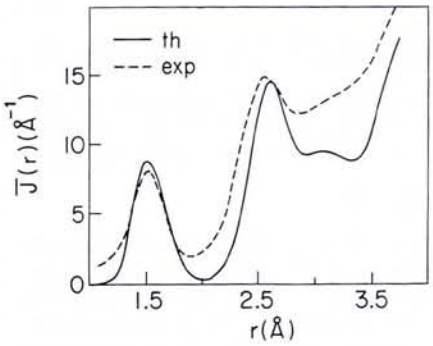

Fig. 5 — Theoretical (full line) and experimental (dotted line) RDF **J**(r) *of amorphous C.* **J**(r) = $4\pi r^2 \rho g(r)$, *where* ρ *is the average density and* g(r) *is the pair correlation function. The theoretical* **J**(r) *has been convoluted with the experimental resolution function.*

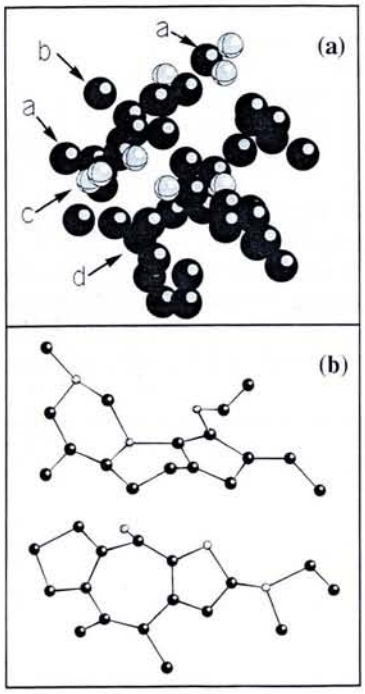

Fig. 6 — Microscopic structure of the computer-generated amorphous C network: the entire set of atoms belonging to the MD cell (a) and several 5-, 6-, and 7-fold ring structures of which the system is composed (b). Black and grey spheres indicate 3- and 4-fold coordinated atoms, respectively.

cal point of view α-C is very attractive, since it combines semiconducting properties, in some way similar to graphite, with a much higher hardness. Disordered forms of carbon are thought to consist of a mixture of threefold and fourfold coordinated atoms, as in graphite and diamond, respectively. The simultaneous presence of two coordinations depends on a delicate balance of different electronic binding forces and makes the simulation of α-C particularly challenging.

The RDF obtained with a 54-atom MD cell is reported in Fig. 5. The corresponding microscopic structure is shown in Fig. 6a, which displays the entire set of atoms belonging to one MD cell. Several 5-, 6- and 7-fold ring structures are shown in Fig. 6b. One sees that disorder introduces 5- and 7-fold rings, in addition to the 6-fold graphitic ones. Five and 7-fold rings are usually coupled as in carbon azulene molecules. Although the structure is truly three dimensional, the atoms are arranged into several *thick planes*, two of which, labelled (a) and (b) in Fig. 6a, are roughly parallel to each other. Four-fold coordinated atoms, indicated by the grey spheres, show a tendency to clustering and bind together the locally planar structures. Thus they contribute significantly to the hardness of the system.

In conclusion, we have presented only a few applications of the MD-DF approach to liquid and amorphous semiconductors, but they are sufficient to demonstrate the power of the method.

Meetings

Corrections and Up-dates

Dates Interchanged, Schools

25-29 Sept. Bad Honnef, FRG
DPG-Schule für Physik, Kurs IV:
Physik in der Mikroelektronik
J. Debrus, Physikzentrum Bad Honnef,
Hauptstr. 5, D-5340 Bad Honnef
A: 2.6.89 / 60 / German /
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2-6 Oct. Bad Honnef, FRG
DPG-Schule für Physik, Kurs V:
Nichtlineare Dynamik in Festkörpern
J. Debrus, Physikzentrum Bad Honnef,
Hauptstr. 5, D-5340 Bad Honnef
A: 2.6.89 / 60 / German /
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New, Workshop

20 Nov. 1989 Rijnhuizen, NL
3rd European Workshop on Free Electron Lasers; collaboration between research institutes and industry
A. Nijsen-Vis, FOM, Postbus 1207,
NL-3430 BE Nieuwegein
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