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Editorial

Giving credit where credit is due: The Stone–(Thrower)–Wales designation revisited

Naming things is a fundamental factor in communication between human beings, and because it has been a factor in transmission, it has been a factor in progress, at least within a given community. Communication became a science as soon as names were used to sort and classify things, and it is no wonder then that science was first and for a long time descriptive. Eventually the knowledge acquired by local observers, named scholars, savants, astronomers, philosophers, or wizards, became a genuine science (meanwhile turning wizards into scientists) as soon as it could become universally shared, which implies two conditions: one is to use a common language (once Latin, now English), another is to name the same thing by the same name. Hence, for science, naming things is not enough, correct naming is compulsory.

Unfortunately, although modern times have made communication and knowledge dissemination easier than ever, which is good for the universality of science, it has allowed wrong information to spread as fast as that which is correct. To give an example within the scope of this journal, the often unique properties and performance of carbon nanoforms have attracted many scientists whose background is not carbon-related, and this has induced a multiplication of the irrelevant use of terms whose meaning was clear and universally shared within the carbon community before the Nobel-recognised nanocarbon saga started. The editors of CARBON journal are struggling daily to identify such misuses – among which the words related to graphite ("graphite", "graphitic", graphitisation") are probably the most frequent – within the tens of manuscripts that are submitted for publication every week. This eventually comes with two potential problems.

The first problem occurs when the misuse has been so widespread that the original meaning has definitely been altered. This is what has happened with the word "graphene". Thanks to the input of H. P. Boehm, graphene was clearly defined in 1995 in a publication openly accessible to all, the International Union of Pure and Applied Chemistry (IUPAC) nomenclature [1], as "*a single carbon layer of the graphite structure, describing its nature by analogy to a polycyclic aromatic hydrocarbon of quasi infinite size*". In spite of this, the expression "few-layer graphene", which is not compatible with the IUPAC definition strictly speaking, has become quite popular and is now understood by everyone as a stack made of few superimposed graphenes. One might think that considering something now to be correct, when it clearly does not conform to the original meaning is a pity, but it is perhaps forgivable? Languages are in constant evolution, new words are always being created and new meanings appear, but what is important is that the same word is understood by everyone as designating the same thing.

The second problem is more of an issue. It occurs when the alteration of the initial meaning results in giving credit to a person that rightly belongs to someone else. One example has already been provided as an editorial in this journal dealing with the credit to be given for the discovery of carbon nanotubes [2]. The other example which will be emphasized here is that of the "Stone–Wales defect". For (almost?) everyone nowadays (including us, until recently) interested in topological defects in graphene, the symmetrical combination of two 5–7 ring pairs (Fig. 1) is designated as such, i.e., a "Stone–Wales defect".

This designation is wrong. After it was found that an earlier work by P. Thrower considered the existence of 5–7 pairs as defects in graphene [3], it was later proposed to rename this defect, as shown in Fig. 1, as a "Stone–Thrower–Wales" defect. This is not correct either. In order to sort this out, one has to go back to the original papers.

The original paper by Stone and Wales in 1986 [4] was not discussing topological defects in graphene or nanotubes, and did not introduce the symmetrical double 5–7 pair defect. It was discussing the possibility of isomerisation in C_{60} fullerene molecules and introduced a symmetrical double 5–6 pair defect, i.e., a pyracylene motif, as shown by the copy of the related figure below (Fig. 2).

This was an important paper at that time, as it introduced the possibility of creating new fullerene isomers by simply rotating the central C—C bond of the defect. This overall mechanism of bond rotation was then referred to as the "Stone–Wales **transformation**" and then was soon generalised under this name as soon as the bond rotation that occurs

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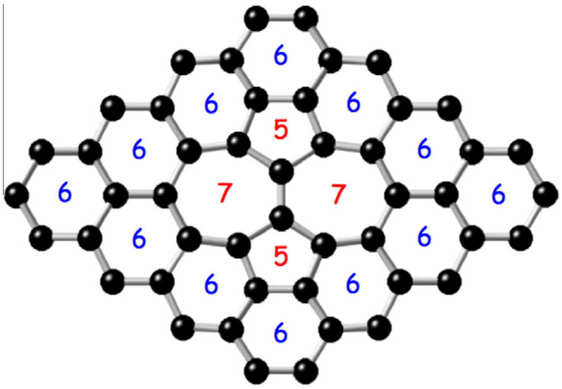

Fig. 1 – Ball-and-stick model of the 5–7-ring double pair defect surrounded by hexagonal (6) rings, so-called “Stone–Wales defect” in the current literature. (A color version of this figure can be viewed online.)

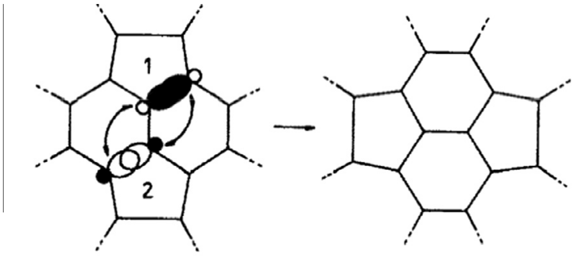

Fig. 1. Structural rearrangement relating isomers of C_{60}. The fragment shown includes pentagons 1 and 2 of the twelve pentagons present in the molecule (see fig. 2). The rearrangement formally requires the two sigma bonds shown to be broken, and new bonds to be formed as indicated by the arrows.

Fig. 2 – Original figure and its related caption from the paper by Stone and Wales [4]. The rotation of the central C—C bond within a symmetrical double 5–6 pair defect was proposed as the possible mechanism for isomerisation in C_{60} fullerenes.

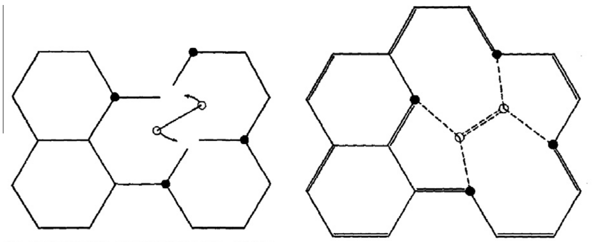

FIG. 4. Diffusion via direct interchange in graphite. FIG. 5. Saddle point configuration for direct interchange.

Fig. 3 – Original figures and their related captions from the paper by Dienes [10]. The rotation of the central C—C bond within a group of four 6-rings (left, yet the fourth ring involved is not fully drawn), turning it into a symmetrical double 5–7-ring pairs (right), was proposed as the preferred mechanism for self-diffusion in graphite.

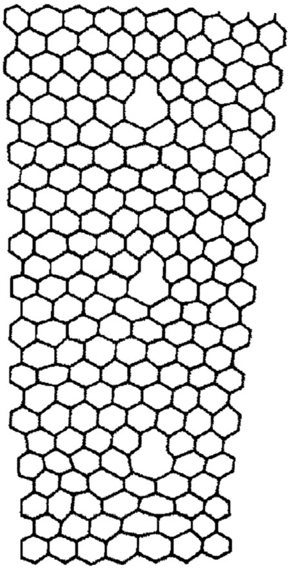

FIG. 10. Configuration (in two dimensions) of the lattice around three edge dislocations, equally spaced, constituting a symmetrical boundary.

Fig. 4 – Original figure and its related caption from the paper by Roscoe and Thomas [11]. All rings are hexagonal, yet highly deformed.

within any kind of four-polygon motif (involving pentagons, hexagons, and heptagons), as a mechanism for moving specific polygons around a fullerene surface [5]. The specific application of the Stone–Wales transformation to double 5–7 pairs came later while discussing growth or deformation mechanisms and subsequent properties in carbon nanotubes [6–8]. Single and double 5–7 ring pairs became far more popular defects to consider with nanotubes and then with graphene [8,9] than with fullerenes because, as opposed to other kinds of defects such as 5–6, double 5–6, 5–6–5 rings and so on, the strains induced by the pentagon and the heptagon mostly compensate, leaving the tube wall (or the graphene plane) topology affected to only a very small extent. Correspondingly, as nanotubes were becoming more and more prevalent over fullerenes in research, the so-called Stone–Wales transformation was increasingly applied to the double 5–7 ring pair defect rather than to any other defect combination. And that is where the confusion comes from: the designation of the specific bond rotation mechanism was rapidly merged with the designation of the double 5–7 pair defect in which the rotation mechanism was then considered to occur, ultimately resulting in naming the double 5–7 ring pair defect also after Stone and Wales even though the central bond rotation was even not considered.

This is not right, because symmetrical double 5–7 ring pairs were first illustrated by Dienes in 1952 [10] as an intermediate configuration that would exist during a proposed theoretical self-diffusion mechanism in graphite (Fig. 3). This mechanism of self-diffusion has, to our knowledge, never been verified or expanded on, and 60 years later Dienes’ work appears to have been forgotten. However it is clear that he was the first person to propose such a configuration. He was also – probably – the first to propose the mechanism of rotation of the central bond within an ensemble of four rings.

One can see that the principle of the rotation of a C—C bond within a group of *sp*^{2}-carbon rings was then proposed

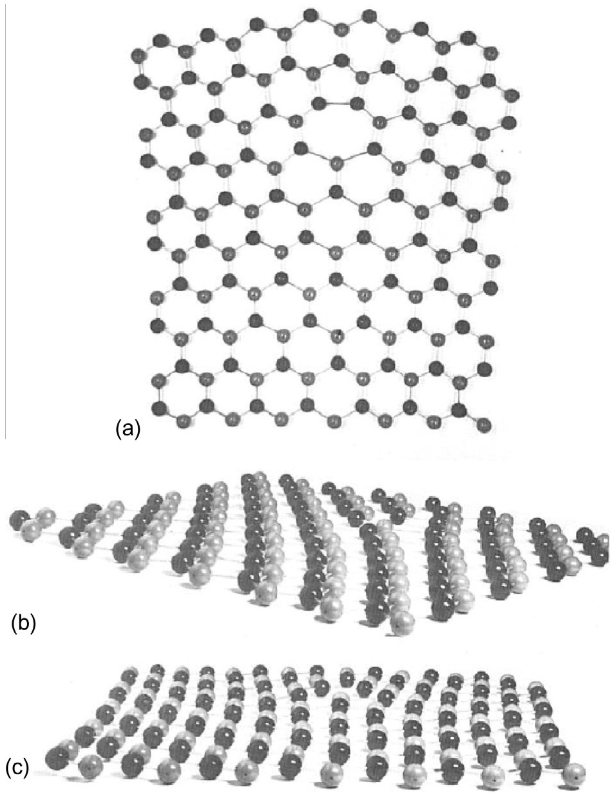

Fig. 25. Model of a unit dislocation of length $c/2[0001]$ such as exists at the ends of vacancy lines: (a) plane view; (b) and (c) oblique views showing two different ways in which the half-plane of atoms can be considered to have been removed.

Fig. 5 – Original figure and its related caption from the paper by Thrower [3]. A ball-and-stick model of graphene lattice is deformed by introducing a vacancy line, at the end of which a 5–7 ring pair exists to accommodate the resulting strain.

– and found energetically valid – long ago before the paper by Stone and Wales, yet both the sp^2-carbon ring combination involved and the authors' goals were different.

Now, what is the input of Peter Thrower in this picture? Back in the early seventies, considering that non-regular rings (i.e., other than 6-rings) could be incorporated within the graphene plane had not really come up to carbon scientists' mind. For example, in 1966, Roscoe and Thomas [11] proposed a model for grain boundaries as shown in Fig. 4.

In Fig. 4, all rings are hexagonal, and the strain is accommodated by considering vacancies at the edge of a dislocation and severe angle deformations. Now that the graphene lattice can be directly imaged by means of near-field microscopy or aberration-corrected transmission electron microscopy, such a model looks definitely unrealistic. This was not true at that time, as it had deserved to be published in CARBON journal! In opposition to this all-6-ring approach, P. Thrower proposed that single 5–7 pairs were present at the ends of vacancy lines in the hexagonal lattice of graphite (Fig. 5) that were produced by, e.g., neutron irradiation [3]. In that case then, even when two 5–7-ring pairs were considered, they were not adjacent since they had to be located at both ends of a vacancy line, and no bond rotation could of course be envisaged.

Incorporating 5- and 7-rings to the graphene lattice as in Fig. 5 ensures that most of the strain is supported by two rings only, as opposed to what was proposed in Fig. 4, where all rings had to be deformed in some extent. Although it is obviously a more favourable situation from the point of view of energetics, it was demonstrated to actually exist only recently [12]. Hence, because he was first to consider the introduction of non-regular cycles in the graphene lattice, P. Thrower appears as a pioneer of the modern vision of graphene topology which developed more than 20 years later starting with the paper by Terrones and Mackay in 1992 [13].

To summarise, the current designation of the defect sketched in Fig. 1 as the "Stone–Wales defect" (or the "Stone–Thrower–Wales defect") is not correct, and is misleading. For the various aspects addressed in this editorial, fairer designations should be:

- To designate the **single 5–7 pair** defect as shown in Fig. 4 as the "**Thrower defect**"
- To designate the **double 5–6 pair** defect as shown in Fig. 2(right) as the "**Stone–Wales defect**"
- To designate the **double 5–7 pair** defect as shown in Figs. 1 and 3(right) as the "**Dienes defect**"
- To designate the **rotation mechanism of the central bond of a group of four polygons** (involving pentagons, hexagons, and heptagons) as "**a Dienes transformation**" or possibly "**a Dienes–Stone–Wales transformation**".

This way, not only will the naming be right, but the credit will go to whom it rightly belongs.

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