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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.

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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1   nanosystem.[4] Although MD simulations can assist in the analysis of nanoresonators
2   for biological applications, it is time-consuming in comparison with continuum
3   models, as it is the case for many other bio-applications at the nanoscale.[5,6] Never-
4   theless, the MD simulations of the silicon nanowire (SiNW) resonator can provide a
5   deeper understanding of the dynamics of targeted nanosystems.
6   Two important approaches for the modeling of nanoresonators include continuum
7   models and MD simulations. Continuum models require less computational effort
8   and provide a relatively straightforward formulation, which can give a qualitative
9   insight into the dynamic behavior of nanoresonators. On the other hand, continuum
10   models neglect the structural discontinuities at the atomic scale, which is one of the
11   intrinsic limitations of such models. This crucial limitation averts continuum models
12   from providing more accurate results and accentuates the need for MD simulations in
13   analyzing the vibration properties of such nanostructures. MD simulations can
14   provide a reliable and precise insight into such properties. Indeed, among different
15   techniques for simulations at the atomic level, MD has shown a great potential for
16   vibration analysis of nanoresonators, and it is a potent tool for understanding me-
17   chanical behaviors of nanoscale systems.[1,7,8] Originally proposed by Alder and
18   Wainwright to study the phase transition of hard spheres,[9] MD now is an advanced
19   tool, which is commonly used for simulations of thousands of atoms, given appro-
20   priate computer facilities,[10] and has been applied to a wide range of nanoscience and
21   nanotechnology applications.[11–19] It is being considered as a well-founded simulation
22   technique that can be applied also to the systems with biological interactions and
23   tiny nanoresonators.[10,20]
24   During the last decade, several types of simulation techniques have been devel-
25   oped based on MD for particular systems such as solvated proteins, protein–DNA
26   complexes, RNA nanostructures, as well as lipid systems, graphene sheets, nano-
27   tubes, and nanowires (NWs).[1,7,21–29] For example, the application of a carbon
28   nanotube for zeptogram-level mass detection has been explored by Joshi *et al.*[30] They
29   used the molecular structural mechanics approach for investigating the dynamic
30   responses of chiral single-walled carbon-nanotube-based nanobiosensors. They
31   showed that single-walled carbon nanotubes can reach the high sensitivity charac-
32   terized by the order of $0.12 \, \text{zg/GHz}$.[30] Carbon nanotubes can also provide advanced
33   capabilities for biological imaging and other medical applications.[31–36] In another
34   work, Adhikari and Chowdhury[37] developed a mathematical framework for the use
35   of graphene sheets in small mass sensing. They considered four different configura-
36   tions for locating the small bio-objects and developed both MD and analytical
37   simulations. The results of this paper indicate that the sensitivity of graphene sensors
38   is in the order of gigahertz/zeptogram. Using MD simulations, Kwon *et al.*[38] showed
39   the potential of graphene-nanoribbon-based resonators for yoctogram mass sensing.
40   Properties of graphene nanoribbons were studied in details in Refs. 39–43. In another
41   interesting work, Duan *et al.*[44] revealed the potential of pillared graphene as an ultra-
42   high mass sensing. Employing MD simulations, they showed that pillared graphene
43   can reach at least $10^{-24} \, \text{g}$ resolution. Recently, they have also shown the ultra-high

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

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

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

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

39
40 ## 2. Modeling and Simulation
41
42 In this study, a rectangular SiNW is simulated as shown in Fig. 1. With the use of a
43 rectangular cross-section NW resonator, it is more practical to locate a molecule of