Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Supercoil Formation During DNA Melting[1] MEHMET SAYAR, BARIS AVSAROGLU, ALKAN KABAKCIOGLU, Koc University — Supercoil formation plays a key role in determining the structure-function relationship in DNA. Biological and technological processes, such as protein synthesis, polymerase chain reaction, and microarrays relys on separation of the two strands in DNA, which is coupled to the unwinding of the supercoiled structure. This problem has been studied theoretically via Peyrard-Bishop and Poland-Scheraga type models, which include a simple representation of the DNA structural properties. In recent years, computational models, which provide a more realtistic representaion of DNA molecule, have been used to study the melting behavior of short DNA chains. Here, we will present a new coarse-grained model of DNA which is capable of simulating sufficiently long DNA chains for studying the supercoil formation during melting, without sacrificing the local structural properties. Our coarse-grained model successfully reproduces the local geometry of the DNA molecule, such as the 3'-5' directionality, major-minor groove structure, and the helical pitch. We will present our initial results on the dynamics of supercoiling during DNA melting.

[1]Tubitak Grant No:108T553

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Date submitted: 21 Nov 2008 Electronic form version 1.4