

Multi-scale, multi-physics modeling of electrochemical actuation of Ni nanohoneycomb in water



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ARTICLE INFO

Article history:

Received 12 August 2016

Received in revised form 11 November 2016

Accepted 12 November 2016

Keywords:

Multiscale modeling

Electrochemical actuation

Nanohoneycomb nickel

Surface stress

Ni/water interface

ABSTRACT

Recent experiments have shown that a composite cantilever structure comprising a Ni nanohoneycomb active layer, backed by a solid constraining layer of Ni, can exhibit bending in an electrolyte environment when a voltage is applied across the cantilever and electrolyte. In this work, a multi-scale, multi-field simulation approach is used to model such an electrochemical actuation behavior. Specifically, molecular dynamics simulations with reactive force-field potentials and a modified charge-equilibrium (QEq) method are used to calculate the surface stress built up in Ni(1 0 0) surface in contact with water electrolyte due to a voltage applied across the interface, as a result of capacitive charging of the double layer in the contacting electrolyte as well as redox reaction of the Ni surface. The calculated surface stress is then used as input in a meso-scale finite-element (FE) model to compute the actuating stress set up in a single hexagonal unit cell of the Ni nanohoneycomb structure. The single-unit actuating stress is eventually used in a continuum FE model at a larger scale, to calculate the bending of an entire bilayered cantilever which replicates experimental conditions. The actuation deflection of the bilayered nanohoneycomb nickel is predicted to be 41.4 μm at 0.43 V vs the point of zero charge (PZC), which corresponds to ~ 0.48 V vs saturated calomel electrode (SCE), and this is in excellent agreement with the experimental value of 45–62 μm at a similar voltage vs SCE. This is the first successful attempt to simulate the electrochemical actuation of a real-sized, nano-porous metallic structure in an electrolytic environment.

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1. Introduction

In recent years, nano-porous metals with high surface-to-volume ratios show great promise as artificial muscles that can be electrochemically actuated to produce relatively large strain amplitudes at low triggering voltages, and yet unlike polymeric counterparts, they possess high stiffness and strength [1–11]. Earlier nano-porous metals exhibiting such electrochemical actuation behavior were noble metals including Au and Pt [1,3–7]. *Ab initio* studies were performed to study the relaxation behavior of electrically charged clean metal surfaces [12–14] in vacuum, and based on these results, multi-scale simulations were carried out to study the charge-induced deformation in nano-porous Au [15,16]. While these studies revealed that surface stress can be induced by charges accumulated in the surface atomic layers, experiments [17–19] have shown that ion adsorption on clean metal surfaces in contact with electrolyte or air (i.e. the double layer) can also sig-

nificantly modify the surface properties and thus induce surface stress.

Recently, in addition to noble metals as mentioned above, cheaper porous materials such as anodic alumina [8] and metallic Ni nanohoneycombs [10] were also found to exhibit similar electrochemical actuation behavior in electrolytic environments. In the case of Ni for which surfaces cannot be clean, experiments, as reviewed in Section 2 later, have indeed shown that the actuation in an electrolytic environment is dominated by faradaic charging involving a redox couple between the Ni(II) and Ni(III) states, in addition to a milder contribution by the non-faradaic mechanism of double-layer capacitive charging that would be the only mechanism for clean metallic surfaces. To model the actuation mechanism in Ni, there are at least two challenges involved: one is the multi-scale nature of the length scales involved in a real-sized nano-porous structure, and another is the multi-physics nature of the problem, involving redox electrochemistry, electric charge transfer, and mechanics.

In this work, we investigate the electrochemical actuation of Ni nanohoneycombs in water electrolyte [10] by a multi-scale, multi-physics simulation approach. While *ab initio* calculations can be

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used to study the surface stress of clean metal surfaces in vacuum, for the case of Ni, the involvement of surface redox reactions in contact with an electrolyte makes the problem practically intractable by *ab initio* approaches. More recently, reactive force-field potentials [20] and charge-equilibrium (QEq) methods [21] for molecular dynamics (MD) have been developed to simulate chemical reactions and solid/liquid interfaces [22,23]. The present work therefore makes use of such advanced MD methods to calculate the surface stress built up due to potential charging through contact with water electrolyte, with the chemical, electrical and mechanical aspects of the problem duly considered. Then, the surface stress is used in finite-element models of two different length scales to study the actuation behavior of a real-sized cantilever structure that replicates experimental conditions.

2. Review of experimental observations

Before the modeling work is described, it is useful to review the experimental observations [10] that the present simulations are aimed for. Fig. 1(a) shows the Ni nanohoneycomb structure which exhibited the actuating property, and the lower-magnification image in Fig. 1(b) shows the cantilever actuator which was composed of a layer of the nanohoneycomb structure in Fig. 1(a), on top of a solid layer of Ni which acted as the constraining layer. This bilayered structure of metallic Ni, with dimensions

10 mm × 3 mm × 3 μm (2 μm porous layer + 1 μm solid layer), was produced by a template electrodeposition process the details of which can be found in Ref. [10]. The actuation experiment setup is illustrated in Fig. 1(c). The bilayered Ni cantilever was immersed in 1 M NaOH electrolyte and an electric potential was applied to the sample with respect to saturated calomel electrode (SCE). In a scanning potential window of [−0.1, 0.5] V vs SCE, reversible actuation was observed at different scanning rates, and as shown in Fig. 1(d), the maximum displacement of the free end of the cantilever ranged from 45–62 μm depending on the potential scan rates [10]. Cyclic voltammetry measurements indicated that at large applied potentials in the range of 0.15–0.5 V vs SCE, the dominating actuation mechanism was a reversible faradic redox reaction of the Ni surface that leads to volume expansion on positive charging [10], while surface stress due to the non-faradic, capacitive charging/discharging of the double layer in the contacting electrolyte produced a milder contribution as indicated by the gray band in Fig. 1(d).

The experiments in Ref. [10] were carried out with the voltage applied with Ref. to the SCE, but in the simulations described below, applied voltages with Ref. to the “point of zero charge” (PZC) condition are more readily studied. A conversion between the SCE and PZC Refs. is thus needed. The potential at PZC for Ni/water interface was reported to be 0.05 V vs Ag/AgCl which corresponds to ~0.006 V vs SCE [24], and 0.33 V vs normal hydrogen electrode (NHE) which corresponds to ~0.089 V vs SCE [25]. The

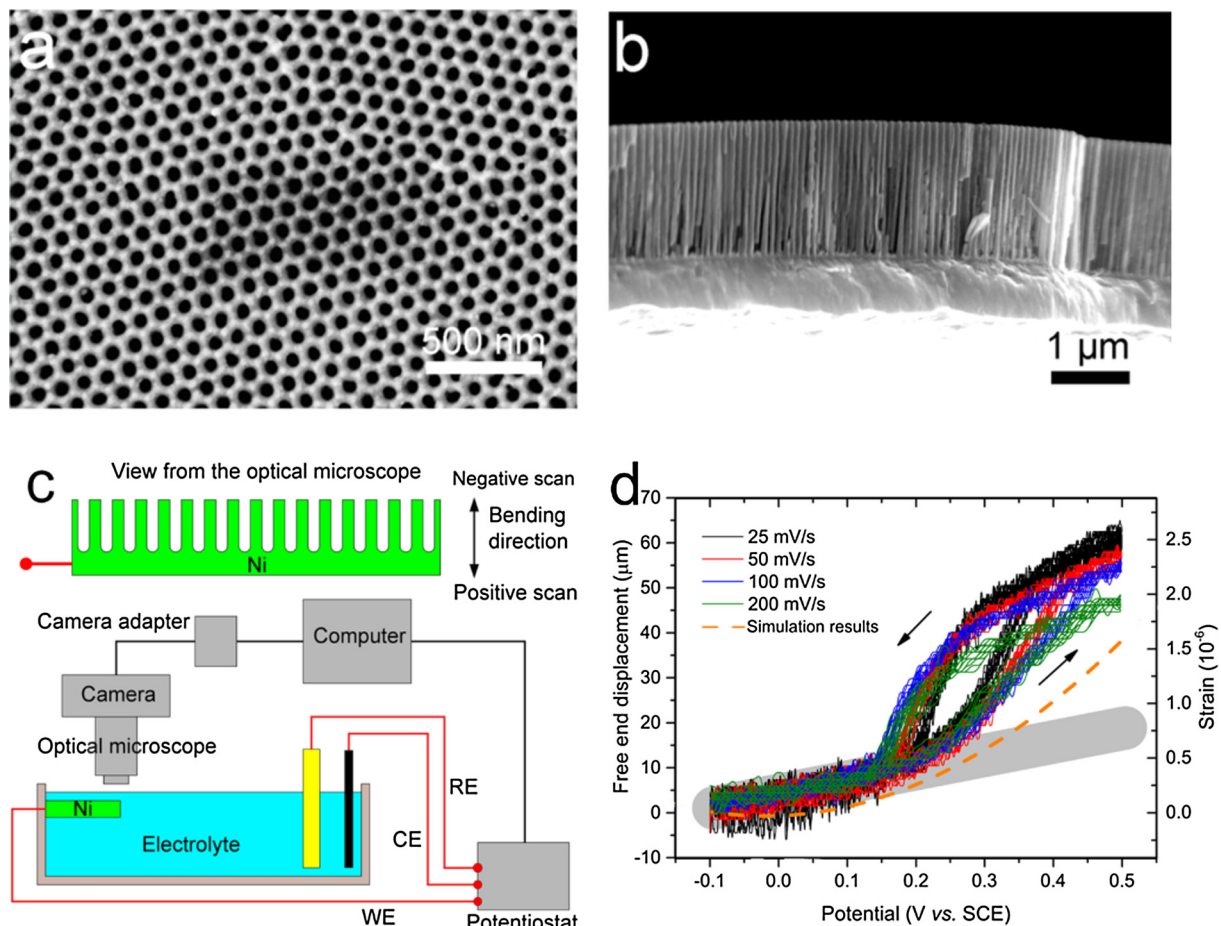


Fig. 1. (a) Top view of the nanohoneycomb Ni. (b) Cross-sectional view of the nanohoneycomb Ni supported by an underlying solid Ni layer. (c) Schematic of the setup in the actuation experiment. (d) Observed free-end displacement of the cantilever actuator against applied potential at different scan rates, with the trend marked by the gray band representing the potential contribution from surface stress due to capacitive charging/discharging of the double layer in the contacting electrolyte. Orange dashed line denotes simulated results. Experimental data adapted from Ref. [10]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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