Impact sensitivity of energetic materials – theory and experiment

Piotr Rozyczko

Data Management and Software Centre
European Spallation Source
Copenhagen, Denmark

Mechanical shock deposits thermal energy into low- frequency phonon modes of the crystal, and ultimately full thermal equilibrium in the sample is achieved by multiphonon scattering into higher frequency modes. Molecular dissociation occurs after sufficient energy is transferred into the internal modes of the molecule.

Finding initial steps of the decomposition reaction is the main problem in evaluating the sensitivity of an energetic material. Once the pathway is known, the (impact) sensitivity can be evaluated and predicted based on the overtone analysis of low energy vibrations coupled to the acoustic phonon bath [1-4].

We propose a new method for evaluation of the initial steps of the decomposition process of an energetic material, using Inelastic Neutron Scattering experiment and high level ab-initio simulations. This approach is aimed at predicting impact sensitivities by determining the lowest energy decomposition pathway.

We performed INS spectroscopy studies on a powdered sample and on a sample dissolved in a solvent, mimicking gas phase. We then performed analysis of low frequency modes and their overtones and compared the two spectra. The comparison allows us to use highly predictive computational methods to accurately model vibrational spectra of molecular solids. Subsequently we will perform a computational modeling of energy transfer rates between acoustic phonon modes and the low energy molecular vibrational modes and between overtones of those low energy modes and reaction- inducing vibrational stretch modes.

We focus primarily on energetic molecular crystals due to wide interest in the safety and short-time reaction kinetics of such materials.

The goal of the project is to be able to computationally predict impact sensitivities of novel energetic materials using single-molecule vibrational calculations. This is done by assuring transferability of high accuracy electron correlated picture of a single molecule into the solid phase description for relevant vibrational modes. To accomplish this, a highly accurate neutron vibrational spectra need to be generated for both phases. INS is the preferred technique, considering some of the decomposition pathways include proton transfer reaction.