MD simulation of nanoparticle transport induced by different mechanisms

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Abstract

Transporting an object from one place to another is a basic and ubiquitous activity in nature. How to manipulate or transport nanoscale objects accurately becomes an inevitable task nowadays, which is vitally important in both engineering and science of NEMS and bio-systems. Non-equilibrium molecular dynamic simulation is carried out in the present paper in order to disclose whether a nanoscale object could be driven by the strain gradient in substrates or by a sliding block moving under the substrate. An inspiring result is that a nanoscale flake on a graphene strip substrate would move spontaneously from the region with higher strain to the one with lower strain or transport from one side to the other side with a sliding block under the substrate. In the first case, we find that the potential energy difference induced by the strain gradient field in the graphene strip substrate can generate sufficient force to overcome the static and kinetic friction forces between the nano-flake and the strip substrate, resulting in the nanoscale flake motion in the direction of gradient reduction. In the second case, we find that as the sliding block moves under the graphene substrate, a driving force is yielded from the van der Waals interaction between the sliding block and the nanoparticle and a pre-tensioned graphene substrate could provide easier nanoparticle transport, based in which a novel nano-sieve can be designed to screen and classify nanoparticles of different sizes spontaneously. In both cases, many factors that will influence the transportation of nano-objects are studied systematically. Our findings may be useful for promising designs of nanoscale manipulation, classification, transportation and smart surfaces.

Keywords: Nanoparticle; Non-uniform field; Nano-transport; Nano-sieve

References

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