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CONDUCTIVITY OF C_{60} FULLERENE CRYSTALS UNDER MULTI-STEP DYNAMIC COMPRESSION UP TO 300 kbar

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Introduction

In the crystalline state C_{60} is a semiconductor with an energy gap E_g of about 2 eV. The excitonic absorption edge corresponds to an energy of about 1.7 eV. The C_{60} molecules are mainly bound by the Van der Waals forces (Young's modulus is about 13.5 GPa). Thus there is an appreciable reduction of distances between neighboring molecules of C_{60} in a crystal under moderate pressure. It leads to rapid increase of overlapping of electronic shells and, accordingly, to rapid reduction of band-gap because of expansion of filled (valent) and unfilled energy zones. It is possible to expect transition of a crystal to a metal state in a limit.

Results and discussion

In the first part of present work specific conductivity of fullerene C_{60} crystals has been measured under smooth quasi-isentropic loading conditions up to 15 GPa at initial temperatures T=293 K and 77 K. We have registered the sharp increase of conductivity more than 6 orders of magnitude in a range of pressure from 0 to 15 GPa, fig.1. Value of conductivity regains initial properties after dynamic load is removed. The

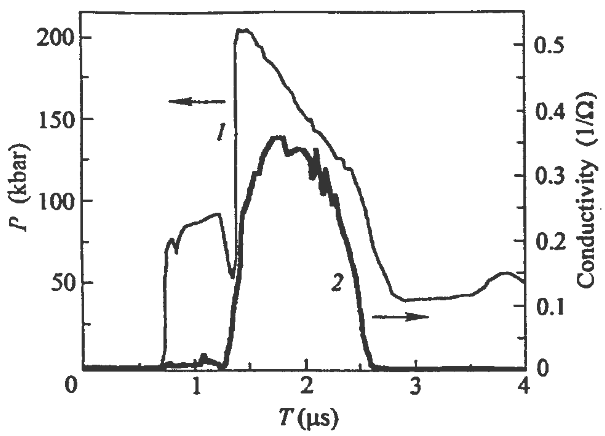

Fig.1 Pressure and conductivity time dependences of the C_{60} crystal under compression by spread shock wave

results received testified about sharply decreasing of band-gap of C_{60} under compression. However the experimental temperature dependence of conductivity under pressure indicated that band-gap haven't decreased down to zero and the sample compressed to 15 GPa have remained semiconducting. The X-Ray analysis has shown that C_{60} samples under these conditions regain the initial phase state after dynamic compression is removed. Similar, but a little less expressed effects in behavior of conductivity of C_{70} crystals were observed in the hydrostatic compression experiments.

The purpose of the second part of the present research is measurement of conductivity of fullerene C_{60} crystals under high pressures more than at the former experiments to find out metallization C_{60} is possible. In the latest experiments we used a mode of multi-step quasi-isentropic compression of fullerene crystals by series of consecutive flat shock waves which enables us to reach much higher pressures without essential warming-up of sample that is common for compression by a unitary shock wave. The idea of the method is as follows presented in [1]. The fullerite sample, which has the form of a rectangular plate with dimensions 8x3x1 mm and also piezoresistivic manganin pressure sensor, are placed between two metal plates (basis and reflector) separated from the sample by 1mm thick teflon film. Dynamic compression of the sample was carried out by series of the shock waves circulating between the basis and the reflector which was initiated by hit of the steel plate accelerated up speed about 2-2.5 km/s by a special explosive equipment.

The result of typical experiment of measurement of conductivity of C_{60} under multi-step quasi-isentropic compression up to final pressure ~ 30 Gpa is presented on fig. 2 as time dependences of sample conductivity and pressure, measured with help of manganin-foil pressure sensor. It is visible as we can see that at the beginning conductivity of a sample sharply increases and then starts to decrease smoothly despite of proceeding increase of pressure. As against to range 0-15 GPa change of the kept samples roentgenograms was observed after higher pressure loading (up to 30 GPa). The complex structure of samples transformations were found out at them.

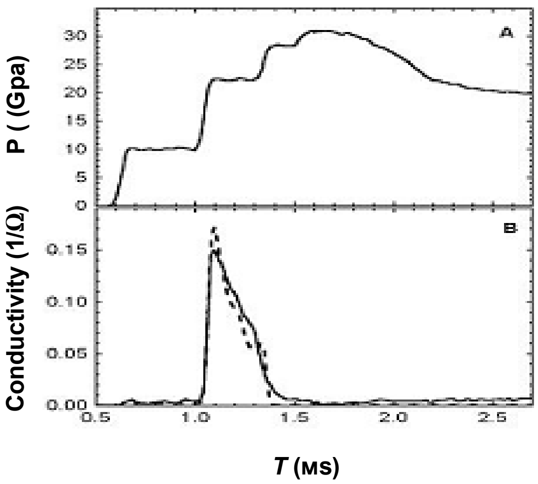

Fig.2 Pressure and conductivity time dependences of the C_{60} crystal under compression by series of the consecutive shock waves

Conclusions

The most essential fact received in the present work that is that at increase in pressure from above 20 GPa conductivity of the sample instead of the further increase on the contrary starts to fall, that formally corresponds to increase in size of effective band-gap energy E_G. It can be connected with phase transformations occurring in system and it is in agreement the data of X-Ray research.

Fundamental fact [2-5] is that at pressures higher than P_0=0.5-1 GPa according to polymeric phase C_{60} which is characterized by formation of covalent bonds between molecules of C_{60} becomes thermodynamically preferable. Thus experimental data obtained can be explained with the assumption that energy barrier of C_{60} polymerization becomes lower with pressure increase about equally the band-gap energy.

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