Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Theory of Activated Relaxation in Nanoscale Confined Liquids STEPHEN MIRIGIAN, KENNETH SCHWEIZER, University of Illinois Urbana-Champaign — We extend the recently developed Elastically Cooperative Nonlinear Langevin Equation(ECNLE) theory of activated relaxation in supercooled liquids to treat the case of geometrically confined liquids. Generically, confinement of supercooled liquids leads to a speeding up of the dynamics(with a consequent depression of the glass transition temperature) extending on the order of tens of molecular diameters away from a free surface. At present, this behavior is not theoretically well understood. Our theory interprets the speed up in dynamics in terms of two coupled effects. First, a direct surface effect, extending two to three molecular diameters from a free surface, and related to a local rearrangement of molecules with a single cage. The second is a longer ranged "confinement" effect, extending tens of molecular diameters from a free surface and related to the long range elastic penalty necessary for a local rearrangement. The theory allows for the calculation of relaxation time and T_g profiles within a given geometry and first principles calculations of relevant length scales. Comparison to both dynamic and pseudo-thermodynamic measurements shows reasonable agreement to experiment with no adjustable parameters.

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Date submitted: 12 Nov 2013 Electronic form version 1.4