating polyelectrolyte solutions”, *submitted to The Journal of Physical Chemistry Letters (under review)*.
- **Arindam Kundagrami**, Rajeev Kumar, and M. Muthukumar. “Simulations and Theories of Single Polyelectrolyte Chains”, invited contribution, edited by P. Gujrati, WILEY-VCH Verlag, Weinheim, Germany.
- **Arindam Kundagrami** and M. Muthukumar. “Effective charge and coil-globule transition of a polyelectrolyte chain”, *submitted to Macromolecules (under review)*.

- Rajeev Kumar, **Arindam Kundagrami**, and M. Muthukumar. “Counterion adsorption on flexible polyelectrolytes : a comparison of theories”, *Macromolecules* **42**, 1370 (2009).
- Peter Loh, Roshan Deen, Doris Vollmer, Karl Fischer, Manfred Schmidt, **Arindam Kundagrami**, and Murugappan Muthukumar. “The collapse of linear polyelectrolyte chains in a poor solvent: When does a collapsing polyelectrolyte collect its counter ions?”, *Macromolecules* **41**, 9352 (2008).
- **Arindam Kundagrami** and M. Muthukumar. “Theory of competitive counterion adsorption on flexible polyelectrolytes : Divalent salts”, *The Journal of Chemical Physics*, **128**, 244901 (2008).
- **Arindam Kundagrami** and M. Muthukumar. “Continuum theory of polymer crystallization”, *The Journal of Chemical Physics* **126**, 144901 (2007).
- **Arindam Kundagrami** and Tom Lubensky. “The Structure of twist-grain-boundary-*C* Phases”, *Physical Review E (Rapid Communications)* **68**, 060703 (2003).
- **Arindam Kundagrami** and Chandan Dasgupta. “Multiscaling in discrete models of epitaxial growth”, *Physica A* **270**, 135 (1999).
- **Arindam Kundagrami**, Chandan Dasgupta, P. Punyindu, and S. Das Sarma. “Extended self-similarity in kinetic surface roughening”, *Physical Review E (Rapid Communications)* **57**, R3703 (1998).

RESEARCH INTERESTS (SUMMARY)

Current:

- Equilibrium statistical mechanics of counterion distribution and conformation of polyelectrolytes in the presence of monovalent and multivalent salts (role of ion-bridging) - in isolated chains, gels, brushes - application to complex formation problems (e. g., adsorption of protein on a polyelectrolyte), semi-flexible polymers (DNA compaction to toroids), and drug delivery (volume transition in gels). Further, kinetics in them starting from single-molecule level.
- Equilibrium and critical phase behaviors of polyelectrolyte gels.
- The nature of coil-globule transition in charged polymers, the role of charges and salt in affecting the order and degree of the transition and locations of the phase boundaries - the scope of the intermediate “pearl-necklace” phase.
- Kinetics of swelling and solvent diffusion in polyelectrolyte gels - role of physical stress relaxation (e. g., in polar solvents) and chemical reaction (e. g., for photoresists in aqueous-base developers) in setting time-scales.
- Polymer crystallization and application of the concept of entropic barrier in the ordering of protein crystals.
- Moving boundary problems in a diffusive system, and its application to soft-matter and biological processes.
- Physics of soft matter and the role of charges in biology.

Previous:

- Phase transitions, topological defects and chiral segregation in liquid crystals.
- Monte Carlo and Molecular Dynamics simulations in soft-matter (liquid crystal droplets) systems.
- Non-equilibrium dynamics of surface growth models.

CONSULTANCY

- Service to **Vistakon** (*Johnson and Johnson Limited, Jacksonville, Florida*):
(as part of commitment from M. Muthukumar's lab, University of Massachusetts, Amherst, USA)
 1. Provided, using moving boundary algorithms, a numerical scheme to assess volume change related to temperature diffusion in polymeric materials of arbitrary shape.
 2. Provided a first-principle based predictive computational tool to model the expansion and power of contact lenses when exposed to solutions of different thermodynamic features.

CONFERENCES AND SCHOOLS

- **American Physical Society - March meeting 2009**, Pittsburgh, PA, USA, March 16-20, 2009. *Physics of charged polymers: effective charge, size, and phase transitions* (oral presentation).
- **Fall Polymer Event 2008, Polymer Science and Engineering, University of Massachusetts**, Amherst, MA, USA, October 14-16, 2008. *Effective charge, collapse, and critical point of linear polyelectrolyte chains: Role of solvent quality and electrostatics* (poster presentation).
- **7th International Symposium on Polyelectrolytes - Polyelectrolytes 2008**, University of Coimbra, Coimbra, PORTUGAL, June 16-19, 2008. *The collapse of linear polyelectrolyte chains in a poor solvent: When does a collapsing polyelectrolyte collect its counter ions?* (poster presented by co-author).
- **American Physical Society - March meeting 2008**, New Orleans, LA, USA, March 10-14, 2008. *Theory of competitive counterion adsorption on flexible polyelectrolytes : Divalent salts* (oral presentation).
- **University of Massachusetts Amherst/University of Heidelberg Workshop, Modeling and Computation in Physics, Mathematics, and Biology**, Amherst, MA, USA, May 21-23, 2007. *Competitive counterion adsorption and charge reversal on a single flexible polyelectrolyte : Divalent salts* (poster presentation).
- **American Physical Society - March meeting 2006**, Baltimore, MD, USA, March 13-17, 2006. *The swelling and dissolution kinetics of polymer thin films* (oral presentation).
- **6-th National Graduate Research Conference**, University of Massachusetts, Amherst, MA, USA, June 15-17, 2005. *Theory of Lamellar Growth in Polymer Crystallization* (oral presentation).
- **American Physical Society - March meeting 2005**, Los Angeles, CA, USA, March 21-25, 2005. *Theory of Lamellar Growth in Polymer Solutions* (oral presentation).
- **American Physical Society - March meeting 2004**, Montreal, QC, CANADA, March 22-26, 2004. Attended.
- **American Physical Society - March meeting 2003**, Austin TX, USA, March 3-7, 2003. *Renn-Lubensky and Bordeaux TGB_C phases near the upper critical field h_{c2}* (oral presentation).
- **Boulder School for Condensed Matter and Materials Physics - 2002, The Physics of Soft Condensed Matter**, Boulder CO, USA, July 1-26, 2002. *The Structure of TGB_C phases near the upper critical field h_{c2}* (poster presentation).

- **American Physical Society - March meeting 2002**, Indianapolis IN, USA, March 18-22, 2002. *The dislocation lattice structure in the TGB_C phases near h_{c2}* (oral presentation).
- **International Conference on Statistical Physics - 2002, STATPHYS - KOLKATA-IV**, S. N. Bose National Centre for Basic Sciences, Kolkata (Calcutta), INDIA, January 14-19, 2002. *The dislocation lattice structure in the TGB_C phases near h_{c2}* (poster presentation).
- **Gordon Research Conferences, Liquid Crystals - 2001**, Colby-Sawyer College, New London NH, USA, June 24-29, 2001. *TGB_C phases near h_{c2}* (poster presentation).
- **American Physical Society - March meeting 2001**, Seattle WA, USA, March 12-16, 2001. *TGB_C phases near h_{c2}* (oral presentation).
- **International Conference on Statistical Physics - 1999, STATPHYS - KOLKATA-III**, S. N. Bose National Centre for the Basic Sciences, Kolkata (Calcutta), INDIA, January 4-9, 1999. Attended.
- **83d Statistical Mechanics Conference**, Rutgers University NJ, USA, May 2000. Attended.
- **Annual symposia on the Physics of Soft Materials**, Laboratory of Research for the Structure of Matter, University of Pennsylvania, Philadelphia, PA, USA 1998 - 2002. Attended.
- **10 Years of TGB Phase : A workshop**, University of Pennsylvania, Philadelphia PA, USA, April 22-24, 1998. Attended.

AWARDS AND HONORS

- **Research Fellowship**: Graduate Program, University of Pennsylvania (1998-2003).
- **Junior Fellowship**: Integrated Doctoral Programme, Indian Institute of Science, Dept. of Science and Technology (Govt. of India) (1994-1997).

COMPUTATION

Simulation:

- Large scale simulation on non-equilibrium dynamics of surface growth models.
- Simulated annealing (e. g., 2-d droplet of nematic molecules) using Monte-Carlo and Molecular Dynamics.

Numerical:

- Solution of diffusion equations in multiple dimensions with time dependent (moving) boundary conditions.
- Solution of nonlinear problems using numerical techniques (for example, multi-dimensional minimization).

TEACHING EXPERIENCE

- **Teaching Assistant**: Dept. of Physics and Astronomy, Univ. of Pennsylvania (1997-1998).
- **Lab Instructor**: Phy101 (Mechanics) - Fall 1997, Phy151 (Electricity and Magnetism) - Spring 1998, Dept. of Physics and Astronomy, Univ. of Pennsylvania.

Reviewer

- Journal of Chemical Physics

Professional Memberships

- American Physical Society (APS) - since 1998.

REFERENCES

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