Supporting Information (SI)

SI1. Verification of the accuracy of FEAwSE by molecular dynamics simulation

FEAThe accuracy of the FEAwSE is verified by comparing the results calculated from MD and FEAwSE. The thickness ratio of the Si and SiGe layers, as well as the composition ratio of Si in SiGe, is fixed at 0.5 throughout this paper. The open source code, LAMMPS,[26] is used as an MD simulation tool, and Tersoff[24] is used as the intermolecular potential. Both Si and SiGe have unreconstructed *p*(1×1) ideal surfaces. Minimum boundary conditions are imposed to remove rigid body motion. On the other hand, the FEAwSE is performed under the same geometry and material properties as those of the MD simulation.

We first calculated the equilibrium configuration of freestanding Si monolayer thin films. In this case, the surface stress is the only driving force for deformation, and there is no other external force. The number of atomic layers is 34 and 33 for even and odd layers, respectively, and the width-to-thickness and length-to-width (L/W) ratios are both 5. The simulated models are <100>/even, <100>/odd, <110>/αα, and <110>/βα. The calculation results are shown in Figs. SI1 and SI2. In the even layer case, there is no out of plane deformation in either <100>/even or <110>/αα. In contrast, when odd layers are used, twisted and bending shapes are obtained in <100>/odd and <110>/βα, respectively. For the twisted shape in the <100>/odd model, the twisting angles between the two edges in the FEAwSE and MD simulations are 25.82° and 25.09°, respectively. For the bending shape in the <110>/βα model, the curvature radiuses in the FEAwSE and MD simulations are 248.5 and 258.8 nm, respectively, and the pitch angles are 0.50 and 0.03 nm, respectively. The resultant configurations obtained from both methods match well, with a slight difference in the degree of twisting or bending. Here we can see the strong effect of the surface when there is no other external force in the odd layer case. In addition, the effects of surface configuration and size contribute considerably to the equilibrium configuration. Even if the size of the thin film is equivalent, the difference in the surface configuration can lead to a very different equilibrium configuration.

We further proceeded to the case of freestanding Si/SiGe bilayer film, in which $Si/Si_{0.5}Ge_{0.5}$ bilayer was used. The number of Si atomic layers is 17, and the number of SiGe atomic layers is 17 and 16 for even and odd, respectively. The width-to-thickness and L/W ratios are both 5. The simulated models are <100>/even, <100>/odd, <110>/αα, and <110>/βα. The results are shown in Figs. SI3 and SI4, and the curvature radius and pitch angle of each model are presented in Table 6. These MD and FEAwSE results also correspond well to each other. The differences of curvature radius in FEAwSE and MD results are less than 10%, and the differences of pitch angle are less than 1°. According to S. Kim *et al.*[17], the nanoband shape is expected in both the <100> and <110> directions if the surface effect is neglected. In the even layer case, the nanoband shape is obtained as expected; however, a different trend is observed when odd layers are used. A helical shape (curl in diagonal direction) is obtained in <100>/odd, and a nanoband shape is obtained in <110>/βα. The most probable cause of such a mismatch between the results of this study and that of S. Kim *et al*. is that the misfit strain between the two layers was assumed the only driving force in the study by S. Kim *et al.*, and the surface effect was neglected. The calculated shapes obtained from this study can be explained by the combination of the two driving forces: the misfit strain, which leads to the nanoband shape, and the surface effect, which adds additional curvature in the <110> direction. Now we can be assured that the FEAwSE can express the atomic features of thin films properly. In addition, it is clear that the surface effect causes the appearance of helical shapes in <100>/odd.

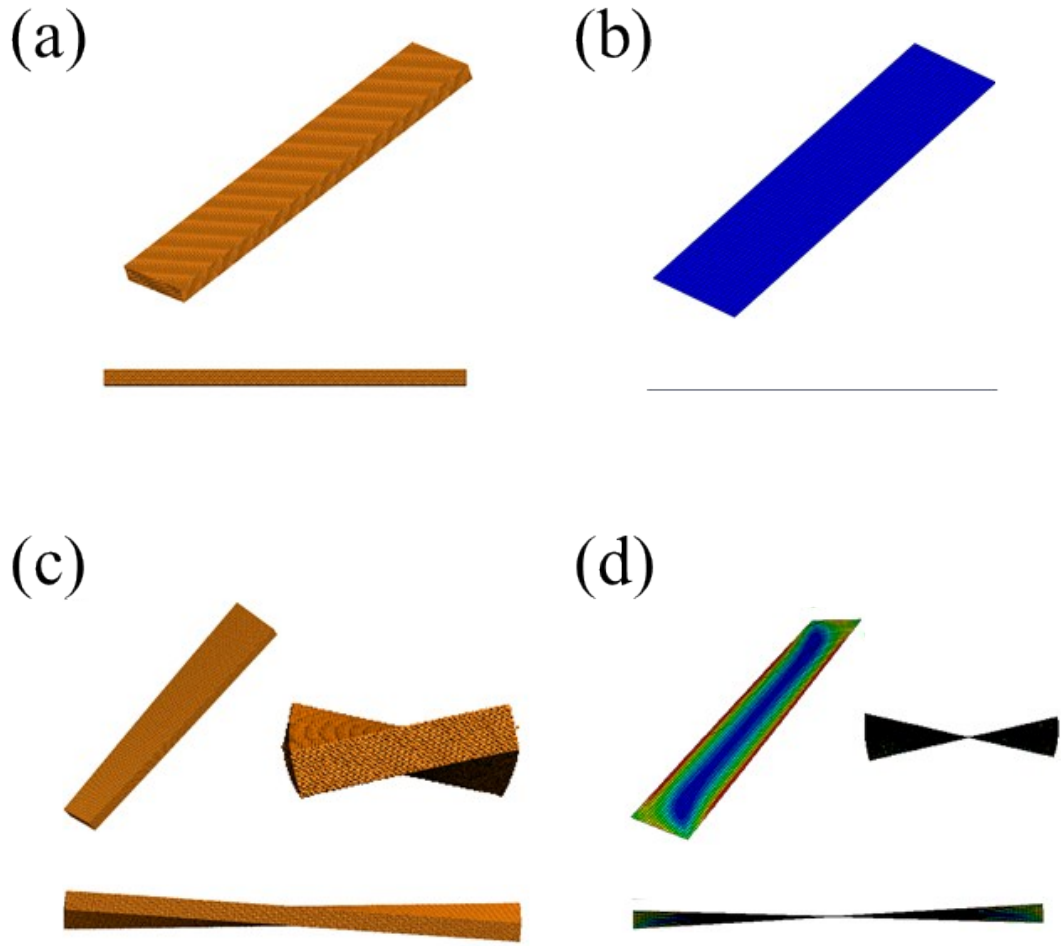

Figure SI1. Equilibrium configurations of freestanding Si monolayer thin films. (a) <100>/even, calculated by MD. (b) <100>/even, calculated by FEAwSE. (c) <100>/odd, calculated by MD. (d) <100>/odd, calculated by FEAwSE. In the MD results, orange colored particles represent Si atoms. In the FEAwSE results, the color indicates the maximum in-plane principal logarithmic strain.

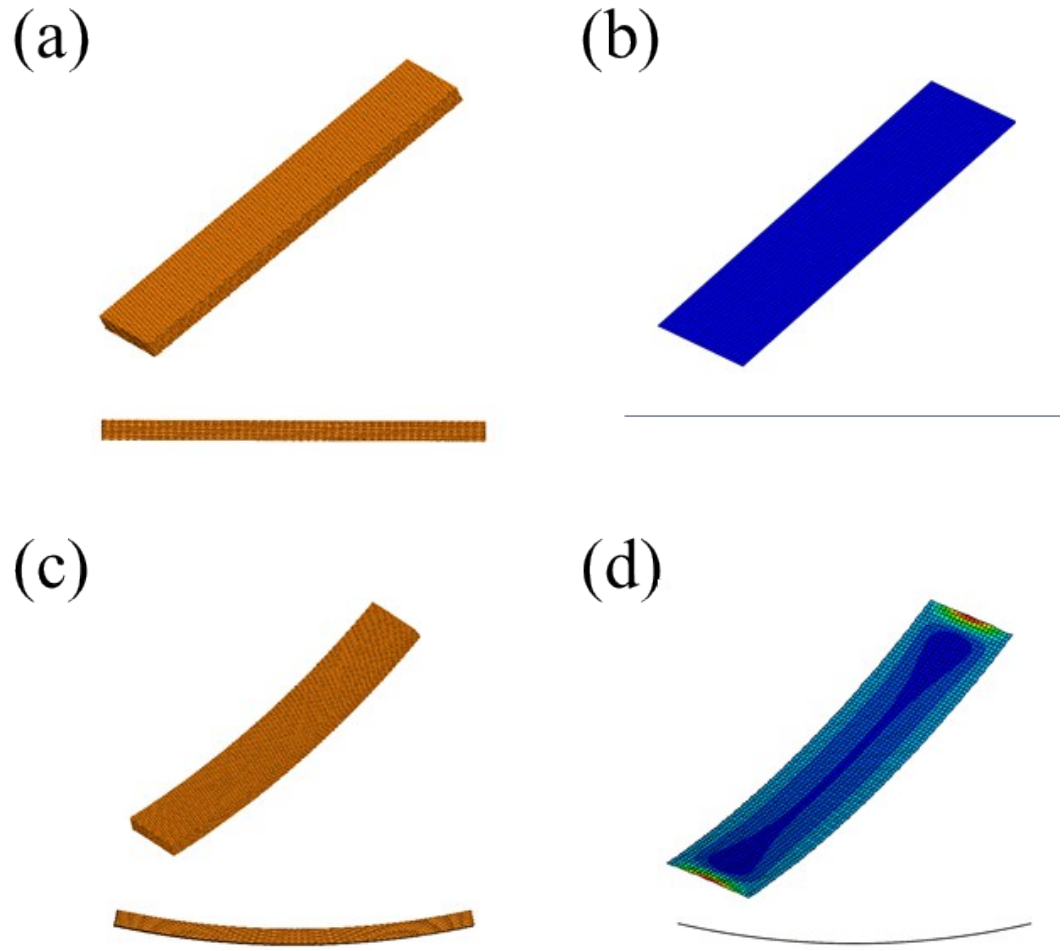

Figure SI2. Equilibrium configurations of freestanding Si monolayer thin films. (a) <110>/αα, calculated by MD. (b) <110>/αα, calculated by FEAwSE. (c) <110>/βα, calculated by MD. (d) <110>/βα, calculated by FEAwSE. In the MD results, orange colored particles represent Si atoms. In the FEAwSE results, the color indicates the maximum in-plane principal logarithmic strain.

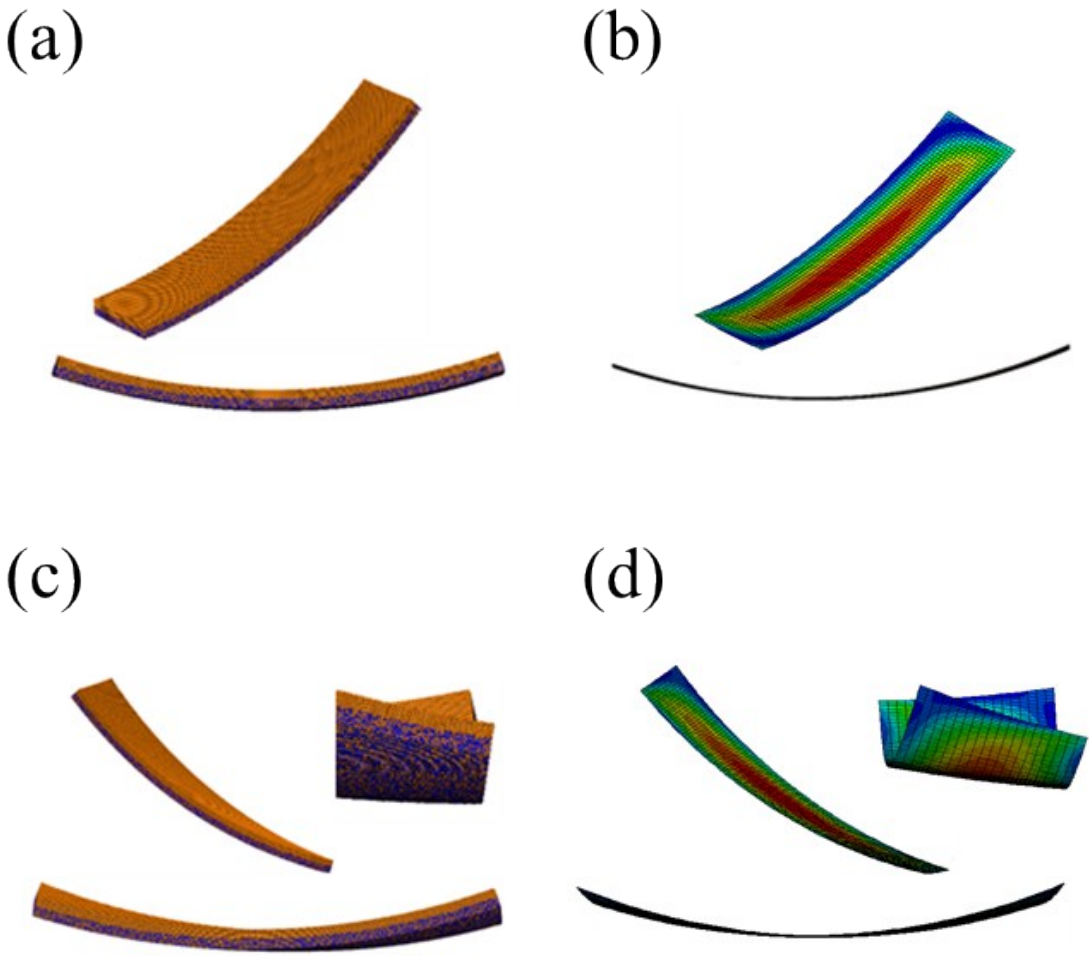

Figure SI3. Equilibrium configurations of freestanding Si/SiGe bilayer thin films. (a) <100>/even, calculated by MD. (b) <100>/even, calculated by FEAwSE. (c) <100>/odd, calculated by MD. (d) <100>/odd, calculated by FEAwSE. In the MD results, orange colored particles represent Si atoms. In the FEAwSE results, the color indicates the maximum in-plane principal logarithmic strain.

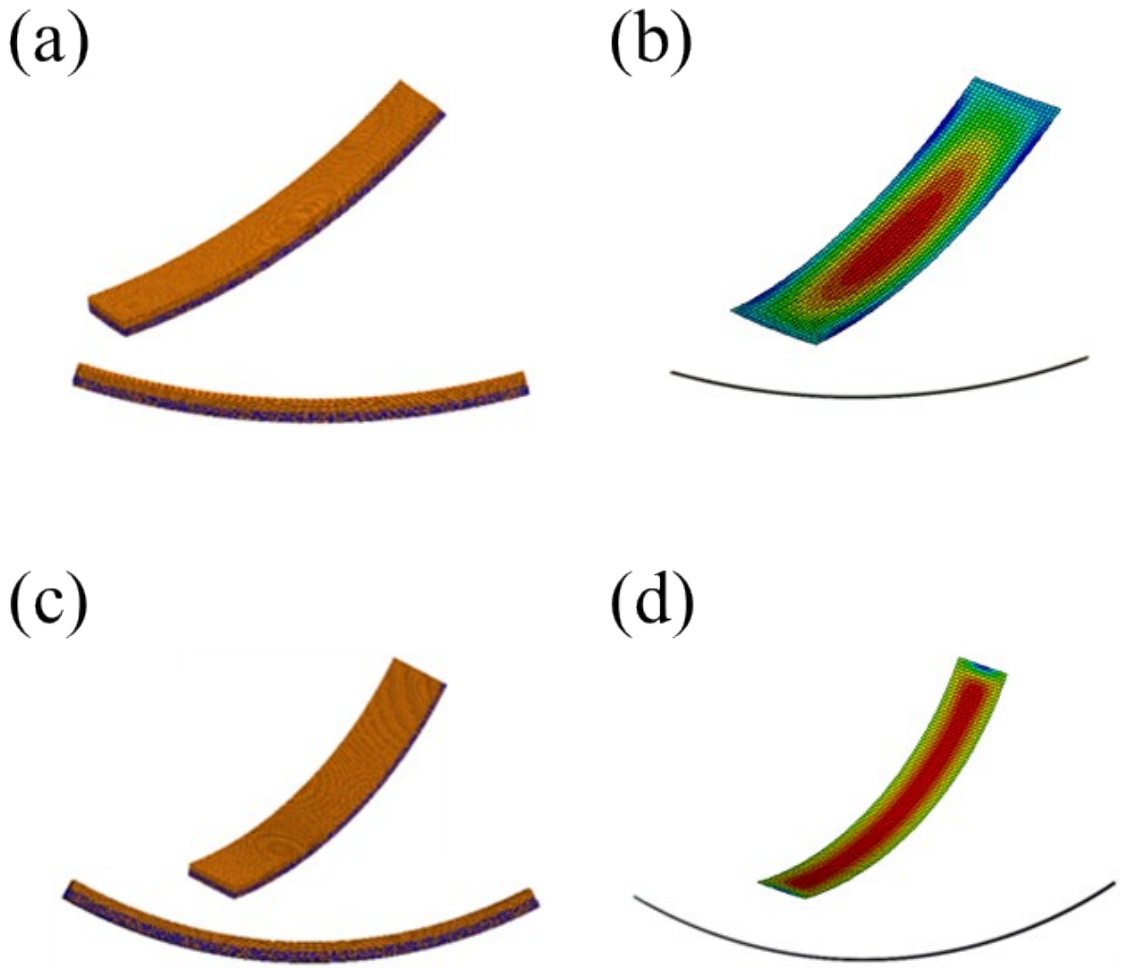

Figure SI4. Equilibrium configurations of freestanding Si/SiGe bilayer thin films. (a) <110>/αα, calculated by MD. (b) <110>/αα, calculated by FEAwSE. (c) <110>/βα, calculated by MD. (d) <110>/βα, calculated by FEAwSE. In the MD results, orange colored particles represent Si atoms. In the FEAwSE results, the color indicates the maximum in-plane principal logarithmic strain.

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