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Characterization of Silicon Surface Elastic Constants Based on Different Interatomic Potentials

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Abstract

Mechanical properties of materials is an important factor in designing nanoscale systems. Several researches and experiments have shown that the mechanical properties of the nano-scale materials is different from those of bulk. One of the major reasons for this difference is that the ratio of surface to volume increases at the nano scale, and the effects of free surfaces become very important. In this paper, we have measured the surface elastic constants of silicon crystalline structure using different interatomic potentials. The potentials employed here are EDIP (Environment-Dependent Interatomic Potential), Stillinger-Weber and Tersoff, and also different crystalline orientations are examined. In order to obtain surface elastic constants, we have first determined the lattice constant resulting in minimum energy of bulk model for each potential, then we have measured the bulk and film elastic constants using respective models. It is observed that by increasing film thickness, elastic constants approach to those of bulk. Next, using the results of the previous sections, the surface elastic constants are measured and discussed for different surfaces using different potentials.

Keywords: Silicon; Surface Elastic Properties; Tersoff; EDIP; Stillinger-Weber

[[1] [2]]

[3] [4] [5] [6]

1. Introduction

When the size of material decreases to nano scale, the ratio of surface to volume increases significantly. Several researches and experiments have shown that material properties such as mechanical, thermal and electrical properties of the nano-scale materials are different from those of large scale systems [1-6]. To design and model nano-scale systems, precise characterization of their mechanical properties is necessary. Considering difficulties of experimentation at small sizes, theoretical computational techniques based on interatomic potentials seems to be useful for determination of the elastic constants.