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TITLE: **SINGLE CRYSTAL ORIENTATION EFFECTS IN SHOCK INITIATION OF PETN EXPLOSIVE**

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SINGLE CRYSTAL ORIENTATION EFFECTS IN SHOCK INITIATION OF PETN EXPLOSIVE*

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ABSTRACT

Over the past nine years in Los Alamos we have studied shock initiation of detonation in single crystals of PETN explosive. We have demonstrated the effects of point defects and crystal orientation on shock sensitivity. Here we report recent work on orientation effects and anomalous detonation in <110> orientation at 4 GPa.

Plane shock initiation of detonation involves conversion of the mechanical energy of uniaxial compression into heat and subsequent chemical decomposition. In many instances there is localization of this energy conversion at hot spots. In some way the work of plastic deformation is converted into heat. In polycrystalline materials or defective single crystals this may involve the multidimensional strain of void collapse. In perfect single crystals it must involve slip on particular lattice planes. Any process due to defects or steric hindrance that increases the plastic work or the dissipation will make the material hotter. The presence of defects or impurities that can act as decomposition sites of lowered activation energy will further sensitize the explosive.

In previous work we have shown that <110> PETN single crystals are shock sensitized by gamma radiation.[1] This sensitization was interpreted as due to increasing the number of initiation sites, these sites being the defect sites of molecules decomposed by the radiation. Exposing crystals to gamma radiation provides a controlled way of adding defect sites to a nearly perfect crystal, although the nature of these defect sites still needs to be characterized and understood.

We also showed that shock sensitivity depends on crystal orientation in PETN.[2] We showed that this may be due to the differing slip systems available for plastic flow in different orientations. Much work remains to be done to establish this more firmly and to elucidate the physical mechanisms involved.

Much remains to be done to understand shock initiation of PETN single crystals at a molecular level. The bulk response can, in many ways, be described as homogeneous or liquid like, but certainly at a molecular level it must be heterogeneous.[3]

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There has been evidence for some time for anomalously large decomposition at 4 GPa in <110> PETN as well as evidence for an intermediate velocity transition. In very recent unpublished work we have shown that <110> PETN detonates at 4 GPa with a shorter run than at 8.5 GPa.

Previous Los Alamos experiments on PETN single crystals at 4 GPa by Dave Vier, Bobby Craig, Stan Marsh, Phil Halleck, and Jerry Wackerle[4,5] have shown unusual behavior indicative of anomalously large amounts of decomposition at this low shock pressure. Recently we did four experiments to explore this regime. In all these experiments the crystals were mounted on 5-mm-thick Kel-F buffer plates that were impacted by 11-mm-thick Vistal discs.

The first experiment was a wedge. The purpose was to confirm evidence for an intermediate velocity transition seen in an experiment done by Bobby Craig around 1970. Craig's crystal was 6-mm thick whereas ours was almost 8-mm thick. Detonation transition was observed at about 6.8 mm and 1.5 μs. This is astounding because it is a shorter run than one gets at 8.5 GPa. It means that there may be a special detonation regime around 4 GPa where the maximum resolved shear stress is reached.

Two shots were done with two image intensifier cameras. The first shot had an X-cut quartz crystal, a fused quartz disc, and a <110> PETN crystal. The purpose was to check techniques and exposure by repeating known results for quartz. The records were underexposed. Emitted light was recorded only from the X-cut quartz. The second shot had PETN crystals of <110>, <101>, and <100> orientations. Vier's work in 1979 showed that the <110> orientation emitted strongly at 4 GPa. The purpose of this experiment was to show that the orientations with easy slip for plastic flow would not emit under the same conditions. This is, in fact, what was observed. Snapshots were taken at 0.2 and 0.5 μs (0.8 and 2 mm) after shock entry into the crystals, based on the pressure excursion beginning at about 0.3 μs seen in an impact-face quartz gauge record for a 4 GPa shock in <110> PETN (Halleck and Wackerle).[4] In our experiments emitted light was recorded from the <110> crystal at both 0.2 and 0.5 μs, but it was six times brighter at 0.5 μs, consonant with the quartz gauge record.

The last of the series was emission spectroscopy of a <110> crystal at 4 GPa, with the data taken beginning 0.5 μs after shock entry for about 0.13 μs. Data were recorded over the wave length range of 360 to 700 nm. A low number of counts was obtained but the results indicate emission that is not in thermal equilibrium. In fact a broad peak at 460 nm can be tentatively attributed to the chemiluminescence of NO_2 radicals formed by PETN decomposition.

Some of this work needs to be checked, but the data confirm our view based on previous work that there is anomalous behavior in PETN at 4 GPa associated with orientation-dependent plastic flow. There is much that can be done to unravel and establish what is going on. It means we can study shock-induced chemistry in a solid explosive at a low pressure.

Willie Spencer helped with shot preparation and did the camera work with some input from Bud Winslow. Don Pettit helped with the spectroscopy shot. Rick Alcon fired the gun. Crystal preparation was done at M-1 using crystals made by Howard Cady some years ago.

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