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Microfluidic devices reduce protein consumption required for identifying crystallization conditions and obtaining well ordered crystals. This nanoliter volumes approach has nevertheless some inconvenient, generally involving higher levels of supersaturation than equivalent experiments at the microliter or milliliter scales.

As the influence of channel depth of the PDMS microcircuits has not yet been evaluated, we have undertaken a comparison of the nucleation depending of this parameter. We observed that it is indeed correlated with the supersaturation needed to get crystals [1]. When the depth of the microchannels is decreasing the number of lysozyme crystals is dramatically reducing whereas their mean size is increasing.

Consequently, in order to uncouple nucleation and crystal growth, we propose original microfluidic chips which can be used to initiate nucleation in its deepest section and facilitate crystal growth in its shallow end.

The data presented in this work can contribute to a better control of the crystallization in microfluidics and shed light for the design of new microcircuits uncoupling nucleation and crystal growth that should facilitate the appearance of single crystals suitable for X-ray diffraction. They can also be used for macroseeding and microseeding experiments to improve the quality and size of crystals obtained after a first random screening.

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**Keywords:** crystallization, microfluidics, nucleation

## MS35.P26

*Acta Cryst.* (2011) **A67**, C465

### Cubic growth of natural diamond

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Natural diamond grows by at least three different modes: (a) Faceted growth on {111} planes giving octahedra; (b) Fibrous growth in <111> directions giving cubes [1]; and (c) Cuboid growth on crinkly surfaces approximating to {100}, which also produces cubes [1]. Combinations may also occur: growth by (a) followed by (b) gives coated stones [2]; and (a) and (c) growth modes may occur together to give combined morphologies. Twinning of (a) gives spinel-type contact twins (called 'macles') [3] and twinning of (b) gives fluorite-type interpenetrant cubes [4]. Subsequent dissolution may greatly modify the morphology: for example, octahedral diamonds grown by mode (a) may dissolve into rounded rhombic dodecahedra [5].

Here we report the existence of a fourth mode of growth: (d) Faceted growth on {100} planes. Flat cube facets are a common occurrence for *synthetic* diamonds grown by high-pressure high-temperature techniques, especially at the lower range of temperatures at which diamonds are formed; but cube facets are so rare in nature that some have denied that they are a true growth form. It is true that they have been seen only on small diamonds (< 1 mm). Their absence from larger diamonds may simply be the result of their growth rate being much larger than that for octahedral facets and thus they grow out.

We also report another finding [6]: a diamond which has grown by fibrous mode (b), followed by octahedral growth (a): an unusual

occurrence, whereas (a) followed by (b) is quite common.

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**Keywords:** diamond, morphology, X-ray topography

## MS35.P27

*Acta Cryst.* (2011) **A67**, C465

### Calculating the interaction energy between 1-D hydrogen bond motifs using semi-empirical methods

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One dimensional hydrogen bond motifs often, but not always, tend to display needle-like morphologies which extend in the motif direction. Perhydropyrimidin-2-one and a highly substituted derivative display identical 1-D hydrogen bonding motifs. However, the former displays a block morphology while the latter grows exclusively as needles. These observations have been investigated by calculating the interaction energy between a motif and its surroundings.

A 7 motif pack was constructed. Each motif was 6 molecules long and the central one was surrounded by its 6 nearest neighbours. MOPAC2009 [1] was used to optimize this pack using the AM1 method. The pack was then split into a core and a shell and these energies were also computed. The difference in the energy of the core + shell and the energy of the pack is taken to be the interaction energy. The interaction energy per 100 Å<sup>2</sup> of core surface (Connolly) was calculated. There is a significantly lower interaction energy calculated for the substituted system. This suggests that in nucleation and crystal growth the structure will advance slower normal to the 1-D motif direction.

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**Keywords:** 1D, hydrogen\_bonding, morphology

## MS35.P28

*Acta Cryst.* (2011) **A67**, C465-C466

### Morphology of synthetic tourmaline crystals

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Single crystals of colored Co-, Ni-, Fe-, (Ni,Cr)-, (Ni,Fe)-, and (Co,Ni,Cr)-bearing tourmalines have been grown on a seed in boric, boric-alkaline, boric-fluoride, boric-chloride-fluoride, and boric-chloride hydrothermal solutions at 400–750°C and 100 MPa [1]. The morphology of spontaneous tourmaline crystals formed in experiments in solutions of different composition has been studied.

Crystals synthesized in boric-chloride solutions, are characterized by the long prismatic habit (needles) formed by the trigonal pyramid {10-11} and the hexagonal prism {11-20} faces. Long prismatic