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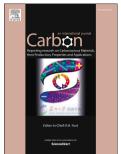
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Evaluation of wetting transparency and surface energy of pristine and aged graphene through nanoscale friction

Peng Gong^a, Zhijiang Ye^b, Lin Yuan^{a,1}, Philip Egberts^{a,*}

Abstract

Friction on few-layer graphene supported by $\mathrm{Si/SiO}_x$ and mica substrates was investigated using atomic force microscopy (AFM) and coordinated molecular dynamics (MD) simulations to examine friction hysteresis and wetting transparency. Experiments showed that graphene exhibited higher overall friction, as well as hysteresis, in high humidity conditions, while the hysteresis was not observed under dry conditions. Additionally, as samples were aged under ambient environmental conditions, the work of adhesion increased by an approximate factor of two, likely from oxidation of the surface or adsorption of oxygen containing species from the lab environment. When graphene was supported by mica substrates no significant friction hysteresis was observed. MD simulations showed similar influences to the friction forces with surface energy. Both experiments and simulations suggest that wetting transparency, or a small variation in surface energy resulting from varying the number of graphene layers, contributes to the layer dependent friction forces measured on graphene.

Keywords: atomic force microscope (AFM), graphene, molecular dynamics (MD) simulation, nanotribology, friction, wetting transparency

1. Introduction

Two-dimensional materials, specifically graphene, have promised to be a key component in a number of technological devices, including low-power flexible electronics [1], membrane separators in fuel cells [2], strength and conductivity additives for composite materials [3, 4], and extremely thin solid lubricants in microelectromechanical systems (MEMS) [5]. While widespread application of graphene in these materials is hindered by several factors, including large scale production of graphene, more basic questions related to the fundamental chemical, mechanical and physical properties of this material also limit widespread application of this material. While several experiments have demonstrated graphene to be the strongest material with respect to the in-plane modulus [6], the out-of-plane modulus has been reported to be much lower, which subsequently has implications on the usefulness of graphene as a tribological material [7]. Furthermore, the surface energy of graphene is a critical parameter required for the mixing of graphene into a composite material. Despite examination of this parameter in several studies, surface energy has been examined in a number of ways, including fracture mechanics experiments [8], atomic force microscopy (AFM) pull-off measurements [9], contact angle measurements [10, 11, 12, 13], and simulations [12, 11], and has resulted in significant scatter in the value. Finally, the quality of the produced films (defect density [14], number of domains [15], etc.), as well as the ability to control the thickness of few-layer-graphene (FLG) used in

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