Simulating the electrostatic interaction of charged thin films by the image charge method and soft computing techniques

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Abstract

Understanding the electric field effect in nanostructured thin films is a key issue in nanoscience nowadays [1]. Recently, single and Few Layer Graphene (FLG) has attracted much attention because of its atypical response to electrostatic fields, which is in sharp contrast with that expected for conventional conducting or semiconducting films [2]. It has been found that values of the dielectric constant that cannot be found in other materials can be easily distinguishable when the sample structure is a graphene-like thin film [3].

To understand the origin of this effect, we combine numerical methods and soft computing to simulate the electrostatic interaction between an EFM tip and a thin film. Soft computing techniques become very useful in this context when the EFM system is not fully defined and some parameters are free or unknown. Using the electrostatic force as input patterns to the ANN, we establish that the thin film sample and substrate can be replaced by a simple semiinfinite sample characterized by an effective dielectric constant. We show that, for typical EFM setups and thin film thicknesses around 1nm, the electrostatic interaction of thin films with ultrahigh dielectric constants is easily distinguishable. We find that, for these specific thin films, dielectric constants between 500 and 10000 give very different electric responses.

To improve the performance of the simulations and the understanding of the electrostatic interaction between thin film layers and metallic EFM tips, we have included a free charge density value to the thin film layer. With this improvement, we are able to study the effects and differences between a dielectric thin film and thin layers with small amounts of charge inside. This effect could be of great interest in the study of thin materials with a high polarizability such as graphene layers since their finite size effects could be understood and characterized by ultrahigh thin film dielectric constants or uniform free charge distributions at the surface.

References

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