ATOMIC-SCALE DISPLACEMENT AND STRAIN FIELDS OF NEAR-SPHERICAL GERMANIUM QUANTUM DOTS IN SILICON

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Displacements and strains, and strain energy densities at the atomic scale have been predicted by multiscale modeling in the neighborhood of near-spherical, coherent germanium 'quantum dots' (QD) in crystalline silicon and near a {001} Si surface, by use of a combination of classical molecular dynamics (MD) and Green's function (GF) techniques. The smallest QDs nearest the surface produce a characteristic pattern of out-of-plane surface displacement, namely, a peak with a depression or indent at its center. This depression was absent in the largest dot. For dots that are large (*e.g.*, 6.5 nm diameter), and perhaps even for smaller dots close to the surface, the patterns of surface displacement are of a magnitude sufficient to be observed by advanced scanned probe force microscopy. Iterative force matching over a 'shell' region of thickness a few lattice parameters joined the GF and MD solutions. A modified-embedded-atom-model interatomic potential was used in both analysis methods. Dots of four sizes were analyzed, ranging in diameter from 1.1 to 6.5 nm. The supercell size was 34.2 nm. Calculations for strains and displacements in the infinite solid were extended to the {001} surface of the semi-infinite solid using the scheme described previously. Atomic displacements in the infinite solid showed trends generally similar to the early estimate of Mott and Nabarro, but differed in detail, especially for the smaller dots. Both our calculated strain in the quantum dot and our far-field atomic displacements were smaller than the Mott-Nabarro estimate. Surface displacements were broadly similar in magnitude and shape to the classic isotropic continuum solution of Mindlin and Cheng. Different surface displacements occur along the <100> and <110> directions because of crystalline anisotropy. For the smallest dot, the elastic energy density at the surface shows a pronounced minimum directly above the center of the dot, while for the largest dot an energy maximum occurs at the projected center position.

This paper shows how to avoid arbitrary and non-physical boundary conditions used in previous treatments of the spherical quantum dot, and compares atomistic calculations, made with correct rather than arbitrary boundary conditions, to two continuum models. For a particular QD shape and a range of QD sizes, we provide details of the atom positions near the QD-matrix interface and the form of the displacements around the QD. We have used the Greens function and related mathematical tools to extend these results to calculate surface displacements and strains for the case of a QD lying beneath the substrate surface. The atomic positions are critical for calculation of the electronic-photonic behavior of the QD. The surface distortions are useful for relating scanned-probe microscopy (SPM) and other surface observations to the size, position, and shape of buried QD. And the surface strains provide an indication of which positions may be favorable for formation of neighboring dots in self-assembled arrays.

Keywords: atomistic, multiscale, quantum dot