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WHY DOES AN EXPLOSIVE EXPLODE?

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At a macroscopic level, the detonation phenomenon is well known. In this aspect, how an energetic molecular crystal detonates has been described perfectly. But the question as to why one molecular compound detonates and why another one does not is still a real fundamental problem in spite of the technical progress both in ultra fast spectroscopy and in super computer simulations of molecular electronic states and molecular dynamics.

However, we should like to emphasize the following fact previously discussed (PEYRARD... paper) in the two dimensional molecular dynamics model: as much as it is well established that the electronic molecular bond structure is involved in the detonation, the crystal structure seems also very strongly implicated in the phenomenon because it controls the energy dissipation factor which is mainly determined by the balance between the energy release when molecules dissociate and the energy transferred into transverse oscillations(1).

As shown in Fig. 2 and 3 (crystal structure effect) both the dimensions a and b of the unit cell along the X and Y axes (Fig. 1) and the position of the intramolecular bond NC axis with the shock wave direction: α angle in Fig. 1, play a role in determining if a 2D lattice can sustain a detonation.

Figure 1

(1) In the case of nitromethane, it has been shown by a quantum theoretical approach that no energy is dissipated into vibrational modes of the nitromethane fragments during the "active" excited electronic state 1A2 dissociation.

The limit detonation velocity $v$ depends on the ratio $a/b$ which affects the way the energy is shared between longitudinal and transverse motions. (Fig. 2)

![Figure 2]

The orientation $\alpha$ of the CN intramolecular bond against the shock wave propagation axis appears as a determining factor, correlated to the sensitivity to shocks $\sigma$, to induce a detonation wave. (Fig. 3). Here, for nitromethane, $\alpha$ angle must be $\geq 45^\circ$

![Figure 3]

This last result agrees with the experimental results showing anisotropic behaviors in PETN and RDX monomolecular crystals (see SAMIRANT, DUFORT's paper and J. DICK, J. Appl. Phys. Lett. 44, 859 (1984)). To our knowledge, nitromethane in solid phase does not explode (SNPE) whereas it does in liquid phase. We think that perhaps in the crystal the C-N fixed bond chains prevent the detonation and that in the liquid, if such supposedly frozen chains would exist, these are in perpetual reorientation and thus, the $\alpha$ values which sustain the detonation do appear frequently.

We suggest that it would be interesting:

1 - to observe by the molecular dynamics 2D simulations, how the detonation wave
propagation can be modified by introducing in the chain some variation in $\alpha$,
2 - to pursue systematic experimental works in order to prove if it does exist
$\alpha$ values which sustain and $\alpha$ values which do not sustain a detonation in a single
molecular crystal. (if possible ! nitromethane)

All these microscopic results would qualitatively account for the connection bet-
ween anisotropic detonation properties of solids, differences between solid and
liquid phases properties, and electronic molecular or crystal structure which
cannot be explained by any macroscopic model which ignores the molecular and crystal
structures.

These investigations could help to begin to answer the question : why does an
explosive explode ? which, in conclusion, to day, has no answer.