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A MOLECULAR DYNAMICS STUDY OF NANOWIRE RESONATOR BIO-OBJECT DETECTION

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This paper presents a comprehensive analysis, carried out by the molecular dynamics (MD) simulations, of the vibrations of silicon nanowire (SiNW) resonators, having diverse applications including biological and medical fields. The chosen approach allows us to obtain a better understanding of the nanowire (NW) materials' characteristics, providing a more detailed insight into the behavior of nanostructures, especially when the topic of interest is relevant to their dynamics, interatomic interactions, and atoms trajectories' prediction. We first simulate a SiNW to study its frequency of vibrations using MD simulations. Then, we add a molecule of human immunodeficiency virus as an example to investigate the potential of the SiNW resonator for the detection of tiny bio-objects. The developed technique and its application to the detection of tiny objects, such as viruses, are discussed in the context of several key effects pertinent to the design of SiNW.

Keywords: Vibrations; nanoscale biosensors; molecular dynamics simulations; virus molecules; silicon nanowires; bio-object detection.

1. Introduction

Molecular dynamics (MD) simulations enable studying nanomaterials' properties with comparable results to those obtained with experimental techniques with a dramatically increasing impact in many areas of biology and medicine.[1–3] MD simulations are the basis for developing essential techniques for the investigation of nanomaterials' dynamics. Based on MD simulations, we can obtain important information about interatomic interactions of nanomaterials and molecular complexes, along with the trajectories' prediction of millions of atoms in the targeted

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nanosystem.[4] Although MD simulations can assist in the analysis of nanoresonators for biological applications, it is time-consuming in comparison with continuum models, as it is the case for many other bio-applications at the nanoscale.[5,6] Nevertheless, the MD simulations of the silicon nanowire (SiNW) resonator can provide a deeper understanding of the dynamics of targeted nanosystems.

Two important approaches for the modeling of nanoresonators include continuum models and MD simulations. Continuum models require less computational effort and provide a relatively straightforward formulation, which can give a qualitative insight into the dynamic behavior of nanoresonators. On the other hand, continuum models neglect the structural discontinuities at the atomic scale, which is one of the intrinsic limitations of such models. This crucial limitation averts continuum models from providing more accurate results and accentuates the need for MD simulations in analyzing the vibration properties of such nanostructures. MD simulations can provide a reliable and precise insight into such properties. Indeed, among different techniques for simulations at the atomic level, MD has shown a great potential for vibration analysis of nanoresonators, and it is a potent tool for understanding mechanical behaviors of nanoscale systems.[1,7,8] Originally proposed by Alder and Wainwright to study the phase transition of hard spheres,[9] MD now is an advanced tool, which is commonly used for simulations of thousands of atoms, given appropriate computer facilities,[10] and has been applied to a wide range of nanoscience and nanotechnology applications.[11–19] It is being considered as a well-founded simulation technique that can be applied also to the systems with biological interactions and tiny nanoresonators.[10,20]

During the last decade, several types of simulation techniques have been developed based on MD for particular systems such as solvated proteins, protein–DNA complexes, RNA nanostructures, as well as lipid systems, graphene sheets, nanotubes, and nanowires (NWs).[1,7,21–29] For example, the application of a carbon nanotube for zeptogram-level mass detection has been explored by Joshi *et al.*[30] They used the molecular structural mechanics approach for investigating the dynamic responses of chiral single-walled carbon-nanotube-based nanobiosensors. They showed that single-walled carbon nanotubes can reach the high sensitivity characterized by the order of 0.12 zg/GHz.[30] Carbon nanotubes can also provide advanced capabilities for biological imaging and other medical applications.[31–36] In another work, Adhikari and Chowdhury[37] developed a mathematical framework for the use of graphene sheets in small mass sensing. They considered four different configurations for locating the small bio-objects and developed both MD and analytical simulations. The results of this paper indicate that the sensitivity of graphene sensors is in the order of gigahertz/zeptogram. Using MD simulations, Kwon *et al.*[38] showed the potential of graphene-nanoribbon-based resonators for yoctogram mass sensing. Properties of graphene nanoribbons were studied in details in Refs. 39–43. In another interesting work, Duan *et al.*[44] revealed the potential of pillared graphene as an ultra-high mass sensing. Employing MD simulations, they showed that pillared graphene can reach at least 10^{-24} g resolution. Recently, they have also shown the ultra-high

mass sensitivity and a very high quality factor of diamond-nanothread-based resonators by applying MD simulations.[45] Zheng *et al.* studied the vibration behavior of FeNWs with MD simulations.[46] In particular, the effect of different lengths and heights on the vibration properties of FeNWs was studied in their work.

In his recent work, Nasr Esfahani[47] has shown the effect of surface stress profile on the tensile properties of SiNWs through MD simulations considering fixed–fixed and fixed–free boundary conditions. It was demonstrated that compressive surface stress and torsional surface stress profiles result in an uniaxial expansion and a twist deformation of Si nanocantilevers, respectively. By using MD simulations, Zhang and Shou[48] showed that resonance frequencies of piezoelectric boron nitride (BN) nanosheets can be tuned using an external electric field. Observation of this phenomenon in BN nanosheets led to a conclusion that it can serve as a good building block for designing NEMS devices. Wang *et al.*[49] analyzed the mechanical behavior of *a*-axis gallium nitride (GaN) NWs under tension or compression loading until failure. Moreover, MD simulations were utilized to explore the mechanical behaviors of *a*-axis GaN NWs under axial loads. They showed that Young's modulus of *a*-axis GaN NWs increases significantly with decreasing cross-sectional size.

Very recently, a novel approach, based on a co-resonant mass detector, was proposed by Twiefel *et al.* to detect tiny masses.[50] They provided both theoretical and fabrication procedures in their study to identify added tiny mass to nanoresonators. Their results show the feasibility of combination of longitudinal and bending modes for the detection of the aforementioned purpose. In another very recent research, Xiang *et al.*[51] developed an analytical frequency model to quantitatively show how the detection sensitivity depends on the interactions between the nanoresonator-based sensor and the biochemical adsorbate measuring of elasticity and density.[51] Dilena *et al.*[52] have examined the effect of boundary conditions on the sensitivity of nanorods in mass detection. Their results provide a guideline for designing nanoresonators to detect tiny mass with high resolution.

In this paper, we use MD simulations to analyze interatomic interactions of SiNW in the targeted nanosystem. The use of MD simulations enables not only investigating the frequency behavior of NW resonators under different situations, but also providing a set of results to explore potency of the nanostructures considered here for the detection of tiny objects such as viruses. Accordingly, to demonstrate the application of SiNW resonators in detecting tiny masses such as biological objects, we simulate the SiNW resonator with a molecule of human immunodeficiency virus (HIV) located in the middle, considering clamped–clamped (CC) boundary conditions. In the next sections, we will discuss the modeling and simulation procedure of our considered nanoresonators.

2. Modeling and Simulation

In this study, a rectangular SiNW is simulated as shown in Fig. 1. With the use of a rectangular cross-section NW resonator, it is more practical to locate a molecule of