1. Introduction

Recently, physical and chemical properties of CNT have been investigated by quite a few researchers all over the world in detail, and their unexpected superior characteristics have been made clear theoretically and experimentally. Both the electronic and mechanical properties of CNT are superior to those of metals and their specific weight is rather light. In addition, they are deformed easily and stable chemically. Therefore, if the resistivity of CNTs changes by applied external strain drastically, it is possible to develop a highly sensitive strain sensor [1, 2].

Thus, the authors have proposed a new highly sensitive strain sensor using a popular resin in which multi-walled CNTs (MWCNTs) are dispersed uniformly [3]. It is easy to make a cheap, flexible and stable sensor by using the CNT-dispersed resin. The measured change rate was 400% strain and 150% strain at tensile side and compressive side that was about a hundred times higher than that of metals. So, the possibility of high sensitivity strain measurement was revealed. However, there was large fluctuation of the measured change rate among test samples. Thus, it is very important to clarify the mechanism of the change of the resistance of a CNT due to its deformation. In this study, in order to discuss the relationship between the deformation of a CNT and its electronic conductivity, both molecular dynamics (MD) and density functional calculation were applied. Since the CNT consists of six-membered ring carbon, the change of the band structure of a graphene sheet was also analyzed.

2. Deformation of CNT under compressive strain

Figure 1 shows the scanning electron micrographs of the structure of MWCNTs dispersed in polycarbonate. Most MWCNTs were bended or buckled significantly and jammed one after another complicatedly, indicating that there should be large distribution of the residual strain in each dispersed MWCNT. Thus, even when uni-axial strain is applied to the CNTs-dispersed resin, the deformation of each CNT should be varied significantly. Therefore, it is not easy to estimate the change of electronic conductivity of the deformed CNTs quantitatively due to the large distribution of residual strain.

In order to estimate influences of bended or buckled deformation of CNT on their electronic conductivity, deformation characteristics of CNT under axial compressive strain were investigated by molecular dynamics (MD) simulations. Simple single-walled CNT structures were modeled and Tersoff potential was used for the simulations. Estimated change of radial distribution functions (RDF) of CNT with chirality of (11,0) caused by the applied compressive strain is shown in Fig. 2. When the amplitude of the applied compressive strain was less than 5%, the RDF shifted to smaller distance side, indicating that most CNTs showed just axial shrinkage. However, it moved again to larger distance side when the amplitude of the applied
strain was 6%. This indicates that the buckling deformation causes the complicated nonlinear change of atomic configuration of six-membered carbon rings. Figure 3 shows an example of the deformation of a six-membered ring in the buckled CNT. In this example, the maximum distortion of the deformed six-membered ring (b/a) reached 1.140 and the shrinkage of the ring was 0.04. This result clearly indicates that buckling deformation of a CNT causes a very complicated strain distribution in the tube. Therefore, the control of the shape of the MWCNTs dispersed in resin is very important to estimate the change of resistivity of the CNT-dispersed resin.

3. Change of electronic band structure of graphene

Since the CNT consists of a periodical structure of a six-membered ring carbon, the electronic characteristic of CNTs should be determined by the electronic band structure of the six-membered ring. Thus, the change of the band structure of a graphene sheet caused by the distortion of the six-membered ring structure was analyzed by applying the density functional theory. Figure 4 shows analysis model of graphene and its unit cell. Two-dimensional periodic boundary condition was assumed in this analysis. To discuss the relationship between the distortion of the six-membered ring and the electronic structure of graphene sheet, the six-membered ring of graphene sheet was deformed by changing the distance between the nearest carbon atoms in the six-membered ring. The magnitude of the distance change was defined as the B/A ratio where A was the bond length along the y axis and B was the other bond length. Bond length of A was constant at 1.42 Å and B was changed in the range of B/A from 0.75 to 1.0. This deformation corresponds to the biaxial compressive strain along x direction. Examples of the calculated band structure are shown in Fig. 5. For graphene sheet without strain, the Dirac point K_0 that is the position in the Brillouin zone where conduction and valence bands touch conically coincides with the symmetry point K in the Brillouin zone. On the other hand, the Dirac point K_0 drifts inside the Brillouin zone from the symmetry point K in the strained graphene sheet. The move of Dirac points K_0 by the distortion of the six-membered ring is summarized in Fig. 6. This figure clearly shows that Dirac points move further from the K points as the applied compressive strain increases. It is well known that the electrical properties of the CNT can be explained by the relationship between the position of the Dirac point and the CNT circumference. Thus, the displacement of the Dirac point of graphene sheet under compressive strain suggests that the electronic conductivity of CNT could be changed drastically due to the distortion of six-membered ring.

4. Conclusions

When the applied axial compressive strain exceeded about 5%, buckling deformation of a CNT occurred and six-membered rings in the buckled CNT were distorted significantly. We found the band structure of a graphene sheet was changed by the distortion of six-membered rings. Therefore, the electronic conductivity of a graphene sheet and thus, a CNT was found to be mainly dominated by the fluctuation of the distance between the nearest carbon atoms due to the residual and external strain.

References