MICROHARDNESS OF HYDROGEN-INTERCALATED C_{60} FULLERITE

Fomenko L.S., Lubenets S.V., Natsik V.D., Stetsenko Yu.E., Izotov A.N.[(1)], Nikolaev R.K[(1)], Sidorov N.S. [(1)]
B.I.Verkin Institute for Low Temperature Physics and Engineering, NAS of Ukraine,
Lenin Ave., 47, Kharkov, 61103, Ukraine,
[(1)]Institute of Solid State Physics, Russian Academy of Sciences, Institute Ave., 15,
Chernogolovka, Moscow Distr., 142432, Russia

Introduction

Considering the arrangement of the centers of gravity of its molecules, fullerite C_{60} forms a face-centered cubic (fcc) lattice through the whole range of existence of its solid phase. For each C_{60} molecule in the lattice there are two tetrahedral sites as well as one octahedral site. The weak van der Waals interaction between the C_{60} molecules as well the presence of comparatively large interstitial sites result in the crystal easily absorbs impurities and is easily amenable to intercalation. The physical and mechanical properties of crystalline C_{60} are considerably affected by intercalation of the crystal by different impurities.

Of possible intercalants, gases occupy a highly important place for C_{60}. Gas atoms and molecules can diffuse into the cavities of the fullerite lattice and form interstitial solutions. This investigation is concerned with the influence of interstitial hydrogen on the mechanical properties of C_{60} fullerite. This question has not previously been studied.

As follows from previous investigations [1-3], the temperature dependence of the microhardness H_V in pure C_{60} single crystals has a step-shaped feature (see Fig. 2). The position of the step correlates with $T_c \approx 260$ K of the orientational *fcc-sc* phase transition. It is known that an impurity, when introduced into the C_{60} lattice, as a rule, suppresses T_c and smears the temperature interval of this transition. The goal of this study was to investigate the effect of saturation of C_{60} with hydrogen upon the value of microhardness and the anomalous behavior of its temperature dependence near the phase transition point.

Experimental procedure

The Vickers microhardness was investigated using a standard PMT-3 device at room temperature and a device with a freely suspended indenter at 77-300 K. The loading on the indenter was 0.05-0.1 N during the time ~ 10 s. The measurement was made in the process of cooling. The microhardness was calculated by the equation $H_V = 1.854P/(2a)^2$, where $2a$ is the indentation diagonal. No less than ten impressions were made on the sample surface at each temperature. The calculated microhardness values were averaged over all impressions.

Experimental results and discussion

The study of intercalation kinetics by microindentation method**.** The dependence of microhardness of two C_{60} single crystals on the H_2-saturation time is shown in Fig. 1. The measurement was made on the habit plane (111) at room temperature. It is seen that the H_2-saturation of the single crystals leads to a considerable (2-3.5 times) increase in their microhardness. Note that during equal times of saturation, different crystals absorb different amounts of hydrogen. This is manifested by different changes in the lattice parameters and microhardness, which may be due to different purity and perfection of the crystals. The microhardness growth correlates with the increase of the lattice parameters.

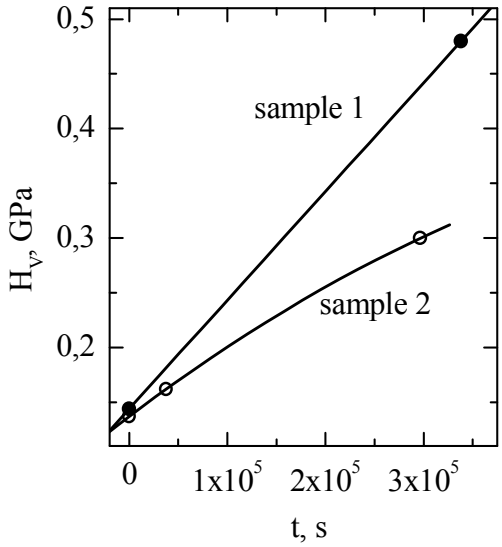

Fig. 1. Dependence of microhardness of two C_{60} single crystals upon H_2-saturation time at T = 290 K. The samples were saturated at H_2 pressure p = 30 atm and T = 259 ^{0}C.

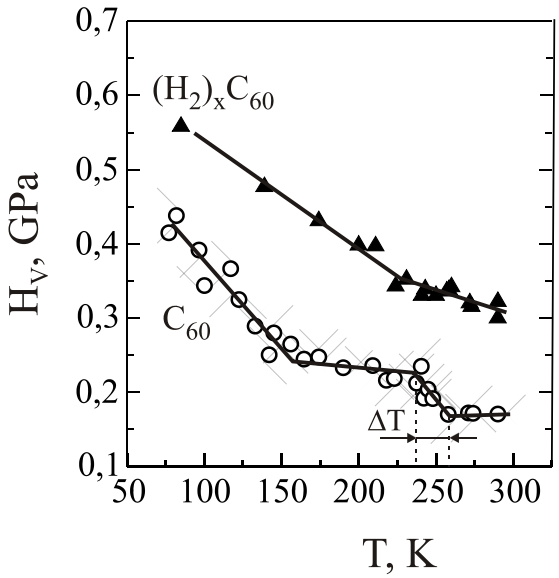

Fig. 2. Temperature dependence of microhardness of pure and H_2 -saturated C_{60}.

Temperature effect on microhardness of pure and intercalated C_{60}. The temperature dependences of microhardness measured on single crystals of pure and H_2-saturated C_{60} are shown in Fig. 2. The basic distinctions in the micromechanical behavior of these materials are as follows:

(1) At room temperature the microhardness of intercalated C_{60} was two times higher than that of pure C_{60}.

(2) The step-like feature in the curve $H_V(T)$ is distinctly seen for pure C_{60} on the transition to *sc* phase below 260 K. In $(H_2)_xC_{60}$ single crystal the phase transition is smeared. As a result the step in the temperature dependence of microhardness is absent but the dependence $H_V(T)$ grows stronger starting with $T \approx 230$ K.

Thus, intercalation of fullerite C_{60} with hydrogen is accompanied by (i) an essential increase in the absolute values ("background") of microhardness and (ii) by an appreciable transformation of the fine features in the temperature dependence $H_V(T)$ in the region of the *fcc-sc* phase transformation. The first effect may be caused by impurity atoms which affect the elastic properties of the material and the mobility of dislocations. The other effect may be attributed to the impurity influence on the dynamics of the orientational degrees of freedom of C_{60} molecules.

The influence of these factors upon the mechanical properties of C_{60} was considered thoroughly in [4]. This investigation prompts the conclusion that the anomalies in the temperature dependences of microhardness in pure and intercalated C_{60} crystals are mainly due to the features of the dislocation-orientational interaction in perfect and interstitial-deformed lattices of fullerite.

Conclusion

Intercalation of pure C_{60} single crystal with hydrogen results in (i) an increase of microhardness (up to 3.5 times), and (ii) the elimination of the step-shaped feature in the temperature dependence of microhardness in the region of the *fcc-sc* phase transformation.

This work was partially supported by the target combined program of the scientific researches "Nanostructured systems, nanomaterials, nanotechnology' of the National Academy of Sciences of Ukraine (project No. 3-025-2004).

References

1. Tachibana M., Michiyama M., Kikuchi K., Achiba Y., Kojima K. Temperature dependence of the microhardness of C_{60} crystals. Phys. Rev. B 1994; 49(21): 14945-14948.
2. Fomenko L.S., Natsik V.D., Lubenets S.V., Lirtsman V.G., Aksenova N.A., Isakina A.P., Prokhvatilov A.I., Strzhemechny M.A., Ruoff R.S. Correlation of low-temperature microplasticity anomalies with structure transformations in C_{60} crystals. Low Temp. Phys. 1995; 21(4): 364-366.
3. Lubenets S.V., Natsik V.D., Fomenko L.S., Isakina A.P., Prokhvatilov A.I., Strzhemechny M.A., Aksenova N.A., Ruoff R.S. The structure, slip systems, and microhardness of C_{60} crystals. Low Temp. Phys. 1997; 23(3), 251-261.
4. Natsik V.D., Lubenets S.V., Fomenko L.S. Effect of orientational ordering of molecules on dislocation mobility in C_{60} crystals. Low Temp. Phys. 1996; 22(3): 264-269.