Molecular dynamics simulation of the growth of carbon films obtained depositing C_{60} fullerenes on silicon substrates

E.B. Halac[1*], M. Reinoso[1], A.G. Dall'Asén[2], H. Huck[1], E. Burgos[2]

1 Dpto Física, C.N.E.A., Argentina- Universidad Nacional de San Martín, Argentina 2 Dpto Física, C.N.E.A., Argentina-CONICET, Argentina

*halac@cnea.gov.ar

INTRODUCTION

Hard carbon materials obtained from polimerized or amorphized C_{60} molecules have shown very interesting properties. Several experimental works have been performed in order to obtain hard carbon coatings from C_{60} molecules accelerated at a defined deposition energy (E_{dep}) [1,2]. From the theoretical point of view only the impact of individual molecules has been studied. We present here a theoretical simulation of the growth of films by sequential deposition of C_{60} molecules on silicon and diamond substrates.

COMPUTATIONAL MODEL

Molecular dynamics

* Semiempirical many-body Tersoff potential for C-C, C-Si and Si-Si interactions [3]

* Berendsen's thermal bath [4]: T = 300 K; $\tau = 50\Delta t$

Substrates

Diamond (100) and **Silicon (100)**: 8 layers (2 fixed) of 50 atoms. Initial conditions: P=0 T=300 K (during 1000 fs)

Deposition of C_{60} molecules

Normal incidence. Initial random orientation.

Molecules vibrating at 300 K.

E_{dep} from 10 to 1000 eV.

Individual molecules: studied during 3000 fs.

Films: ~ 30 molecules; 5000 fs between impacts.

RESULTS

Deposition of individual C_{60} molecules

* On Si (100) and diamond (100) substrates

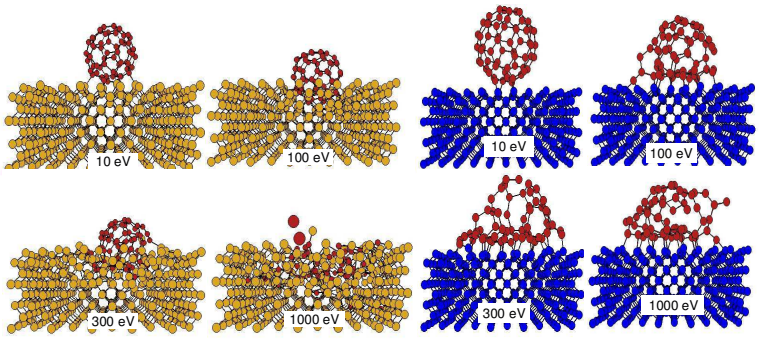
$E_{dep} \leq$ 10 eV: the molecule either bounces away or remain weakly bonded to the substrate.

100 eV < E_{dep} < 300 eV: increasing number of bonds and distortion of the fullerene cage with E_{dep}.

E_{dep} > 300 eV: the molecule is fragmented, some pieces bond to the sustrate and others bounce away.

* On diamond (111) substrates

The threshold energy for fragmentation of fullerenes is significantly lower (~100 eV).



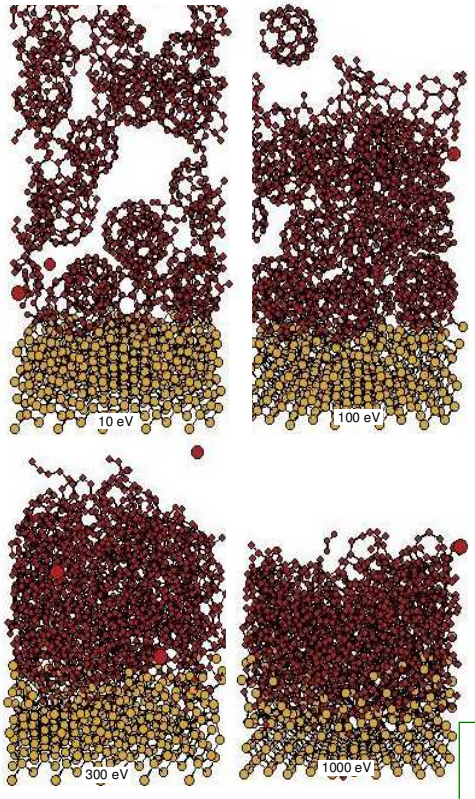
Snapshots of C_{60} molecules thrown at different E_{dep} on Si (100).

Snapshots of C_{60} molecules thrown on diamond (100).

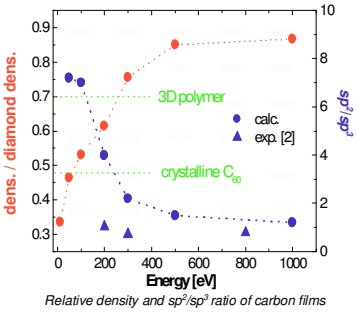
Growth of carbon films by deposition of C_{60} molecules

E_{dep} < 300 eV: C_{60} preserve the molecular identity, but some intermolecular covalent bonds begin to insinuate.

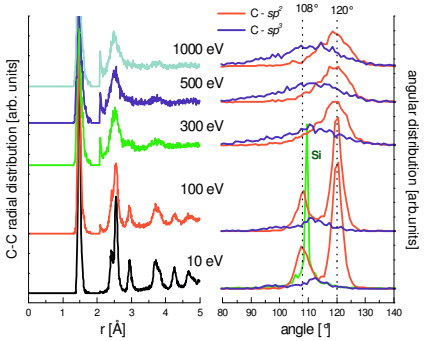
E_{dep} > 300 eV: C_{60} molecules are fragmented forming high density films. Density and substrate distortion increase with E_{dep}.



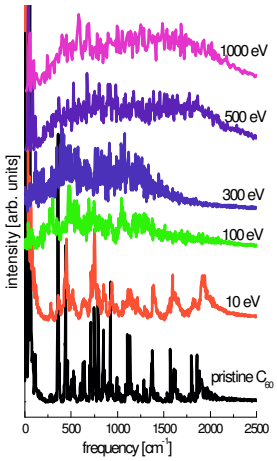
Films grown throwing C_{60} molecules on Si (100).



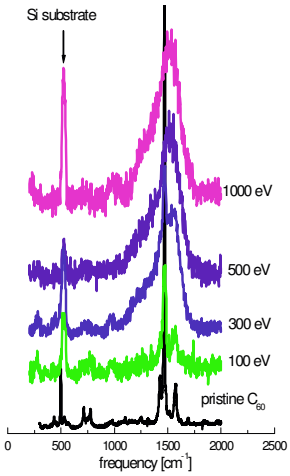
Relative density and sp^2/sp^3 ratio of carbon films grown on Si (100) vs. E_{dep}.



Radial and angular distribution functions for carbon films grown on Si (100).



Vibrational DOS for carbon films grown on Si (100) at different E_{dep}.



Experimental Raman spectra of films grown from a C_{60} ion beam on Si (100).

CONCLUSIONS

The penetration depth of C_{60} is higher for Si than for diamond substrates, but in both cases is lower than the corresponding to C atoms [5]. This is in agreement with the experimentally observed poor adherence for C_{60} on Si.

Molecular identity is preserved for E_{dep} < 300 eV; for higher energies the films exhibit an increasing disorder until reaching the characteristics of amorphous carbon films resembling to those obtained from individual carbon atoms (the peaks corresponding to C_{60} molecules are lost in radial and angular distribution functions; long range order is lost). This is in agreement with structural changes evidenced by experimental Raman spectra of films grown from C_{60} ion beams [1].

The use of C_{60} molecules as projectiles allows to grow dense amorphous carbon films in a wide range of energies and it is reasonable to assume that they would have interesting tribological properties, based on hardness measurements from similar films grown by other methods.

REFERENCES

[1] H. Huck et al. Diamond and Related Materials, **11/3-6** (2002), 964.

[2] H. Huck et al. "Recent Research Developments In Physics", Transworld Research Network, 5 (2004) 217.

[3] J. Tersoff. *Phys. Rev. B* 39 (1989) 5566

[4] H.J.C. Berendsen et al. *J. Chem. Phys.* 81 (1994) 3684.

[5] E.B. Halac et al. ""MD simulation of the growth of thin films by deposition of carbon atoms and C_{60} molecules on diamond and silicon substrates". *Unpublished.*