Buckling of Boron Sheets and Nanotubes: A First Principle Study

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Boron probably has one of the most peculiar nanostructures among all the elements. Boron nanotubes were expected to be all metallic, which might be better conducting systems than carbon nanotubes. The two-dimensional atomically thin boron sheets, which provide the surface structures of boron nanotubes, are made of mixtures of triangular and hexagonal motifs [1]. These sheets can be constructed by removing atoms from a flat triangular sheet. The "hexagon hole density" η is defined as

$$\eta = \frac{\text{No. of removal}}{\text{No. of atoms in the original triangular sheet}}.$$

The stability of these sheets changes smoothly with η. The most stable boron sheet, α sheet, occurs at $\eta = 1/9$. Although α sheet is flat and metallic, small nanotubes made from α sheet can be semiconducting due to the buckling of tube surfaces [2]. Moreover, why two-dimensional boron sheets and clusters buckle is also a universal question.

Using density functional theory, we have studied the buckling of boron sheets and nanotubes. We have discovered that sheets with small η like to become buckled while sheets with large η prefer to stay flat, except for very unstable structures ($\eta > 1/5$). The separational point between these two classes of sheets occurs at $\eta = 1/9$, which coincides with the optimal structure, α sheet. By studying how kinetic energy, electrostatic energy and exchange-correlation energy change with buckling, we show that kinetic energy is the driven force for the buckling. Moreover, we apply the knowledge to boron nanotubes to understand their buckling. In the end, we discuss the stability of buckling patterns of boron nanotubes and the possible consequences.

[1] H. Tang, and S. Ismail-Beigi, Phys. Rev. Lett. **99**, 115501 (2007).

[2] X. Yang, Y. Ding, and J. Ni, Phys. Rev. B **77**, 041402(R) (2008).