Supplementary Material (ESI) for Nanoscale

Supporting Information for: Safer energetic materials by a nanotechnological approach

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1 Preparation of V_2O_5@CNF/Al nanothermites

Oxidized carbon nanofibers. In a one-neck flask, 2 g of Pyrograf carbon nanofibers (PR-24-XT-HHT grade, graphitized at 3000°C, bought from Applied Sciences, Cedarville, OH) are suspended in 125 mL of concentrated nitric acid (65%, Acros). A reflux condenser is added, and the mixture is heated to 125°C for 3 h under constant magnetic stirring. After cooling down to room temperature, the suspension is filtrated over a 450 nm Omnipore membrane (Merck Millipore). The filter cake is washed two times with water and once with acetone. It is dried for 2 h at 80°C. Yield $\sim$ 95 wt%.

V_2O_5@CNF nanocomposite. In a beaker with high form, 260 mg of ammonium metavanadate (NH_4VO_3, Strem) are dissolved in 20 mL of ultrapure water. The beaker is placed on an oil bath and heated to 70°C under magnetic stirring. After the complete dissolution of the vanadium salt, 200 mg of the oxidized carbon nanofibers are added. The suspension is stirred at a temperature of 70°C until the water is completely evaporated (about 12 hours). The dry black residue is calcined for 1 h in a tubular furnace at 325°Cand with a heating rate of 1 K/min under an argon flow of 9 L/h. Yield: about 400 mg of a V_2O_5@CNF nanocomposite containing about 50 wt% of oxide.

V_2O_5@CNF/Al nanothermite. In a pear-shaped one-neck flask, 340 mg of the V_2O_5@CNF nanocomposite (48.6 wt% of oxide) are added to 400 mL of acetonitrile. The flask is placed on an ice bath, and the suspension is homogenized by sonicating it for 30 min with a 400 W sonotrode (Hielscher

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Ultrasound) whose tip is placed in the solution, with 80% power and an 80% duty cycle. 160 mg of nano-aluminum (Al 50 P, 50 nm particle size, 60.85 wt% active Al content) are added to the suspension, which is then magnetically stirred for 15 min and sonicated for another 15 min in a bath sonicator. Finally, the acetonitrile is removed on a rotary evaporator under vacuum. The final pressure is below 0.1 mbar.

The sensitivity (friction, impact, ESD) of the nanothermite is measured on the powdered sample. The unconfined combustion measurement by TRC is carried out on pellets of 50 mg each, which are formed in a hydraulic press with a pressure of 95 MPa. Their diameter and their height are about 4 mm.

2 X-ray diffractogram of V_2O_5@CNF/Al combustion residues

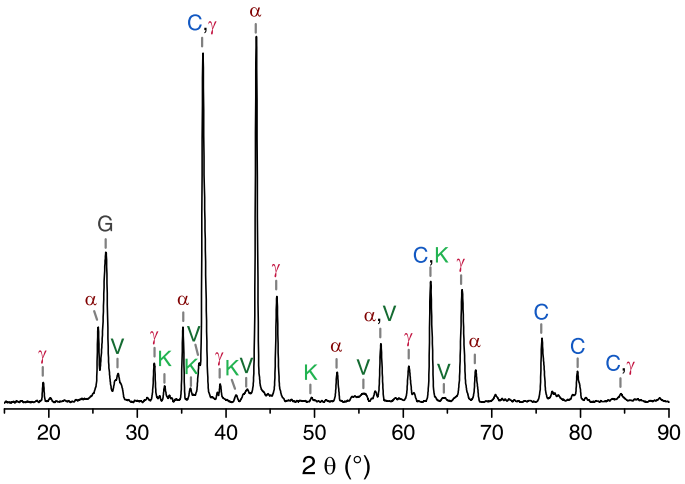

Figure S1: X-ray diffractogram of the combustion residues of the V_2O_5@CNF/Al nanothermite. The annotated phases are Graphite (56-159, **G**), vanadium(IV) oxide (44-252, **V**), Karelianite (vanadium(III) oxide, V_2O_3, 34-187, **K**), vanadium carbide (V_8C_7, 35-786, **C**), Corundum (α-Al_2O_3, 10-173, $\boldsymbol{\alpha}$) and $\boldsymbol{\gamma}$-Al_2O_3 (50-741, $\boldsymbol{\gamma}$).

3 Instructions for *nt-timeline*

3.1 Installation

nt-timeline is a program to create "timeline" images from combustion videos. It is written in the Go programming language, which is an Open Source project by Google. Before using *nt-timeline*, it must be compiled. For this,

you will need to install the Go language compiler on your computer. The source code for the Go language, which works under Linux, Mac OS X and a few other operating systems, can be downloaded at `http://golang.org/`. Binaries for Windows can be downloaded at `http://code.google.com/p/gomingw/`. The program has been tested under the release r56 from March 7, 2011. After installing the Go compiler, the compilation is carried out in two steps:

1. Compile the source: execute the command `8g nt-timeline.go`.
2. Create the executable program: execute the command
   `8l -o nt-timeline nt-timeline.8` (Linux, Mac OS) or
   `8l -o nt-timeline.exe nt-timeline.8` (Windows).

3.2 Use

The program *nt-timeline* requires the frames of the combustion video as jpg files, one for each frame. It extracts one line of pixels of each image and puts them one below the other in the output image, which is saved as a png image. For basic use, the program is called on the command line as follows:

```
nt-timeline -o output.png -l 104 *.jpg
```

In this example, all jpg files in the current directory (`*.jpg`) will be used as inputs, and the output file name will be `output.png`. Line 104 (from the `-l` flag) will be extracted from each image. The width of the output image (the x axis) is equal to the width of the input, while its height (the t axis) is equal to the number of input files.

The output image can be further analyzed to find the the position of the combustion front at each point in time. At the moment, this has to be done manually in an image manipulation software.