Using Molecular Dynamics Simulations to Model the DC Electrical Behavior of Confined Layers

Nathan G. Beougher, Jason McIntosh, Jason A. Djuren, and M.W. Roth
Department of Physics
University of Northern Iowa
Cedar Falls, Iowa 50614 USA

Carlos Wexler
Department of Physics and Astronomy
University of Missouri
Columbia, Missouri 65211 USA

Carl Thurman
Department of Biology
University of Northern Iowa
Cedar Falls, Iowa 50614-0421 USA

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ABSTRACT

A Molecular Dynamics (MD) computer simulation is utilized to qualitatively understand the DC electrical conduction behavior of pentadecane ($C_{15}H_{32}$) layers confined between two graphite slabs as related to the dynamics of the layer. At low temperatures the patch remains together and perpendicular to the confining layers. Then, as temperature is increased, tilting of the molecules begins. The molecules tend to remain straight as they tilt with increasing temperature which, in our model, affects the capacitance somewhat but the resistance little. As temperature is increased further, the molecules exhibit gauche defects which accompany patch collapse. During patch collapse, the system shows dramatic changes in its calculated DC resistance and capacitance. Calculated specific capacitance values are in remarkable agreement with recent experimental measurements. Results for two different confining layer separations are discussed as well as future work related to lipid bilayer systems.

I. INTRODUCTION

Biological membranes are composed of a combination of proteins, carbohydrates, and lipids. These lipids form stable bilayer structures and are present in animal and plant matter. The structure of lipid bilayer membranes is typically comprised of varied head groups and hydrocarbon tails [1]. Of interest in studies of electrical properties of lipid bilayers are membranes which have highly polar head groups, due in part to the geometry of such bilayer systems solvated in water. The structure of lipid bilayer membranes lends itself to exhibiting two key DC electrical properties: capacitance and resistance. When constructed as a bilayer system, the polar head groups may be considered to be attached at opposite ends with the hydrocarbon chains stretching towards each other in the space between the opposing polar head attachments. Considering the distance between the placement of one layer of molecules and the respect to the placement of the other layer, a gap will likely exist between the hydrocarbon chains. The chains can be considered as tails of the molecules that contribute to the resistance of the system. In addition, the gap between the molecules must also contribute to the