

**Okada, Saito, and Oshiyama Reply:** As we mentioned [1], there are only three polymerized  $C_{60}$  phases which have been synthesized under pressure *and* whose atomic structure has been identified to date; one-dimensional orthorhombic, two-dimensional tetragonal, and two-dimensional rhombohedral phases [2]. Although there have been a lot of experimental studies to explore new phases of carbon using pressure synthesis from solid  $C_{60}$  [3–6] as Brazhkin and Lyapin commented [7], in most cases it is not clear what type of atomic structure the synthesized material has: Sometimes amorphous, sometimes crystal, sometimes a mixture of diamond and graphite, and sometimes totally unidentified at all.

Some materials obtained via pressure synthesis from solid  $C_{60}$  were reported to be superhard or even “ultra-hard” (harder than diamond) and were inferred to be three-dimensional (3D)  $C_{60}$  polymers from their broad x-ray diffraction profiles [8,9]. For these “superhard 3D  $C_{60}$  polymers,” atomic-scale network topologies had not been reported so far. Only quite recently, candidates for the atomic coordinates have been proposed [10] for the first time.

In our Letter [1] we tried to provide a firm theoretical framework to consider synthesis and properties of 3D  $C_{60}$  polymers. Starting from the tetragonal phase of 2D  $C_{60}$  polymer, we found an ordered 3D  $C_{60}$  polymer which had not been identified before and exhibited fascinating properties as described in the Letter. From the point of synthesis, for instance, the radial distribution function which experimentalists sometimes rely on to determine the structure is found to *not* be a simple reflection of the microscopic structures. Also the system is expected to be a candidate for a new elemental superconductor consisting entirely of carbon. At the same time, we found that our system was not a superhard or ultrahard material. Its bulk modulus is found to be 1 order of magnitude smaller than diamond [1].

The present theoretical treatment (density-functional pseudopotential procedure) is expected to have enough accuracy to discuss relative hardness of various carbon based materials [11,12]. Hence there is no doubt that the system we found does not correspond directly to so-called superhard 3D  $C_{60}$  polymers. On the other hand, generally it is useful to compare theoretical and experimental results carefully to innovate new materials. It is especially important in the field of nanostructure materials consisting of carbon and/or other covalent-bond elements. Their physical properties are known to depend strongly on the network topology of covalent bonds as has been clearly demonstrated in the case of carbon nanotubes [13,14].

Sometimes the target new materials, with novel properties to be synthesized, can be given from the theoretical study. In this respect, a comparison between theory and experiment done by Brazhkin and Lyapin [7] is worth further consideration. The possibility of the presence of various different phases in pressure-polymerized 3D  $C_{60}$  is an interesting issue to be studied theoretically. In fact, from the density-functional study, we recently found several other stable 3D  $C_{60}$  polymer phases as well. Details will be reported in the future [15].

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