Ab Initio Simulation on Mechanical and Electronic Properties of Nanostructures under Deformation

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ABSTRACT

Nanostructures have been attracting attention because of their prominent properties, and their applications for novel devices with advanced functions have been attemted. Large stress and strain occur in local regions in materials with nanostructures owing to their complex structures. In this study, we conduct *ab initio* simulations to elucidate the mechanical and electronic properties of materials, which are essential for designing functional nanomaterials. Firstly, we investigate in detail the deformation of crystals, such as silicon and nickel, and the change in their electronic structures under deformation. We find that the strain largely changes the electronic structures of the crystals, resulting in the changes in the electric conductivity of silicon and the magnetic property of nickel. Secondly, we conduct simulations on the deformation of carbon nanotubes, which are among greatly notable nanomaterials. We find that the electric conductivity of the carbon nanotubes shows transitions from metallic to semiconducting and vice versa under axial tension. We also find that the semiconducting nanotubes become metallic under radial compression, while the metallic nanotubes do not show the transition.

Keywords: ab initio, deformation, mechanical property, electronic structure, nanostructure

1 Introduction

With the advent of the nano-processing technology, microscopic devices, which include complex structures in nanometer scale, have been intensively developed and their size is continuously reducing. The complex structure may cause local strain condition owing to the mismatch of bimaterials, and this leads to the change in the electronic structure in the local region. As the size of the device is reduced, the effect of the local strain becomes beyond negligible degree, which results in the deterioration of the functions of the device. Conversely, such effect can be utilized for designing novel devices with preferable functions as various properties may be controlled by making use of local strain. Therefore, it is of great importance to clarify the correlation between the electronic properties and the deformation behavior of materials.

We have conducted simulations on the problem by using the *ab initio* DFT calculation based on the pseudopotential plane wave method, by which the mechanical and electronic properties are easily evaluated. In this paper, simulation results about the effect of deformation on the electronic properties in the cases of single crystals and carbon nanotubes are presented.

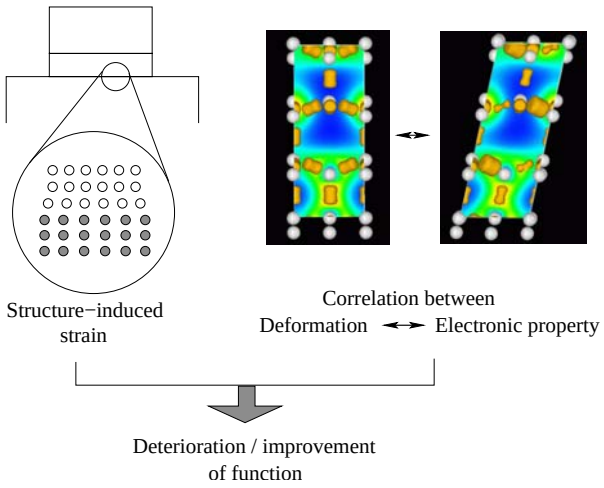
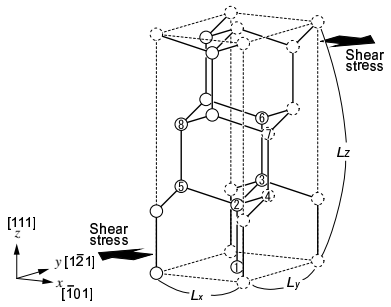


Figure 1: Schematic of local strain caused by nanostructure.

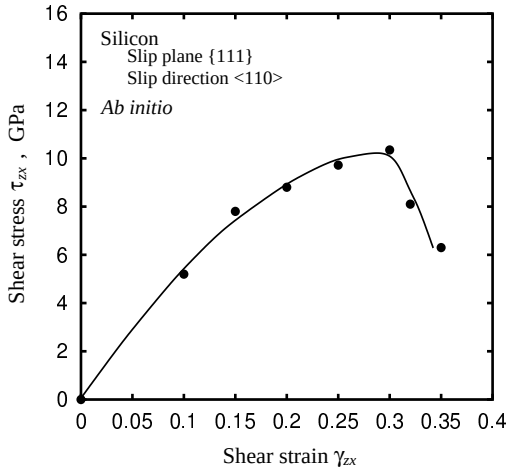
2 Mechanical and Electronic Properties under Deformation

2.1 Single crystal

The ideal deformation of the silicon single crystal, which is commonly used for the substrate of electronic devices, is simulated by the *ab initio* pseudopotential method[1] based on the LDA. The simulation cell shown in Fig. 2(a) is used and the shear strain, γ_{zx}, which corresponds to $[\bar{1}01]$, is applied. All the stress components except τ_{zx} are controlled to be zero by adjusting the cell size, and the atom configuration is relaxed during the shear deformation. Figure 2(b) shows the stress-strain relation. The curve shows the peak, $\tau_{zx} = 10$GPa



(a) Simulation cell.



(b) Shear stress as a function of shear strain.

Figure 2: Ideal shear deformation of silicon single crystal.

at $\gamma_{zx} = 0.3$, which indicates the ideal shear strength. The deformation in the region up to $\gamma_{zx} = 0.3$ is elastic without the bond breaking. The crystal becomes back to the initial state when unloaded. On the other hand, the rapid decrease in the shear stress over $\gamma_{zx} = 0.3$ corresponds to the bond breaking, which we can denote the "mechanical fracture" under this deformation mode.

Figure 3 shows the change in the density of states (DOS) during the shear. The initial state has the band gap energy and it is eliminated at $\gamma_{zx} = 0.2$, which means that the crystal loses the electronic property as the semiconductor under the shear deformation. These results suggest that the electrical deterioration may take place before the mechanical fracture.

The deformation of the nickel crystal, which is one of typical ferromagnetic metals used for magnetic devices, is investigated by *ab initio* calculations based on the LSDA, where the partial core correction[2] is taken into account. Figure 4 shows the magnetic moment of the nickel single crystal, μ, as a function of the isotropic strain, ε. The magnetic moment, μ, increases with the isotropic strain. On the other hand, μ is reduced under

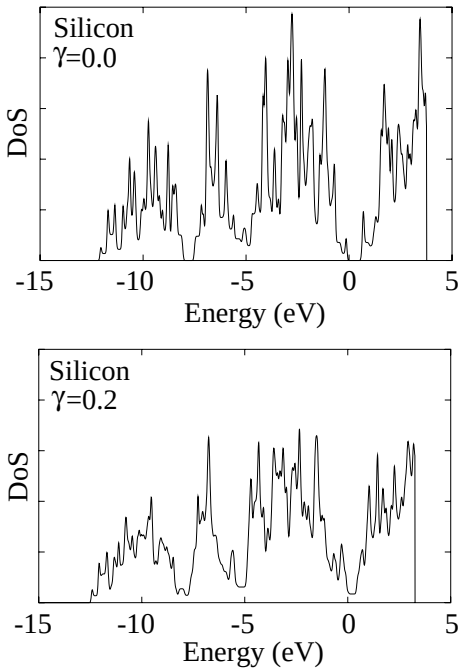


Figure 3: Change in density of states under shear deformation.

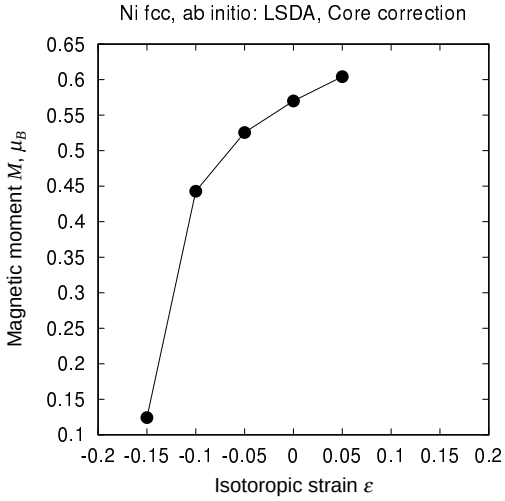


Figure 4: Magnetic moment as a function of isotropic strain in nickel single crystal.

contraction and becomes almost zero at ε = -0.15, which means the crystal is no longer ferromagnetic. This corresponds to the similar calculation conducted by Černý *et al.* [3]. The result can be applied for the device designing, for example, if the tensile strain condition is created by the component structure, the magnetic property of the device can be improved.

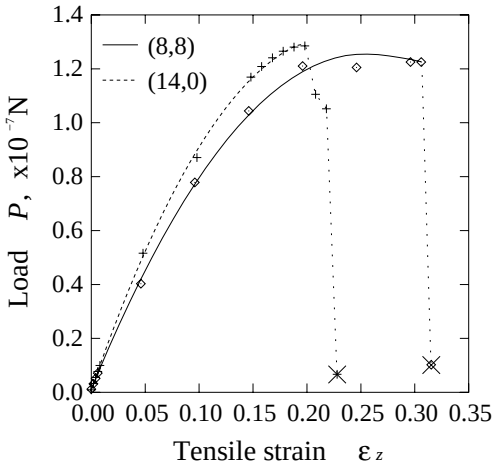


Figure 5: Load-strain relation of CNT under axial tension.

2.2 Carbon nanotube

Carbon nanotubes (CNTs) have been attracting attention because of their prominent mechanical and electronic properties. The deformation of single-walled carbon nanotubes (SWCNTs) is investigated by tight-binding calculations and the change in the band gap energy is examined [4]. The focus is placed on the dependency of the mechanical and electronic properties on the CNT structure, which is denoted by the chiral vector, (m, n). The validity of the tight-binding calculations is verified by *ab initio* DFT calculations based on the pseudopotential method as preliminaly calculations. Two deformation modes, axial tension and radial compression, are considered.

The axial load as a function of the axial strain for the (14,0) and the (8,8) tubes is shown in Fig. 5. This result points out that CNTs can show large elastic elongation in the axial tension and that the elongation depends on the chiral structure. This suggests that it is meaningful to investigate the change in the electronic properties of CNTs under high axial strain. Figure 6 shows the change in the band gap energy, $E_{\rm gap}$ during the axial tension. CNTs are classified into three groups; A:$m-n=3q$, B:$m-n=3q+1$, and C:$m-n=3q+2$. The CNTs show different patterns of transition of the electric conductivity under the deformation. Type A shows M→S→M, where M and S denote "metallic" and "semiconducting", respectively. On the other hand, The transition of Types B and C is S→M→S.

Figure 7 shows the relationship between the applied load, P, and the normalized displacement, δ, under the radial compression. The curves show the difference in the deformation behavior because of the difference in the diameters of the tubes. In the case of the (8,0) tube, the diameter of which is 0.626nm, the load gradually

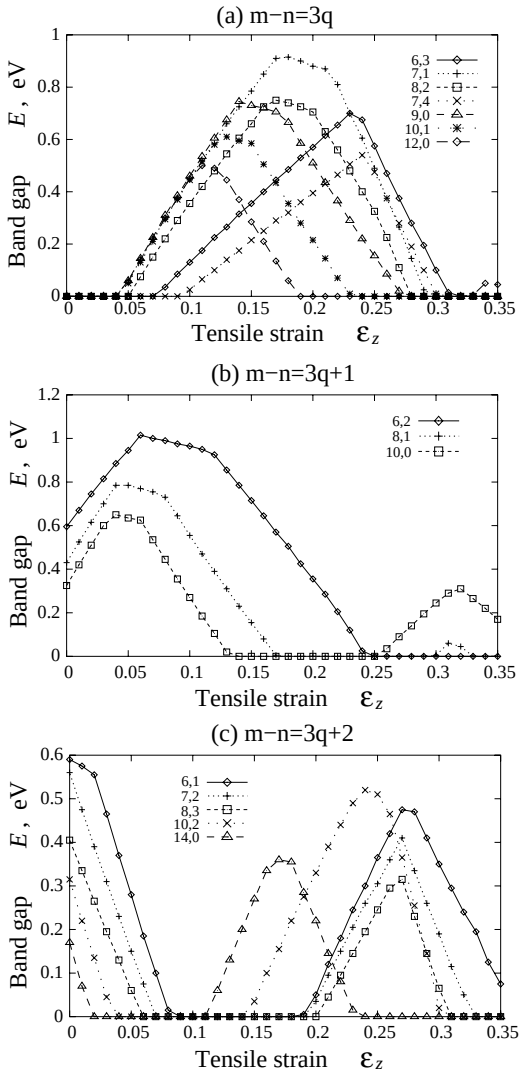
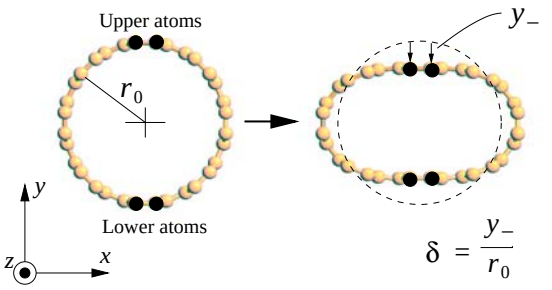


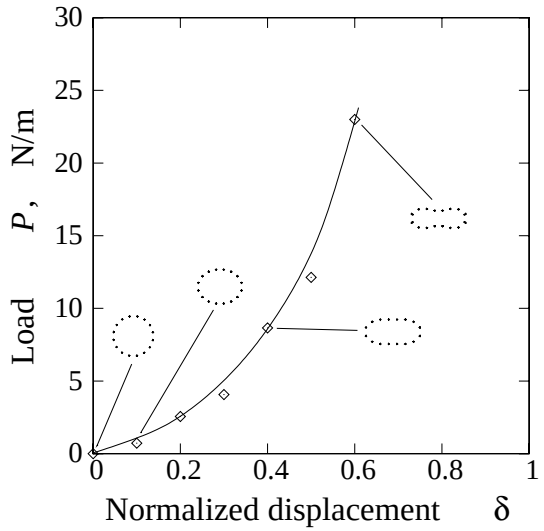
Figure 6: Change in band gap energy during axial tension.

increases with the displacement. The inclination, which corresponds to the resistance against the deformation, also shows monotonic increase. This is becase the CNT wall has elasticity so that it has the resistance against the curvature change. On the other hand, in the case of the (14,0) tube, which has a larger diameter, 1.10nm, the inclination of the curve is relatively low up to $\delta = 0.7$ and then it increases rapidly. The rapid increase of the load at $\delta > 0.7$ indicates the tube becomes stiffer, which is explained by the repulsion between the top and the bottom walls of the CNT because the distance between the upper and the lower wall when the curve shows the rapid increase is about 0.33nm, which is a little smaller than the interlayer distance in graphite, 0.335nm.

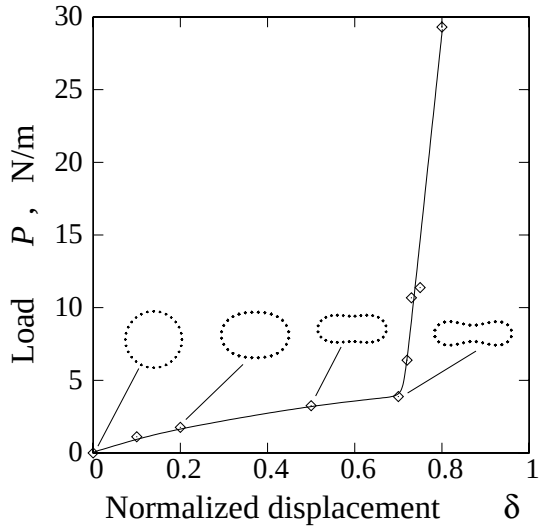
It should be noted that the shape of the tubes becomes back to the initial state when unloaded.

Figure 8 shows the change in the band gap energy of





(a) (8,0) tube



(b) (14,0) tube

Figure 7: Change in load during radial compression of CNT.

the (8,0) and the (14,0) tubes under the radial compression. Both tubes have the band gap energy at the initial state, which decreases with the displacement and finally becomes zero. However, the (8,0) tube needs much smaller displacement ($\delta = 0.1$) and load ($P = 0.9$N/m)

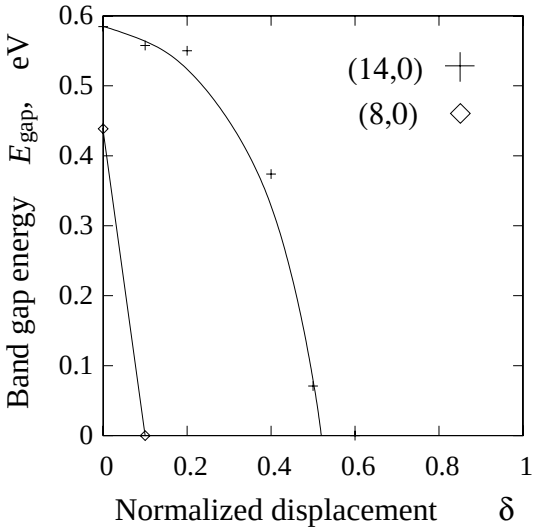


Figure 8: Change in band gap energy during radial compression of CNT.

to eliminate the band gap than the (14,0) tube ($\delta = 0.5$ and $P = 4.1$N/m). The result indicates that it is possible to control the sensitivity of the band gap energy to the deformation by the diameter.

3 Summary

We presented simulation results on the mechanical and electronic properties under deformation of crystals and CNTs. We found these materials have the close correlation in those properties. *Ab initio* and semi-empirical band calculations are suitable for evaluating the correlation, which is essential for designing functional nanodevices.

Acknowledgment

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REFERENCES

[1] Umeno,Y. and Kitamura,T., *Mater. Sci. Eng.*, B, **88**(2002), 79–84.

[2] Louie,S.G., Froyen,S. and Cohen,M.L., *Phys. Rev.*, B, **26**(1982), 1738–1742.

[3] Černý,M., Pokluda,J., Šob,M., Friák,M. and Šandera,P., *Phys. Rev.*, B, **67**(2003), 035116.

[4] Umeno,Y., Kitamura,T. and Kushima,A., *Comp. Mater. Sci.*, submitted.