THE CHARGE-INDUCED ACTUATION OF NANOPOROUS METALS

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Summary In this study we modified the embedded atom method by fitting the potential to the surface-stress-charge coefficient of Au(100) surfaces obtained from density functional theory (DFT) calculations. We use atomistic simulations to study the effect of cross-sectional size and the crystal orientation of the ligament on the stiffness and charge-induced strain of gold nanofoams having a gyroidal morphology.

INTRODUCTION

Experimental studies have shown that nanoporous metals can undergo considerable dimensional changes when a potential difference is applied [1]. The primary actuation mechanism is the electric double-layer charging of the internal surface in combination with a large surface to volume ratio. Charge is injected on the metal surface in an electrochemical environment, see Fig. 1. The induced charge changes the interatomic bond length on the surface, causing the metal to expand or contract macroscopically.

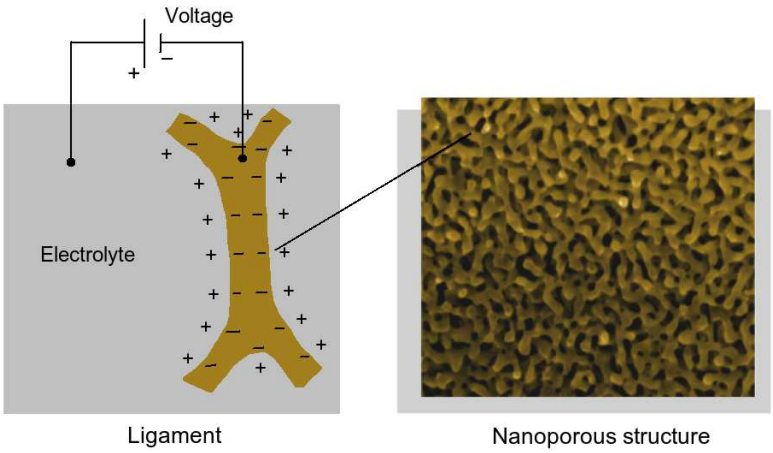

Figure 1: Electrochemical actuation of nanoporous gold.

ATOMISTIC MODEL AND RESULTS

We use atomistic potentials to model the charge-induced strain in gold. Experiments on gold nanoporous structures and DFT calculations [2] on gold surfaces have shown that the metal contracts when a negative charge is injected on its surface and expands with positive charge. In order to model this trend the embedding function of the embedded atom method is modified by adding an extra term to account for the excess charge. The modified potential is fitted to the surface-stress-charge coefficient of Au(100) surface, which is obtained from DFT calculations.

In this presentation, we will report on recent atomistic simulations in which we study the size-dependent stiffness and electrochemical actuation of nanoporous gold. First we explore the charge-induced deformation of a gold nanowire using atomistic simulations. Our simulations indicate that the actuation strain depends on the cross-sectional dimensions of the wire, the magnitude and sign of the charge, and the crystallographic orientation. The stiffness of the nanowires is dictated by the surface-stress-induced nonlinear effects of the core of the wire. We present a simple continuum model

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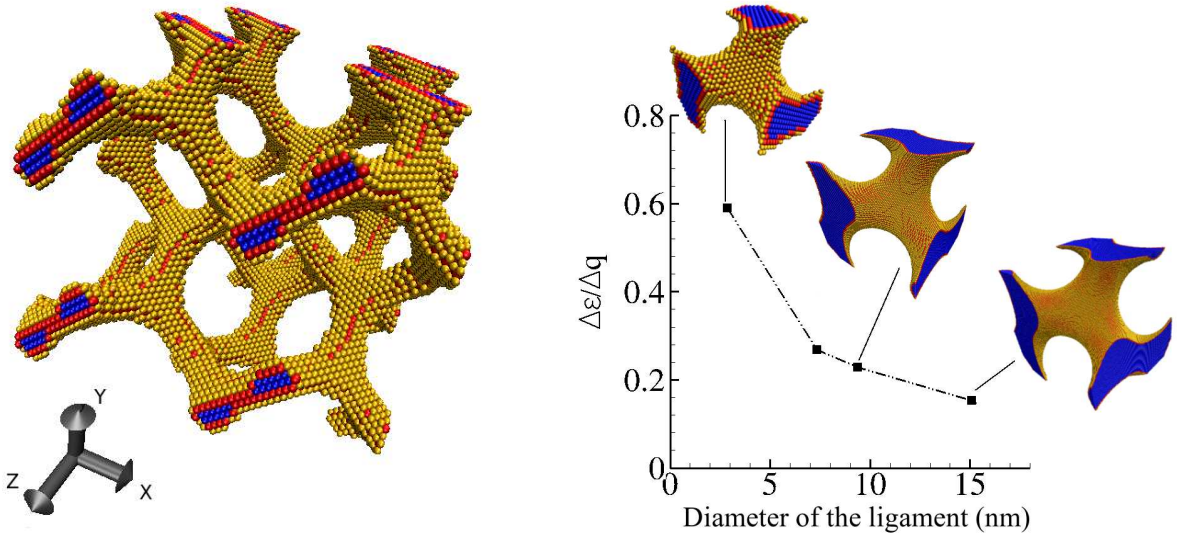
for the charge-induced strain and compare it with the results of the atomistic simulations. Furthermore, we study the size-dependent stiffness and charge-induced strain of gold nanofoams. We found that the stiffness of nanoporous metals depends on the crystal orientation, cross-sectional size of the ligaments and the relative density. We present a scaling relation between the stiffness and the relative density. Similar to our studies on the stiffness, we also explored the effect of relative density, ligament size and crystal orientation on the charge-induced strain of nanoporous gold, based on a gyroidal microstructural representation, see Fig. 2.



(a) (b)

Figure 2: (a) Gyroid with charged atoms. Gold colored atoms are the surface atoms which are assigned with 80% charge, red colored ones are the sub-surface atoms with 20% charge and the blue ones are the core atoms with zero charge. (b) Strain-charge response $\frac{\Delta\epsilon}{\Delta q}$ of gyroids with different ligament diameters and a relative density of 0.3, where ϵ is the strain and q is the surface charge density.

CONCLUSIONS

We modified the embedded atom potential by fitting it to the surface-stress-charge coefficient of Au(100) which is obtained from DFT calculations. The stiffness and charge-induced strain of nanowires depend on their cross-sectional size and crytal orientation. The charge-induced strain of nanowires predicted by continuum theory is in good agreement with the results obtained from atomistic simulations. Similar studies on gyroids have shown that the stiffness and charge-induced strain depend on the cross-sectional size and crystal orientation of the ligaments, and the relative density of the structure.

References

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[2] Umeno Y., Elsasser C., Meyer B., Gumbsch P., Nothacker M., Weissmuller J. and Evers F.: Ab initio study of surface stress response to charging. *EPL (Europhysics Letters)* **78**:13001-p1–p5,2007.