CRYSTAL GROWTH MORPHOLOGY AS A CRITERION OF IMPACT SENSITIVITY FOR POLYCRYSTALLINE EXPLOSIVES

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An important property of a solid explosive is its impact sensitivity. This determines a minimum force (or energy) which is needed for initiation of detonation. To measure impact sensitivity one can apply conventional drop weight test. The result of such experiment, the h_{50} value (cm), determines a minimum drop height which is needed to reproduce 50 % of successful trials. Previously, a number of the quantitative structure-activity relationships (QSAR), including very complex artificial neutral networks, were developed to predict the h_{50} values. These models are based on estimation of the molecular features (topological, electrostatic potential, volume, orbital information, etc) and provide satisfactory results.

On the other hand, the abovementioned QSAR models do not account the solid-state-derived properties of explosives. Conventional appearance of the drop weight test sample is granulated polycrystalline form. Thus, when dropped on the sample surface, the mechanical energy is shared through the contact points between separated neighboring crystals. The pressure formed upon dropping weight is extremely high in these points, which leads to changes in electronic band structure of the solid. Thus, it is clear that the crystal habit shape should affect the energy distribution efficiency and, subsequently, the impact sensitivity.

Hypothetically, the most closely packed polycrystalline materials should have ideally spherical habit shape. The real crystal habits are more or less deviated from the ideal spherical shape. Thus, the more the crystal habit deviates from sphericity, the more compressibility of this polycrystalline material is; graphically, this can be illustrated as in Fig. 1 a, b.

In the present report we introduce a measure of such deviation of the crystal habit shape (θ). This is based on the relation between the volume-surface ratio in an ideal sphere and a real crystal sample. Thus, if $V_1 = V_2$ and R is the radius of the sphere with V_1 (Fig. 1 a, b) than the crystal shape deviation (θ) can be expressed as the following.

$$\theta_1 = \frac{4\pi R^2}{V_{cryst}};\ \theta_2 = \frac{S_{cryst}}{V_{cryst}};\ \theta = \frac{\theta_2}{\theta_1} = \frac{S_{cryst}}{6^{2/3} V_{cryst}^{2/3} \pi^{1/3}}$$

In order to support this hypothesis, we have applied a series of calculations of the crystal morphology using the known crystal structures of the TKX-50 family explosives with the measured impact sensitivity. Figure 1 demonstrates the calculated results for highly explosive phenyldiazonium chloride (c) and insensitive tetrafluoroborate (d) as preliminary models. On the basis of the calculated results for the TKX-50 family explosives we can safely conclude that a dependence exists between the crystal habit shape and the corresponding h_{50} value.

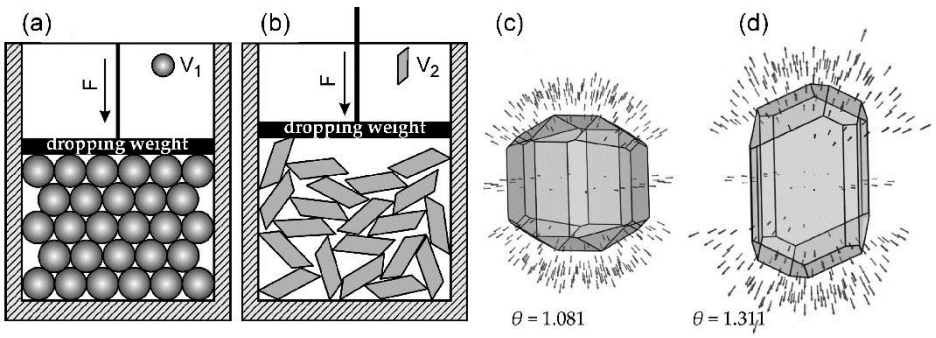

Fig. 1. The influence of the crystal habit shape on the energy distribution (a, b) and the calculated crystal habits for phenyldiazonium chloride (c) and tetrafluoroborate (d)