Analysis of vibrational properties of C-doped hexagonal boron nitride (h-BN)
University of Fukui, 1, Kyushu University 2, Md. Shearjul Islam 1, T. Hirooka 1, T. Makino 1, S. Tanaka 2, A. Hashimoto 1
E-mail: sheraj_ruet@yahoo.com

Mono-layer hexagonal boron nitride (h-BN), a structural analogue to graphene, has stimulated people’s great interest recently due to its novel properties and potential applications in electronic devices. However, pristine h-BN structures are unsuitable for many functional applications because of their large insulating band gap. In most recent, h-BN is doped with C atom to explore the possibilities for creating hybrid BCN systems, with the electronic properties defined by the relative concentration of B, C, and N atoms [1]. Lattice vibrations have a significant effect on the electron transport properties. The vibrational properties in hybrid BCN network are thus of fundamental importance for the electron transport in electronic devices and of great general interest. Here, we first systematically investigated the vibrational properties of C doped h-BN using forced vibrational method suitable to treat physical systems. We inserted C atoms randomly into the h-BN sheets using bond percolation procedure. Only interactions up to the fourth neighbor atoms are used. Figure 1 shows the calculated phonon density of states for h-BN in the total of 10500 atoms. The calculated PDOS is considerable agree with the PDOS calculated by force constant method [2]. The PDOS for the hybrid BCN network for different concentration of B, C and N atoms is shown in Fig. 2. We determine a critical value of C concentration for the onset of this C-induced vibrational transition in the hybrid BCN network. We find that for C concentrations of 10% and higher, the $E_{2g}$ peak of h-BN has been reduced into a shoulder or it has completely disappeared.

References